HEWES: Heisenberg-Euler Weak-Field Expansion Simulator

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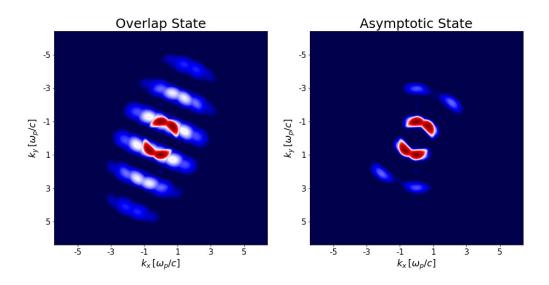


Figure 1.1 Harmonic Generation

The Heisenberg-Euler Weak-Field Expansion Simulator is a solver for the all-optical QED vacuum. It solves the equations of motion for electromagnetic waves in the Heisenberg-Euler effective QED theory in the weak-field expansion with up to six-photon processes.

There is a <code>paper</code> that introduces the algorithm and shows remarkable scientific results. Check that out before the code if you are interested in this project!

1.1 Contents

· Preparing the Makefile

- · Short User Manual
 - Hints for Settings
 - Note on Resource Occupation
 - Note on Output Analysis
- · Authors

1.2 Preparing the Makefile

The following descriptions assume you are using a Unix-like system.

The make utility is used for building and a recent compiler version supporting OpenMP is required. Features up to the C++20 standard are used.

Additionally required software:

· An MPI implementation.

While Intel (R) MPI has mostly been used for scientific work on high-performance computing systems, the provided Makefile here is by default created for use with the *open* implementations OpenMPI or MPICH. While some useful Intel(R) processor specific optimizations and compiler options are not available with the latter, they are easier to get and set up on a personal device simply via the corresponding package manager.

• The SUNDIALS package with the CVode solver.

Version 6 is required. The code is presumably compliant with the upcoming version 7.

For the installation of SUNDIALS, CMake is required. Follow the installation guide and do not forget to enable MPI and specify the directory of the mpicxx wrapper for use of the MPI-based NVECTOR_←

PARALLEL module. Make sure to edit the SUNDIALS binary and library paths in the Makefile.

A minimal Makefile template is provided. Further compiler options might be beneficial, depending on the used system and software; e.g., higher vectorization and register usage instructions.

1.3 Short User Manual

You have full control over all high-level simulation settings via the main.cpp file.

- First, specify the path you want the output data to go via the variable output Directory.
- Second, decide if you want to simulate in 1D, 2D, or 3D and uncomment only that full section.
 You can then specify
 - the relative and absolute integration tolerances of the CVode solver.
 Recommended values are between 1e-12 and 1e-18.
 - the order of accuracy of the numerical scheme via the stencil order.
 You can choose an integer in the range 1-13.
 - the physical side lengths of the grid in meters.
 - the number of lattice points per dimension.
 - the slicing of the lattice into patches (only for 2D and 3D simulations, automatic in 1D) this determines
 the number of patches and therefore the required distinct processing units for MPI.
 The total number of processes is given by the product of patches in any dimension.
 Note: In the 3D case you better insure that every patch is cubic in terms of lattice points. This is decisive for computational efficiency.

1.3 Short User Manual 3

- whether to have periodic or vanishing boundary values (currently has to be chosen periodic).
- whether you want to simulate on top of the linear vacuum only 4-photon processes (1), 6-photon processes (2), both (3), or none (0) the linear Maxwell case.
- the total time of the simulation in units c=1, i.e., the distance propagated by the light waves in meters.
- the number of time steps that will be solved stepwise by CVode.
 In order to keep interpolation errors small do not choose this number too small.
- the multiple of steps at which you want the data to be written to disk.
- the output format. It can be 'c' for comma separated values (csv), or 'b' for binary. For csv format the name of the files written to the output directory is of the form {step_number}_{process_\cup number}.csv. For binary output all data per step is written into one file and the step number is the name of the file.
- which electromagnetic waveform(s) you want to propagate.
 You can choose between a plane wave (not much physical content, but useful for checks) and implementations of Gaussians in 1D, 2D, and 3D. Their parameters can be tuned.
 A description of the wave implementations is given in ref.pdf. Note that the 3D Gaussians, as they are implemented up to now, should be propagated in the xy-plane. More waveform implementations will follow in subsequent versions of the code.

A doxygen-generated complete code reference is provided with ref.pdf.

- Third, in the src directory, build the executable Simulation via the make command.
- Forth, run the simulation.

Make sure to use src as working directory as the code uses a relative path to log the configuration in main.cpp.

You determine the number of processes via the MPI execution command. Note that in 2D and 3D simulations this number has to coincide with the actual number of patches, as described above.

Here, the simulation would be executed distributed over four processes: $mpirun -np \ 4$./Simulation

Monitor stdout and stderr. The unique simulation identifier number (starting timestep = name of data directory), the process steps, and the used wall times per step are printed on stdout. Errors are printed on stderr.
 Note: Convergence of the employed CVode solver can not be guaranteed and issues of this kind can hardly be predicted. On top, they are even system dependent. Piece of advice: Only pass decimal numbers for the grid settings and initial conditions.

CVode warnings and errors are reported on stdout and stderr.

A config.txtfile containing the relevant part of main.cpp is written to the output directory in order to save the simulation settings of each particular run.

You can remove the object files and the executable via make clean.

1.3.1 Note on Simulation Settings

You may want to start with two Gaussian pulses in 1D colliding head-on in a pump-probe setup. For this event, specify a high-frequency probe pulse with a low amplitude and a low-frequency pump pulse with a high frequency. Both frequencies should be chosen to be below a forth of the Nyquist frequency to avoid nonphysical dispersion effects. The wavelengths should neither be chosen too large (bulky wave) on a fine patchwork of narrow patches. Their communication might be problematic with too small halo layer depths. You would observe a blurring over time. The amplitudes need be below 1 – the critical field strength – for the weak-field expansion to be valid.

You can then investigate the arising of higher harmonics in frequency space via a Fourier analysis. The signals from the higher harmonics can be highlighted by subtracting the results of the same simulation in the linear Maxwell vacuum. You will be left with the nonlinear effects.

Choosing the probe pulse to be polarized with an angle to the polarization of the pump you may observe a fractional polarization flip of the probe due to their nonlinear interaction.

Decide beforehand which steps you need to be written to disk for your analysis.

Example scenarios of colliding Gaussians are preconfigured for any dimension.

1.3.2 Note on Resource Occupation

The computational load depends mostly on the grid size and resolution. The order of accuracy of the numerical scheme and CVode are rather secondary except for simulations running on many processing units, as the communication load is dependent on the stencil order.

Simulations in 1D are relatively cheap and can easily be run on a modern laptop within minutes. The output size per step is less than a megabyte.

Simulations in 2D with about one million grid points are still feasible for a personal machine but might take about an hour of time to finish. The output size per step is in the range of some dozen megabytes.

Sensible simulations in 3D require large memory resources and therefore need to be run on distributed systems. Even hundreds of cores can be kept busy for many hours or days. The output size quickly amounts to dozens of gigabytes for just a single state.

1.3.3 Note on Output Analysis

The field data are either written in csv format to one file per MPI process, the ending of which (after an underscore) corresponds to the process number, as described above. This is not an elegant solution, but a portable way that also works fast and is straightforward to analyze.

Or, the option recommended for many larger write operations, in binary format with a single file per output step. Raw bytes are written to the files as they are in memory. This option is more performant and achieved with MPI IO. However, there is no guarantee of portability; postprocessing/conversion is required. The step number is the file name.

A SimResults folder is created in the chosen output directory if it does not exist and a folder named after the starting timestep of the simulation (in the form $yy-mm-dd_hh-MM-ss$) is created where the output files are written into. There are six columns in the csv files, corresponding to the six components of the electromagnetic field: E_x , E_y , E_z

Postprocessing is required to read-in the files in order. A Python module taking care of this is provided.

Likewise, a Python module is provided to read the binary data of a selected field component into a numpy array – its portability, however, cannot be guaranteed.

The process numbers first align along dimension 1 until the number of patches is that direction is reached, then continue on dimension two and finally fill dimension 3. For example, for a 3D simulation on 4x4x4=64 cores, the field data is divided over the patches as follows:

The axes denote the physical dimensions that are each divided into 4 sectors in this example. The numbers inside the 4x4 squares indicate the process number, which is the number of the patch and also the number at the end of the corresponding output csv file. The ordering of the array within a patch follows the standard C convention and can be reshaped in 2D and 3D to the actual size of the path.

More information describing settings and analysis procedures used for actual scientific results are given in the open-access paper.

Some example Python analysis scripts can be found in the examples. The first steps demonstrate how the simulated data is accurately read-in from disk to numpy arrays using the provided get field data module. Harmonic generation in various forms is sketched as one application showing nonlinear quantum vacuum effects. There is however no simulation data provided as it would make the repository size unnecessarily large.

1.4 Authors 5

1.4 Authors

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6	HEWES: Heisenberg-Euler Weak-Field Expansion Simulator

Hierarchical Index

2.1 Class Hierarchy

This inheritance list is sorted roughly, but not completely, alphabetically:

Gauss1D	
Gauss2D	19
	25
gaussian1D	30
3	32
9	34
ICSetter	36
	45
LatticePatch	
OutputManager	
PlaneWave	109
PlaneWave1D	114
PlaneWave2D	
PlaneWave3D	119
planewave	113
Simulation	122
TimeEvolution	141

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Data Structure Index

3.1 Data Structures

Here are the data structures with brief descriptions:

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Class for Gaussian waves in 1D	13
Gauss2D	
Class for Gaussian waves in 2D	19
Gauss3D	
	25
gaussian1D	
	30
gaussian2D	
	32
gaussian3D	
	34
ICSetter	
71	36
Lattice	
1 9	45
LatticePatch	
	60
OutputManager	
	02
PlaneWave	
	09
planewave	
	13
PlaneWave1D	
Class for plane waves in 1D	14
	16
Class for plane waves in 2D	10
	10
Class for plane waves in 3D	19
	00
Simulation class to instantiate the whole walkthrough of a Simulation	
Monostate TimeEvolution Class to propagate the field data in time in a given order of the HE	
weak-field expansion	44
wear-new expansion	41

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File Index

4.1 File List

Here is a list of all files with brief descriptions:

src/DerivationStencils.cpp	
Empty. All definitions in the header	145
src/DerivationStencils.h	
Definition of derivation stencils from order 1 to 13	146
src/ICSetters.cpp	
Implementation of the plane wave and Gaussian wave packets in 1D, 2D, 3D	184
src/ICSetters.h	
Declaration of the plane wave and Gaussian wave packets in 1D, 2D, 3D	188
src/LatticePatch.cpp	
Costruction of the overall envelope lattice and the lattice patches	193
src/LatticePatch.h	
Declaration of the lattice and lattice patches	210
src/main.cpp	
Main function to configure the user's simulation settings	217
src/Outputters.cpp	
Generation of output writing to disk	230
src/Outputters.h	000
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src/SimulationClass.cpp Interface to the whole Simulation procedure: from wave settings over lattice construction, time	
evolution and outputs (also all relevant CVODE steps are performed here)	233
src/SimulationClass.h	233
Class for the Simulation object calling all functionality: from wave settings over lattice construc-	
tion, time evolution and outputs initialization of the CVode object	238
src/SimulationFunctions.cpp	200
Implementation of the complete simulation functions for 1D, 2D, and 3D, as called in the main	
function	241
src/SimulationFunctions.h	
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src/TimeEvolutionFunctions.cpp	
Implementation of functions to propagate data vectors in time according to Maxwell's equations,	
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src/TimeEvolutionFunctions.h	
Functions to propagate data vectors in time according to Maxwell's equations, and various orders	
in the HE weak-field expansion	295

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Data Structure Documentation

5.1 Gauss1D Class Reference

```
class for Gaussian waves in 1D
```

```
#include <src/ICSetters.h>
```

Public Member Functions

• Gauss1D (vector< sunrealtype > k={1, 0, 0}, vector< sunrealtype > p={0, 0, 1}, vector< sunrealtype > xo={0, 0, 0}, sunrealtype phig_=1.0l, vector< sunrealtype > phi={0, 0, 0})

construction with default parameters

• void addToSpace (sunrealtype x, sunrealtype y, sunrealtype z, sunrealtype *pTo6Space) const function for the actual implementation in space

Private Attributes

```
· sunrealtype kx
```

wavenumber k_x

• sunrealtype ky

wavenumber k_y

sunrealtype kz

wavenumber k_z

sunrealtype px

polarization & amplitude in x-direction, p_x

• sunrealtype py

polarization & amplitude in y-direction, p_y

• sunrealtype pz

polarization & amplitude in z-direction, p_z

• sunrealtype phix

phase shift in x-direction, ϕ_x

· sunrealtype phiy

phase shift in y-direction, ϕ_y

sunrealtype phiz

```
\begin{array}{c} \textit{phase shift in z-direction,} \ \phi_z \\ \bullet \ \ \text{sunrealtype x0x} \\ \quad \textit{center of pulse in x-direction,} \ x_0 \\ \bullet \ \ \text{sunrealtype x0y} \\ \quad \textit{center of pulse in y-direction,} \ y_0 \\ \bullet \ \ \text{sunrealtype x0z} \\ \quad \textit{center of pulse in z-direction,} \ z_0 \\ \bullet \ \ \text{sunrealtype phig} \\ \quad \textit{pulse width} \ \Phi_q \end{array}
```

5.1.1 Detailed Description

```
class for Gaussian waves in 1D
```

```
They are given in the form \vec{E} = \vec{p} \exp \left(-(\vec{x} - \vec{x}_0)^2/\Phi_g^2\right) \cos(\vec{k} \cdot \vec{x})
```

Definition at line 86 of file ICSetters.h.

5.1.2 Constructor & Destructor Documentation

5.1.2.1 Gauss1D()

```
Gauss1D::Gauss1D (  \mbox{vector} < \mbox{sunrealtype} > k = \{1, 0, 0\}, \\ \mbox{vector} < \mbox{sunrealtype} > p = \{0, 0, 1\}, \\ \mbox{vector} < \mbox{sunrealtype} > xo = \{0, 0, 0\}, \\ \mbox{sunrealtype} \mbox{phig} = 1.01, \\ \mbox{vector} < \mbox{sunrealtype} > phi = \{0, 0, 0\} \}
```

construction with default parameters

Gauss1D construction with

- wavevectors k_x
- k_y
- k_z normalized to $1/\lambda$
- amplitude (polarization) in x-direction
- amplitude (polarization) in y-direction
- amplitude (polarization) in z-direction
- phase shift in x-direction
- · phase shift in y-direction
- · phase shift in z-direction
- width

- · shift from origin in x-direction
- · shift from origin in y-direction
- · shift from origin in z-direction

Definition at line 125 of file ICSetters.cpp.

```
00127
                            /** - wavevectors \f$ k_x \f$ */
/** - \f$ k_y \f$ */
/** - \f$ k_z \f$ normalized to \f$ 1/\lambda \f$*/
00128
          kx = k[0]:
00129
          ky = k[1];
00130
         kz = k[2];
                            /** - amplitude (polarization) in x-direction */
         px = p[0];
                             /** - amplitude (polarization) in y-direction */  
/** - amplitude (polarization) in z-direction */
00132
          py = p[1];
          pz = p[2];
00133
          phix = phi[0]; /** - phase shift in x-direction */
phiy = phi[1]; /** - phase shift in y-direction */
00134
00135
          phiz = phi[2]; /** - phase shift in z-direction */
00136
00137
          phig = phig_; /** - width */
00138
          x0x = xo[0];
                            /** - shift from origin in x-direction*/
00139
          x0y = xo[1];
                             /** - shift from origin in y-direction*/
         x0z = xo[2];
                            /** - shift from origin in z-direction*/
00140
00141 }
```

References kx, ky, kz, phig, phix, phiy, phiz, px, py, pz, x0x, x0y, and x0z.

5.1.3 Member Function Documentation

5.1.3.1 addToSpace()

function for the actual implementation in space

Gauss1D implementation in space

```
Definition at line 145 of file ICSetters.cpp.
```

```
00146
00147
         const sunrealtype wavelength =
            sqrt(kx * kx + ky * ky + kz * kz); /* f$ 1/\lambda f$ */
00148
         x = x - x0x; /* x-coordinate minus shift from origin */
00149
00150
        y = y - x0y; /* y-coordinate minus shift from origin */
00151
         z = z - x0z; /* z-coordinate minus shift from origin */
        const sunrealtype kScalarX = (kx * x + ky * y + kz * z) * 2 * numbers::pi; /* \f$ 2\pi \ \vec{k} \cdot \vec{x} \f$ */
00152
00153
        const sunrealtype envelopeAmp =
00154
00155
            \exp(-(x * x + y * y + z * z) / phig) / phig); /* enveloping Gauss shape */
00156
        // Gaussian wave definition
00157
        const array<sunrealtype, 3> E{
00158
                                                                  /* E-field vector */
                                                                 /* \f$ E_x \f$ */
/* \f$ E_y \f$ */
00159
               px * cos(kScalarX - phix) * envelopeAmp,
               py * cos(kScalarX - phiy) * envelopeAmp, /* \f$ E_y \f$ */
pz * cos(kScalarX - phiz) * envelopeAmp}); /* \f$ E_z \f$ */
00160
00161
00162
        // Put E-field into space
00163
        pTo6Space[0] += E[0];
00164
        pTo6Space[1] += E[1];
00165
        pTo6Space[2] += E[2];
00166
         // and B-field
        pTo6Space[3] += (ky * E[2] - kz * E[1]) / wavelength;
pTo6Space[4] += (kz * E[0] - kx * E[2]) / wavelength;
00167
00168
         pTo6Space[5] += (kx * E[1] - ky * E[0]) / wavelength;
00169
00170 }
```

References kx, ky, kz, phig, phix, phiy, phiz, px, py, pz, x0x, x0y, and x0z.

5.1.4 Field Documentation

```
5.1.4.1 kx
```

```
sunrealtype Gauss1D::kx [private] wavenumber k_x Definition at line 89 of file ICSetters.h. Referenced by addToSpace(), and Gauss1D().
```

5.1.4.2 ky

```
sunrealtype Gauss1D::ky [private] wavenumber k_y Definition at line 91 of file ICSetters.h. Referenced by addToSpace(), and Gauss1D().
```

5.1.4.3 kz

```
sunrealtype Gauss1D::kz [private]  \label{eq:causs1D:kz}  wavenumber k_z Definition at line 93 of file ICSetters.h.  \label{eq:causs1D}  Referenced by addToSpace(), and Gauss1D().
```

5.1.4.4 phig

```
sunrealtype Gauss1D::phig [private]  \label{eq:pulse}    \text{pulse width } \Phi_g  Definition at line 113 of file ICSetters.h.     \text{Referenced by addToSpace(), and Gauss1D().}
```

5.1.4.5 phix

5.1.4.6 phiy

```
sunrealtype Gauss1D::phiy [private] \label{eq:phise} \mbox{phase shift in y-direction, } \phi_y \mbox{Definition at line 103 of file ICSetters.h.} \mbox{Referenced by addToSpace(), and Gauss1D().}
```

5.1.4.7 phiz

5.1.4.8 px

```
sunrealtype Gauss1D::px [private]  \label{eq:polarization} \mbox{polarization \& amplitude in x-direction, } p_x  Definition at line 95 of file ICSetters.h.  \mbox{Referenced by addToSpace(), and Gauss1D().}
```

5.1.4.9 py

```
sunrealtype Gauss1D::py [private]  \label{eq:polarization} \mbox{polarization \& amplitude in y-direction, } p_y  Definition at line 97 of file ICSetters.h.  \mbox{Referenced by addToSpace(), and Gauss1D().}
```

5.1.4.10 pz

```
sunrealtype Gauss1D::pz [private]  \label{eq:polarization} \mbox{polarization \& amplitude in z-direction, } p_z  Definition at line 99 of file ICSetters.h.  \mbox{Referenced by addToSpace(), and Gauss1D().}
```

5.1.4.11 x0x

```
sunrealtype Gauss1D::x0x [private] center of pulse in x-direction, x_0 Definition at line 107 of file ICSetters.h. Referenced by addToSpace(), and Gauss1D().
```

5.1.4.12 x0y

```
sunrealtype Gauss1D::x0y [private] center of pulse in y-direction, y_0 Definition at line 109 of file ICSetters.h. Referenced by addToSpace(), and Gauss1D().
```

5.1.4.13 x0z

```
sunrealtype Gauss1D::x0z [private] center of pulse in z-direction, z_0 Definition at line 111 of file ICSetters.h. Referenced by addToSpace(), and Gauss1D().
```

The documentation for this class was generated from the following files:

- src/ICSetters.h
- src/ICSetters.cpp

5.2 Gauss2D Class Reference

```
class for Gaussian waves in 2D
#include <src/ICSetters.h>
```

Public Member Functions

Gauss2D (vector< sunrealtype > dis_={0, 0, 0}, vector< sunrealtype > axis_={1, 0, 0}, sunrealtype Amp
 =1.0l, sunrealtype phip=0, sunrealtype w0_=1e-5, sunrealtype zr_=4e-5, sunrealtype Ph0_=2e-5, sunrealtype PhA =0.45e-5)

construction with default parameters

• void addToSpace (sunrealtype x, sunrealtype y, sunrealtype z, sunrealtype *pTo6Space) const function for the actual implementation in space

Private Attributes

```
    vector< sunrealtype > dis
distance maximum to origin
```

vector< sunrealtype > axis

normalized propagation axis

• sunrealtype Amp

amplitude A

sunrealtype phip

polarization rotation from TE-mode around propagation direction

• sunrealtype w0

taille ω_0

• sunrealtype zr

Rayleigh length $z_R = \pi \omega_0^2 / \lambda$.

sunrealtype Ph0

center of beam Φ_0

sunrealtype PhA

length of beam Φ_A

sunrealtype A1

amplitude projection on TE-mode

sunrealtype A2

amplitude projection on xy-plane

• sunrealtype lambda

wavelength λ

5.2.1 Detailed Description

class for Gaussian waves in 2D

They are given in the form $\vec{E}=A\,\vec{\epsilon}\,\sqrt{\frac{\omega_0}{\omega(z)}}\,\exp\left(-r/\omega(z)\right)^2\,\exp\left(-((z_g-\Phi_0)/\Phi_A)^2\right)\,\cos\left(\frac{k\,r^2}{2R(z)}+g(z)-k\,z_g\right)$ with

- propagation direction (subtracted distance to origin) \boldsymbol{z}_q
- radial distance to propagation axis $r=\sqrt{\vec{x}^2-z_g^2}$
- $k = 2\pi/\lambda$
- waist at position z, $\omega(z)=w_0\,\sqrt{1+(z_g/z_R)^2}$
- Gouy phase $g(z) = \tan^{-1}(z_q/z_r)$
- beam curvature $R(z)=z_{g}\left(1+(z_{r}/z_{g})^{2}
 ight)$ obtained via the chosen parameters

Definition at line 140 of file ICSetters.h.

5.2.2 Constructor & Destructor Documentation

5.2.2.1 Gauss2D()

```
Gauss2D::Gauss2D (

vector< sunrealtype > dis_{-} = \{0, 0, 0\},

vector< sunrealtype > axis_{-} = \{1, 0, 0\},

sunrealtype Amp_{-} = 1.01,

sunrealtype phip_{-} = 0,

sunrealtype w0_{-} = 1e-5,

sunrealtype zr_{-} = 4e-5,

sunrealtype Ph0_{-} = 2e-5,

sunrealtype PhA_{-} = 0.45e-5)
```

construction with default parameters

Gauss2D construction with

- · center it approaches
- · direction form where it comes
- amplitude
- · polarization rotation from TE-mode
- taille
- · Rayleigh length
- · beam center
- · beam length

Definition at line 173 of file ICSetters.cpp.

```
00176
         dis = dis_;
                                      /** - center it approaches */
                                    /** - direction form where it comes */
00177
         axis = axis_;
                                     /** - amplitude */
         Amp = Amp_;
00178
00179
                                      /** - polarization rotation from TE-mode */
         phip = phip ;
         w0 = w0_{;}
                                     /** - taille */
00180
00181
         zr = zr_;
                                      /** - Rayleigh length */
                                     /** - beam center */
/** - beam length */
00182
         Ph0 = Ph0_;
         PhA = PhA_;
00183
        A1 = Amp * cos(phip); // amplitude in z-direction
A2 = Amp * sin(phip); // amplitude on xy-plane
lambda = numbers::pi * w0 * w0 / zr; // formula for wavelength
00184
00185
00186
00187 }
```

References A1, A2, Amp, axis, dis, lambda, Ph0, PhA, phip, w0, and zr.

5.2.3 Member Function Documentation

5.2.3.1 addToSpace()

function for the actual implementation in space

```
Definition at line 190 of file ICSetters.cpp.
```

```
00191
00192
                   //\f$ \vec{x} = \vec{x}_0-\vec{dis} \f$ // coordinates minus distance to
00193
                  //origin
00194
                  x -= dis[0];
00195
                  y -= dis[1];
00196
                  // z-=dis[2];
                  z = NAN;
00197
00198
                  // \f$ z_g = \vec{x}\cdot\vec{e}_g \f$ projection on propagation axis
                 const sunrealtype zg =
00199
                          x * axis[0] + y * axis[1]; //+z*axis[2]; // =z-z0 -> propagation
00200
00201
                                                                                            //direction, minus origin
                 // \f$ r = \sqrt{\vec{x}^2 -z_g^2} \f$ -> pythagoras of radius minus
00202
                 // \lf f = \sqrt(\vector | z - z_g z \), \rf f \rf projection on prop axis const sunrealtype r = sqrt((x * x + y * y /*+z*z*/) - zg * zg); // radial distance to propagation axis // \f$ w(z) = w0\sqrt{1+(z-g/z_R)^2} \f$
00203
00204
00205
00206
00207
                 const sunrealtype wz = w0 * sqrt(1 + (zg * zg / zr / zr)); // waist at position z
00208
                  // \ f$ g(z) = atan(z_g/z_r) \f$
                 const surrealtype gz = atan(zg / zr); // Gouy phase // \f$ R(z) = z_g*(1+(z_r/z_g)^2) \f$ surrealtype Rz = NAN; // beam curvature
00209
00210
00211
00212
                  if (zg != 0)
00213
                      Rz = zg * (1 + (zr * zr / zg / zg));
00214
                 else
00215
                      Rz = 1e308;
                 // wavenumber \f$ k = 2\pi/\lambda \sqrt{\frac{1}{2}}
00216
                 // wavefunder \forall \fo
00217
00218
00219
                 const sunrealtype PhF =
                 00220
00221
00222
                 \ensuremath{//} CVode is a diva, no chance to remove the square in the second exponential
00223
                 // -> h too small
00224
                 const sunrealtype G2D = sqrt(w0 / wz) * exp(-r * r / wz / wz) *
00225
                                                             \exp(-(zg - Ph0) * (zg - Ph0) / PhA / PhA) *
00226
                                                             cos(PhF); // gauss shape
00227
                 // \f$ c_\alpha =\vec{e}_x\cdot\vec{axis} \f$
                 // projection components; do like this for CVode convergence -> otherwise
00228
00229
                 // results in machine error values for non-existant field components if
00230
                 // axis[0] and axis[1] are given
                 const sunrealtype ca =
```

References A1, A2, axis, dis, lambda, Ph0, PhA, w0, and zr.

5.2.4 Field Documentation

5.2.4.1 A1

```
sunrealtype Gauss2D::A1 [private]
```

amplitude projection on TE-mode

Definition at line 160 of file ICSetters.h.

Referenced by addToSpace(), and Gauss2D().

5.2.4.2 A2

```
sunrealtype Gauss2D::A2 [private]
```

amplitude projection on xy-plane

Definition at line 162 of file ICSetters.h.

Referenced by addToSpace(), and Gauss2D().

5.2.4.3 Amp

```
sunrealtype Gauss2D::Amp [private]
```

 ${\it amplitude} \; A$

Definition at line 147 of file ICSetters.h.

Referenced by Gauss2D().

5.2.4.4 axis

```
vector<sunrealtype> Gauss2D::axis [private]
normalized propagation axis

Definition at line 145 of file ICSetters.h.
```

Referenced by addToSpace(), and Gauss2D().

5.2.4.5 dis

```
vector<sunrealtype> Gauss2D::dis [private]
distance maximum to origin
Definition at line 143 of file ICSetters.h.
```

Referenced by addToSpace(), and Gauss2D().

5.2.4.6 lambda

```
sunrealtype Gauss2D::lambda [private] wavelength \lambda Definition at line 164 of file ICSetters.h. Referenced by addToSpace(), and Gauss2D().
```

5.2.4.7 Ph0

5.2.4.8 PhA

```
sunrealtype Gauss2D::PhA [private]
```

length of beam Φ_A

Definition at line 158 of file ICSetters.h.

Referenced by addToSpace(), and Gauss2D().

5.2.4.9 phip

```
sunrealtype Gauss2D::phip [private]
```

polarization rotation from TE-mode around propagation direction

Definition at line 150 of file ICSetters.h.

Referenced by Gauss2D().

5.2.4.10 w0

```
sunrealtype Gauss2D::w0 [private]
```

taille ω_0

Definition at line 152 of file ICSetters.h.

Referenced by addToSpace(), and Gauss2D().

5.2.4.11 zr

```
sunrealtype Gauss2D::zr [private]
```

Rayleigh length $z_R = \pi \omega_0^2 / \lambda$.

Definition at line 154 of file ICSetters.h.

Referenced by addToSpace(), and Gauss2D().

The documentation for this class was generated from the following files:

- src/ICSetters.h
- src/ICSetters.cpp

5.3 Gauss3D Class Reference

class for Gaussian waves in 3D

```
#include <src/ICSetters.h>
```

Public Member Functions

Gauss3D (vector< sunrealtype > dis_={0, 0, 0}, vector< sunrealtype > axis_={1, 0, 0}, sunrealtype Amp
 =1.0l, sunrealtype phip=0, sunrealtype w0_=1e-5, sunrealtype zr_=4e-5, sunrealtype Ph0_=2e-5, sunrealtype PhA_=0.45e-5)

construction with default parameters

• void addToSpace (sunrealtype x, sunrealtype y, sunrealtype z, sunrealtype *pTo6Space) const function for the actual implementation in space

Private Attributes

```
    vector< sunrealtype > dis

      distance maximum to origin
vector< sunrealtype > axis
      normalized propagation axis

    sunrealtype Amp

      amplitude A

    sunrealtype phip

      polarization rotation from TE-mode around propagation direction
• sunrealtype w0
      taille \omega_0
• sunrealtype zr
      Rayleigh length z_R = \pi \omega_0^2 / \lambda.
• sunrealtype Ph0
      center of beam \Phi_0

    sunrealtype PhA

      length of beam \Phi_A
• sunrealtype A1
      amplitude projection on TE-mode (z-axis)

    sunrealtype A2

      amplitude projection on xy-plane
• sunrealtype lambda
      wavelength \lambda
```

5.3.1 Detailed Description

class for Gaussian waves in 3D

They are given in the form $\vec{E} = A \vec{\epsilon} \frac{\omega_0}{\omega(z)} \exp\left(-r/\omega(z)\right)^2 \exp\left(-((z_g - \Phi_0)/\Phi_A)^2\right) \cos\left(\frac{k \, r^2}{2R(z)} + g(z) - k \, z_g\right)$ with

- propagation direction (subtracted distance to origin) \boldsymbol{z}_q
- radial distance to propagation axis $r=\sqrt{\vec{x}^2-z_g^2}$
- $k = 2\pi/\lambda$
- waist at position z, $\omega(z)=w_0\,\sqrt{1+(z_g/z_R)^2}$
- Gouy phase $g(z) = \tan^{-1}(z_q/z_r)$
- beam curvature $R(z)=z_q\left(1+(z_r/z_q)^2\right)$ obtained via the chosen parameters

Definition at line 192 of file ICSetters.h.

5.3.2 Constructor & Destructor Documentation

5.3.2.1 Gauss3D()

```
Gauss3D::Gauss3D (

vector< sunrealtype > dis_{-} = \{0, 0, 0\},

vector< sunrealtype > axis_{-} = \{1, 0, 0\},

sunrealtype Amp_{-} = 1.01,

sunrealtype phip_{-} = 0,

sunrealtype w0_{-} = 1e-5,

sunrealtype zr_{-} = 4e-5,

sunrealtype Ph0_{-} = 2e-5,

sunrealtype PhA_{-} = 0.45e-5)
```

construction with default parameters

Gauss3D construction with

- · center it approaches
- · direction from where it comes
- amplitude
- · polarization rotation form TE-mode
- taille
- · Rayleigh length
- · beam center
- · beam length

Definition at line 246 of file ICSetters.cpp.

```
00251
            dis = dis_; /** - center it approaches */
           axis = axis_; /** - direction from where it comes */
Amp = Amp_; /** - amplitude */
00252
00253
00254
           // pol=pol_;
           phip = phip_; /** - polarization rotation form TE-mode */
           phip = phip_; /** - pointization rocat
w0 = w0_; /** - taille */
zr = zr_; /** - Rayleigh length */
Ph0 = Ph0_; /** - beam center */
PhA = PhA_; /** - beam length */
00256
00257
00258
00259
00260
           lambda = numbers::pi * w0 * w0 / zr;
00261 A1 = Amp * cos(phip);
00262 A2 = Amp * sin(phip);
00263 }
```

References A1, A2, Amp, axis, dis, lambda, Ph0, PhA, phip, w0, and zr.

5.3.3 Member Function Documentation

5.3.3.1 addToSpace()

function for the actual implementation in space

Gauss3D implementation in space

```
Definition at line 266 of file ICSetters.cpp.
```

```
00268
           x -= dis[0];
          y -= dis[1];
00269
          z -= dis[2];
00270
          const sunrealtype zg = x * axis[0] + y * axis[1] + z * axis[2];
          const sunrealtype r = \operatorname{sqrt}((x * x + y * y + z * z) - zg * zg);

const sunrealtype wz = w0 * \operatorname{sqrt}(1 + (zg * zg / zr / zr));
00273
           const sunrealtype gz = atan(zg / zr);
00274
          sunrealtype Rz = NAN;
if (zg != 0)
  Rz = zg * (1 + (zr * zr / zg / zg));
00275
00276
00277
00278
          else
00279
             Rz = 1e308;
00280
          const sunrealtype k = 2 * numbers::pi / lambda;
          const sunrealtype PhF = -k * r * r / (2 * Rz) + gz - k * zg;

const sunrealtype G3D = (w0 / wz) * exp(-r * r / wz / wz) *

exp(-(zg - Ph0) * (zg - Ph0) / PhA / PhA) * cos(PhF);
00281
00282
00283
00284
          const sunrealtype ca = axis[0];
00285
          const sunrealtype sa = sqrt(1 - ca * ca);
          pTo6Space[0] += sa * (G3D * A2);
pTo6Space[1] += -ca * (G3D * A2);
pTo6Space[2] += G3D * A1;
00286
00287
00288
00289
           pTo6Space[3] += -sa * (G3D * A1);
           pTo6Space[4] += ca * (G3D * A1);
00290
00291
          pTo6Space[5] += G3D * A2;
00292 }
```

References A1, A2, axis, dis, lambda, Ph0, PhA, w0, and zr.

5.3.4 Field Documentation

5.3.4.1 A1

```
sunrealtype Gauss3D::A1 [private]
amplitude projection on TE-mode (z-axis)

Definition at line 214 of file ICSetters.h.

Referenced by addToSpace(), and Gauss3D().
```

5.3.4.2 A2

```
sunrealtype Gauss3D::A2 [private]
amplitude projection on xy-plane
Definition at line 216 of file ICSetters.h.
Referenced by addToSpace(), and Gauss3D().
```

5.3.4.3 Amp

5.3.4.4 axis

```
vector<sunrealtype> Gauss3D::axis [private]
normalized propagation axis

Definition at line 197 of file ICSetters.h.

Referenced by addToSpace(), and Gauss3D().
```

5.3.4.5 dis

```
vector<sunrealtype> Gauss3D::dis [private]
```

distance maximum to origin

Definition at line 195 of file ICSetters.h.

Referenced by addToSpace(), and Gauss3D().

5.3.4.6 lambda

```
sunrealtype Gauss3D::lambda [private]
```

wavelength λ

Definition at line 218 of file ICSetters.h.

Referenced by addToSpace(), and Gauss3D().

5.3.4.7 Ph0

```
sunrealtype Gauss3D::Ph0 [private]
```

center of beam Φ_0

Definition at line 210 of file ICSetters.h.

Referenced by addToSpace(), and Gauss3D().

5.3.4.8 PhA

```
sunrealtype Gauss3D::PhA [private]
```

length of beam $\Phi_{\cal A}$

Definition at line 212 of file ICSetters.h.

Referenced by addToSpace(), and Gauss3D().

5.3.4.9 phip

```
sunrealtype Gauss3D::phip [private]
```

polarization rotation from TE-mode around propagation direction

Definition at line 202 of file ICSetters.h.

Referenced by Gauss3D().

5.3.4.10 w0

```
sunrealtype Gauss3D::w0 [private]
```

taille ω_0

Definition at line 206 of file ICSetters.h.

Referenced by addToSpace(), and Gauss3D().

5.3.4.11 zr

```
sunrealtype Gauss3D::zr [private]
```

Rayleigh length $z_R = \pi \omega_0^2 / \lambda$.

Definition at line 208 of file ICSetters.h.

Referenced by addToSpace(), and Gauss3D().

The documentation for this class was generated from the following files:

- src/ICSetters.h
- src/ICSetters.cpp

5.4 gaussian1D Struct Reference

1D Gaussian wave structure

```
#include <src/SimulationFunctions.h>
```

Data Fields

- vector< sunrealtype > k
- vector< sunrealtype > p
- vector< sunrealtype > x0
- sunrealtype phig
- vector< sunrealtype > phi

5.4.1 Detailed Description

1D Gaussian wave structure

Definition at line 27 of file SimulationFunctions.h.

5.4.2 Field Documentation

5.4.2.1 k

```
vector<sunrealtype> gaussian1D::k
```

wavevector (normalized to $1/\lambda$)

Definition at line 28 of file SimulationFunctions.h.

Referenced by main().

5.4.2.2 p

```
vector<sunrealtype> gaussian1D::p
```

amplitude & polarization vector

Definition at line 29 of file SimulationFunctions.h.

Referenced by main().

5.4.2.3 phi

vector<sunrealtype> gaussian1D::phi

phase shift

Definition at line 32 of file SimulationFunctions.h.

Referenced by main().

5.4.2.4 phig

```
sunrealtype gaussian1D::phig
```

width

Definition at line 31 of file SimulationFunctions.h.

Referenced by main().

5.4.2.5 x0

```
vector<sunrealtype> gaussian1D::x0
```

shift from origin

Definition at line 30 of file SimulationFunctions.h.

Referenced by main().

The documentation for this struct was generated from the following file:

· src/SimulationFunctions.h

5.5 gaussian2D Struct Reference

2D Gaussian wave structure

```
#include <src/SimulationFunctions.h>
```

Data Fields

- vector< sunrealtype > x0
- vector< sunrealtype > axis
- sunrealtype amp
- sunrealtype phip
- sunrealtype w0
- · sunrealtype zr
- sunrealtype ph0
- sunrealtype phA

5.5.1 Detailed Description

2D Gaussian wave structure

Definition at line 36 of file SimulationFunctions.h.

5.5.2 Field Documentation

5.5.2.1 amp

sunrealtype gaussian2D::amp

amplitude

Definition at line 39 of file SimulationFunctions.h.

5.5.2.2 axis

vector<sunrealtype> gaussian2D::axis

direction to center

Definition at line 38 of file SimulationFunctions.h.

5.5.2.3 ph0

sunrealtype gaussian2D::ph0

beam center

Definition at line 43 of file SimulationFunctions.h.

5.5.2.4 phA

sunrealtype gaussian2D::phA

beam length

Definition at line 44 of file SimulationFunctions.h.

5.5.2.5 phip

sunrealtype gaussian2D::phip

polarization rotation

Definition at line 40 of file SimulationFunctions.h.

5.5.2.6 w0

sunrealtype gaussian2D::w0

taille

Definition at line 41 of file SimulationFunctions.h.

5.5.2.7 x0

vector<sunrealtype> gaussian2D::x0

center

Definition at line 37 of file SimulationFunctions.h.

5.5.2.8 zr

sunrealtype gaussian2D::zr

Rayleigh length

Definition at line 42 of file SimulationFunctions.h.

The documentation for this struct was generated from the following file:

• src/SimulationFunctions.h

5.6 gaussian3D Struct Reference

3D Gaussian wave structure

#include <src/SimulationFunctions.h>

Data Fields

- vector< sunrealtype > x0
- vector< sunrealtype > axis
- sunrealtype amp
- sunrealtype phip
- sunrealtype w0
- sunrealtype zr
- sunrealtype ph0
- sunrealtype phA

5.6.1 Detailed Description

3D Gaussian wave structure

Definition at line 48 of file SimulationFunctions.h.

5.6.2 Field Documentation

5.6.2.1 amp

sunrealtype gaussian3D::amp

amplitude

Definition at line 51 of file SimulationFunctions.h.

5.6.2.2 axis

vector<sunrealtype> gaussian3D::axis

direction to center

Definition at line 50 of file SimulationFunctions.h.

5.6.2.3 ph0

sunrealtype gaussian3D::ph0

beam center

Definition at line 55 of file SimulationFunctions.h.

5.6.2.4 phA

sunrealtype gaussian3D::phA

beam length

Definition at line 56 of file SimulationFunctions.h.

5.6.2.5 phip

sunrealtype gaussian3D::phip

polarization rotation

Definition at line 52 of file SimulationFunctions.h.

5.6.2.6 w0

sunrealtype gaussian3D::w0

taille

Definition at line 53 of file SimulationFunctions.h.

5.6.2.7 x0

vector<sunrealtype> gaussian3D::x0

center

Definition at line 49 of file SimulationFunctions.h.

5.6.2.8 zr

sunrealtype gaussian3D::zr

Rayleigh length

Definition at line 54 of file SimulationFunctions.h.

The documentation for this struct was generated from the following file:

• src/SimulationFunctions.h

5.7 ICSetter Class Reference

ICSetter class to initialize wave types with default parameters.

#include <src/ICSetters.h>

Public Member Functions

• void eval (sunrealtype x, sunrealtype y, sunrealtype z, sunrealtype *pTo6Space)

function to set all coordinates to zero and then add the field values

• void add (sunrealtype x, sunrealtype y, sunrealtype z, sunrealtype *pTo6Space)

function to fill the lattice space with initial field values

• void addPlaneWave1D (vector< sunrealtype > k={1, 0, 0}, vector< sunrealtype > p={0, 0, 1}, vector< sunrealtype > phi={0, 0, 0})

function to add plane waves in 1D to their container vector

void addPlaneWave2D (vector< sunrealtype > k={1, 0, 0}, vector< sunrealtype > p={0, 0, 1}, vector< sunrealtype > phi={0, 0, 0})

function to add plane waves in 2D to their container vector

• void addPlaneWave3D (vector< sunrealtype > k={1, 0, 0}, vector< sunrealtype > p={0, 0, 1}, vector< sunrealtype > phi={0, 0, 0})

function to add plane waves in 3D to their container vector

• void addGauss1D (vector< sunrealtype > k={1, 0, 0}, vector< sunrealtype > p={0, 0, 1}, vector< sunrealtype > xo={0, 0, 0}, sunrealtype phig_=1.0l, vector< sunrealtype > phi={0, 0, 0})

function to add Gaussian waves in 1D to their container vector

void addGauss2D (vector< sunrealtype > dis_={0, 0, 0}, vector< sunrealtype > axis_={1, 0, 0}, sunrealtype Amp_=1.0l, sunrealtype phip_=0, sunrealtype w0_=1e-5, sunrealtype zr_=4e-5, sunrealtype Ph0_=2e-5, sunrealtype PhA_=0.45e-5)

function to add Gaussian waves in 2D to their container vector

• void addGauss3D (vector< sunrealtype > dis_={0, 0, 0}, vector< sunrealtype > axis_={1, 0, 0}, sunrealtype Amp_=1.0l, sunrealtype phip_=0, sunrealtype w0_=1e-5, sunrealtype zr_=4e-5, sunrealtype Ph0_=2e-5, sunrealtype PhA_=0.45e-5)

function to add Gaussian waves in 3D to their container vector

Private Attributes

vector< PlaneWave1D > planeWaves1D

container vector for plane waves in 1D

vector< PlaneWave2D > planeWaves2D

container vector for plane waves in 2D

vector< PlaneWave3D > planeWaves3D

container vector for plane waves in 3D

vector < Gauss1D > gauss1Ds

container vector for Gaussian waves in 1D

vector< Gauss2D > gauss2Ds

container vector for Gaussian waves in 2D

vector< Gauss3D > gauss3Ds

container vector for Gaussian waves in 3D

5.7.1 Detailed Description

ICSetter class to initialize wave types with default parameters.

Definition at line 236 of file ICSetters.h.

5.7.2 Member Function Documentation

5.7.2.1 add()

function to fill the lattice space with initial field values

Add all initial field values to the lattice space

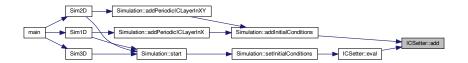
Definition at line 308 of file ICSetters.cpp.

```
00309
          for (const auto &wave : planeWaves1D)
         wave.addToSpace(x, y, z, pTo6Space);
for (const auto &wave : planeWaves2D)
00311
00312
00313
           wave.addToSpace(x, y, z, pTo6Space);
00314
         for (const auto &wave : planeWaves3D)
         wave.addToSpace(x, y, z, pTo6Space);
for (const auto &wave : gauss1Ds)
00315
00316
00317
           wave.addToSpace(x, y, z, pTo6Space);
00318
         for (const auto &wave : gauss2Ds)
         wave.addToSpace(x, y, z, pTo6Space);
for (const auto &wave : gauss3Ds)
00319
00320
00321
            wave.addToSpace(x, y, z, pTo6Space);
00322 }
```

References gauss1Ds, gauss2Ds, gauss3Ds, planeWaves1D, planeWaves2D, and planeWaves3D.

Referenced by Simulation::addInitialConditions(), and eval().

Here is the caller graph for this function:



5.7.2.2 addGauss1D()

```
void ICSetter::addGauss1D (  \mbox{vector} < \mbox{sunrealtype} > k = \{1, 0, 0\}, \\ \mbox{vector} < \mbox{sunrealtype} > p = \{0, 0, 1\}, \\ \mbox{vector} < \mbox{sunrealtype} > xo = \{0, 0, 0\}, \\ \mbox{sunrealtype} \mbox{phig} = 1.01, \\ \mbox{vector} < \mbox{sunrealtype} > phi = \{0, 0, 0\} \}
```

function to add Gaussian waves in 1D to their container vector

Add Gaussian waves in 1D to their container vector

```
Definition at line 343 of file ICSetters.cpp.

00345

00346 gauss1Ds.emplace_back(Gauss1D(k, p, xo, phig_, phi));

00347 }
```

References gauss1Ds.

Referenced by Sim1D().

Here is the caller graph for this function:



5.7.2.3 addGauss2D()

```
void ICSetter::addGauss2D (

vector< sunrealtype > dis_{-} = \{0, 0, 0\},

vector< sunrealtype > axis_{-} = \{1, 0, 0\},

sunrealtype Amp_{-} = 1.01,

sunrealtype phip_{-} = 0,

sunrealtype w0_{-} = 1e-5,

sunrealtype zr_{-} = 4e-5,

sunrealtype Ph0_{-} = 2e-5,

sunrealtype PhA_{-} = 0.45e-5)
```

function to add Gaussian waves in 2D to their container vector

Add Gaussian waves in 2D to their container vector

```
Definition at line 350 of file ICSetters.cpp.
```

```
00352

00353 gauss2Ds.emplace_back(

00354 Gauss2D(dis_, axis_, Amp_, phip_, w0_, zr_, Ph0_, PhA_));

00355 }
```

References gauss2Ds.

Referenced by Sim2D().

Here is the caller graph for this function:



5.7.2.4 addGauss3D()

```
void ICSetter::addGauss3D (

vector< sunrealtype > dis_{-} = \{0, 0, 0\},

vector< sunrealtype > axis_{-} = \{1, 0, 0\},

sunrealtype Amp_{-} = 1.01,

sunrealtype phip_{-} = 0,

sunrealtype w0_{-} = 1e-5,

sunrealtype zr_{-} = 4e-5,

sunrealtype Ph0_{-} = 2e-5,

sunrealtype PhA_{-} = 0.45e-5)
```

function to add Gaussian waves in 3D to their container vector

Add Gaussian waves in 3D to their container vector

Definition at line 358 of file ICSetters.cpp.

```
00360

00361 gauss3Ds.emplace_back(

00362 Gauss3D(dis_, axis_, Amp_, phip_, w0_, zr_, Ph0_, PhA_));

00363 }
```

References gauss3Ds.

Referenced by Sim3D().

Here is the caller graph for this function:



5.7.2.5 addPlaneWave1D()

```
void ICSetter::addPlaneWave1D (  \mbox{vector} < \mbox{sunrealtype} > k = \{1, \ 0, \ 0\}, \\ \mbox{vector} < \mbox{sunrealtype} > p = \{0, \ 0, \ 1\}, \\ \mbox{vector} < \mbox{sunrealtype} > phi = \{0, \ 0, \ 0\} \ )
```

function to add plane waves in 1D to their container vector

Add plane waves in 1D to their container vector

```
Definition at line 325 of file ICSetters.cpp.
```

```
00326
00327 planeWaves1D.emplace_back(PlaneWave1D(k, p, phi));
00328 }
```

References planeWaves1D.

Referenced by Sim1D().

Here is the caller graph for this function:



5.7.2.6 addPlaneWave2D()

```
void ICSetter::addPlaneWave2D (  \mbox{vector} < \mbox{sunrealtype} > k = \{1, \ 0, \ 0\}, \\ \mbox{vector} < \mbox{sunrealtype} > p = \{0, \ 0, \ 1\}, \\ \mbox{vector} < \mbox{sunrealtype} > phi = \{0, \ 0, \ 0\} \ )
```

function to add plane waves in 2D to their container vector

Add plane waves in 2D to their container vector

```
Definition at line 331 of file ICSetters.cpp.
```

```
00332
00333 planeWaves2D.emplace_back(PlaneWave2D(k, p, phi));
00334 }
```

References planeWaves2D.

Referenced by Sim2D().

Here is the caller graph for this function:



5.7.2.7 addPlaneWave3D()

```
void ICSetter::addPlaneWave3D (  \mbox{vector} < \mbox{sunrealtype} > k = \{1, \ 0, \ 0\}, \\ \mbox{vector} < \mbox{sunrealtype} > p = \{0, \ 0, \ 1\}, \\ \mbox{vector} < \mbox{sunrealtype} > phi = \{0, \ 0, \ 0\} \ )
```

function to add plane waves in 3D to their container vector

Add plane waves in 3D to their container vector

```
Definition at line 337 of file ICSetters.cpp.

00338

00339 planeWaves3D.emplace_back(PlaneWave3D(k, p, phi));

00340 }
```

References planeWaves3D.

Referenced by Sim3D().

Here is the caller graph for this function:



5.7.2.8 eval()

function to set all coordinates to zero and then add the field values

Evaluate lattice point values to zero and add field values

Definition at line 296 of file ICSetters.cpp.

```
00297

00298    pTo6Space[0] = 0;

00299    pTo6Space[1] = 0;

00300    pTo6Space[2] = 0;

00301    pTo6Space[3] = 0;

00302    pTo6Space[4] = 0;

00303    pTo6Space[5] = 0;

00304    add(x, y, z, pTo6Space);

00305 }
```

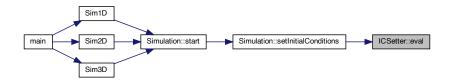
References add().

Referenced by Simulation::setInitialConditions().

Here is the call graph for this function:



Here is the caller graph for this function:



5.7.3 Field Documentation

5.7.3.1 gauss1Ds

vector<Gauss1D> ICSetter::gauss1Ds [private]

container vector for Gaussian waves in 1D

Definition at line 245 of file ICSetters.h.

Referenced by add(), and addGauss1D().

5.7.3.2 gauss2Ds

vector<Gauss2D> ICSetter::gauss2Ds [private]

container vector for Gaussian waves in 2D

Definition at line 247 of file ICSetters.h.

Referenced by add(), and addGauss2D().

5.7.3.3 gauss3Ds

```
vector<Gauss3D> ICSetter::gauss3Ds [private]
container vector for Gaussian waves in 3D

Definition at line 249 of file ICSetters.h.

Referenced by add(), and addGauss3D().
```

5.7.3.4 planeWaves1D

```
vector<PlaneWave1D> ICSetter::planeWaves1D [private]
container vector for plane waves in 1D
Definition at line 239 of file ICSetters.h.
Referenced by add(), and addPlaneWave1D().
```

5.7.3.5 planeWaves2D

```
vector<PlaneWave2D> ICSetter::planeWaves2D [private]
container vector for plane waves in 2D

Definition at line 241 of file ICSetters.h.

Referenced by add(), and addPlaneWave2D().
```

5.7.3.6 planeWaves3D

```
vector<PlaneWave3D> ICSetter::planeWaves3D [private]
container vector for plane waves in 3D
Definition at line 243 of file ICSetters.h.
Referenced by add(), and addPlaneWave3D().
```

The documentation for this class was generated from the following files:

- src/ICSetters.h
- src/ICSetters.cpp

5.8 Lattice Class Reference 45

5.8 Lattice Class Reference

Lattice class for the construction of the enveloping discrete simulation space.

```
#include <src/LatticePatch.h>
```

Public Member Functions

· void initializeCommunicator (const int nx, const int ny, const int nz, const bool per)

function to create and deploy the cartesian communicator

• Lattice (const int StO)

default construction

- void setDiscreteDimensions (const sunindextype _nx, const sunindextype _ny, const sunindextype _nz)
 component function for resizing the discrete dimensions of the lattice
- void setPhysicalDimensions (const sunrealtype _lx, const sunrealtype _ly, const sunrealtype _lz) component function for resizing the physical size of the lattice
- const sunrealtype & get_tot_lx () const
- const sunrealtype & get_tot_ly () const
- const sunrealtype & get_tot_lz () const
- const sunindextype & get tot nx () const
- · const sunindextype & get_tot_ny () const
- · const sunindextype & get tot nz () const
- const sunindextype & get_tot_noP () const
- const sunindextype & get_tot_noDP () const
- · const sunrealtype & get_dx () const
- const sunrealtype & get_dy () const
- const sunrealtype & get_dz () const
- constexpr int get_dataPointDimension () const
- const int & get_stencilOrder () const
- const int & get_ghostLayerWidth () const

Data Fields

• int n prc

number of MPI processes

int my_prc

number of MPI process

MPI_Comm comm

personal communicator of the lattice

SUNContext sunctx

SUNContext object.

SUNProfiler profobj

SUNProfiler object.

Private Attributes

• sunrealtype tot_lx

physical size of the lattice in x-direction

· sunrealtype tot_ly

physical size of the lattice in y-direction

• sunrealtype tot_lz

physical size of the lattice in z-direction

• sunindextype tot_nx

number of points in x-direction

sunindextype tot_ny

number of points in y-direction

sunindextype tot_nz

number of points in z-direction

sunindextype tot_noP

total number of lattice points

• sunindextype tot_noDP

number of lattice points times data dimension of each point

sunrealtype dx

physical distance between lattice points in x-direction

· sunrealtype dy

physical distance between lattice points in y-direction

• sunrealtype dz

physical distance between lattice points in z-direction

· const int stencilOrder

stencil order

· const int ghostLayerWidth

required width of ghost layers (depends on the stencil order)

unsigned char statusFlags

char for checking if lattice flags are set

Static Private Attributes

static constexpr int dataPointDimension = 6
 dimension of each data point -> set once and for all

5.8.1 Detailed Description

Lattice class for the construction of the enveloping discrete simulation space.

Definition at line 46 of file LatticePatch.h.

5.8.2 Constructor & Destructor Documentation

5.8.2.1 Lattice()

```
Lattice::Lattice (
const int StO)
```

default construction

Construct the lattice and set the stencil order.

```
Definition at line 39 of file LatticePatch.cpp.
```

```
00039 : stencilOrder(StO),

00040 ghostLayerWidth(StO/2+1) {

00041 statusFlags = 0;

00042 }
```

References statusFlags.

5.8.3 Member Function Documentation

5.8.3.1 get dataPointDimension()

```
constexpr int Lattice::get_dataPointDimension ( ) const [inline], [constexpr]
```

getter function

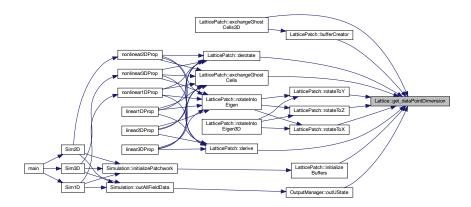
```
Definition at line 114 of file LatticePatch.h.
```

```
00114
00115 return dataPointDimension;
00116 }
```

References dataPointDimension.

Referenced by LatticePatch::bufferCreator(), LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::exchangeGhostCells(), LatticePatch::exchangeGhostCells3D(), LatticePatch::initializeBuffers(), OutputManager::outUState(), LatticePatch::rotateToX(), LatticePatch::rotateToX(), and LatticePatch::rotateToZ().

Here is the caller graph for this function:



5.8.3.2 get_dx()

```
const sunrealtype & Lattice::get_dx ( ) const [inline]
getter function

Definition at line 111 of file LatticePatch.h.
00111 { return dx; }
```

References dx.

5.8.3.3 get_dy()

```
const sunrealtype & Lattice::get_dy ( ) const [inline]
getter function

Definition at line 112 of file LatticePatch.h.
00112 { return dy; }
```

References dy.

5.8.3.4 get_dz()

```
const sunrealtype & Lattice::get_dz ( ) const [inline]
```

getter function

Definition at line 113 of file LatticePatch.h. 00113 { return dz; }

References dz.

5.8.3.5 get_ghostLayerWidth()

```
const int & Lattice::get_ghostLayerWidth ( ) const [inline]
getter function
```

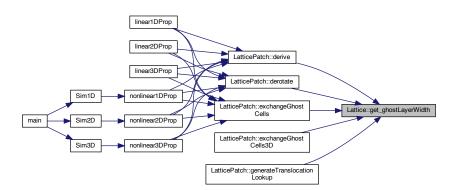
Definition at line 118 of file LatticePatch.h.

```
00118
00119    return ghostLayerWidth;
00120 }
```

References ghostLayerWidth.

Referenced by LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::exchangeGhostCells(), La

Here is the caller graph for this function:



5.8.3.6 get_stencilOrder()

```
const int & Lattice::get_stencilOrder ( ) const [inline]
```

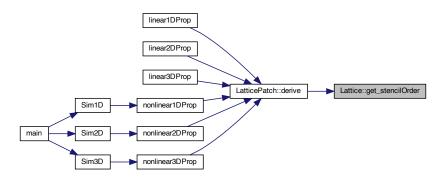
getter function

Definition at line 117 of file LatticePatch.h. 00117 { return stencilOrder; }

References stencilOrder.

Referenced by LatticePatch::derive().

Here is the caller graph for this function:



5.8.3.7 get_tot_lx()

```
const sunrealtype & Lattice::get_tot_lx ( ) const [inline]
```

getter function

Definition at line 103 of file LatticePatch.h.

00103 { return tot_lx; }

References tot_lx.

Referenced by Simulation::addInitialConditions().

Here is the caller graph for this function:



5.8.3.8 get_tot_ly()

```
const sunrealtype & Lattice::get_tot_ly ( ) const [inline]
```

getter function

Definition at line 104 of file LatticePatch.h.

00104 { return tot_ly; }

References tot_ly.

Referenced by Simulation::addInitialConditions().

Here is the caller graph for this function:



5.8.3.9 get_tot_lz()

```
const sunrealtype & Lattice::get_tot_lz ( ) const [inline]
```

getter function

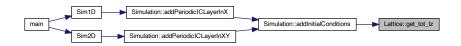
Definition at line 105 of file LatticePatch.h.

00105 { return tot_lz; }

References tot_lz.

Referenced by Simulation::addInitialConditions().

Here is the caller graph for this function:



5.8.3.10 get_tot_noDP()

```
const sunindextype & Lattice::get_tot_noDP ( ) const [inline]
```

getter function

Definition at line 110 of file LatticePatch.h.

00110 { return tot_noDP; }

References tot_noDP.

```
5.8.3.11 get_tot_noP()

const sunindextype & Lattice::get_tot_noP ( ) const [inline]

getter function

Definition at line 109 of file LatticePatch.h.
00109 { return tot_noP; }

References tot_noP.
```

5.8.3.12 get_tot_nx()

```
const sunindextype & Lattice::get_tot_nx ( ) const [inline]
```

getter function

```
Definition at line 106 of file LatticePatch.h. 00106 { return tot_nx; }
```

References tot_nx.

5.8.3.13 get_tot_ny()

```
const sunindextype & Lattice::get_tot_ny ( ) const [inline]
```

getter function

```
Definition at line 107 of file LatticePatch.h.
00107 { return tot_ny; }
```

References tot_ny.

5.8.3.14 get_tot_nz()

```
const sunindextype & Lattice::get_tot_nz ( ) const [inline]
```

getter function

```
Definition at line 108 of file LatticePatch.h. 00108 { return tot_nz; }
```

References tot_nz.

5.8 Lattice Class Reference 53

5.8.3.15 initializeCommunicator()

function to create and deploy the cartesian communicator

Initialize the cartesian communicator.

Definition at line 15 of file LatticePatch.cpp.

```
00017
         const int dims[3] = \{nz, ny, nx\};
00018
         const int periods[3] = {static_cast<int>(per), static_cast<int>(per),
         static_cast<int>(per));

// Create the cartesian communicator for MPI_COMM_WORLD
00019
00020
        MPI_Cart_create(MPI_COMM_WORLD, 3, dims, periods, 1, &comm);
00021
00022
         // Set MPI variables of the lattice
00023
         MPI_Comm_size(comm, &(n_prc));
00024
        MPI_Comm_rank(comm, &(my_prc));
00025
         // Associate name to the communicator to identify it \rightarrow for debugging and
        // Associate Name to the communication to Identify // nicer error messages constexpr char lattice_comm_name[] = "Lattice";
00026
00027
00028
         MPI_Comm_set_name(comm, lattice_comm_name);
00029
00030
         \ensuremath{//} Test if process naming is the same for both communicators
00031
00032
         int MYPRC:
         MPI_Comm_rank (MPI_COMM_WORLD, &MYPRC);
cout«"\r"«my_prc«"\t"«MYPRC«endl;
00033
00034
00035
00036 }
```

References comm, my_prc, and n_prc.

Referenced by Simulation::Simulation().

Here is the caller graph for this function:



5.8.3.16 setDiscreteDimensions()

component function for resizing the discrete dimensions of the lattice

Set the number of points in each dimension of the lattice.

Definition at line 45 of file LatticePatch.cpp.

```
00047
         // copy the given data for number of points
00048
         tot_nx = _nx;
        tot_ny = _ny;
tot_nz = _nz;
00049
00050
00051
        // compute the resulting number of points and datapoints
00052
         tot_noP = tot_nx * tot_ny * tot_nz;
00053
         tot_noDP = dataPointDimension * tot_noP;
00054
         // compute the new Delta, the physical resolution
        dx = tot_lx / tot_nx;
dy = tot_ly / tot_ny;
dz = tot_lz / tot_nz;
00055
00056
00057
00058 }
```

References dataPointDimension, dx, dy, dz, tot_lx, tot_ly, tot_lz, tot_noDP, tot_noP, tot_nx, tot_ny, and tot_nz.

Referenced by Simulation::setDiscreteDimensionsOfLattice().

Here is the caller graph for this function:



5.8.3.17 setPhysicalDimensions()

component function for resizing the physical size of the lattice

Set the physical size of the lattice.

Definition at line 61 of file LatticePatch.cpp.

References dx, dy, dz, FLatticeDimensionSet, statusFlags, tot lx, tot ly, tot lz, tot nx, tot ny, and tot nz.

Referenced by Simulation::setPhysicalDimensionsOfLattice().

Here is the caller graph for this function:



5.8.4 Field Documentation

5.8.4.1 comm

MPI_Comm Lattice::comm

personal communicator of the lattice

Definition at line 85 of file LatticePatch.h.

Referenced by LatticePatch::exchangeGhostCells(), LatticePatch::exchangeGhostCells3D(), Simulation::get_cart_comm(), initializeCommunicator(), Simulation::initializeCVODEobject(), OutputManager::outUState(), and Simulation::Simulation().

5.8.4.2 dataPointDimension

constexpr int Lattice::dataPointDimension = 6 [static], [constexpr], [private]

dimension of each data point -> set once and for all

Definition at line 63 of file LatticePatch.h.

Referenced by get_dataPointDimension(), and setDiscreteDimensions().

5.8.4.3 dx

sunrealtype Lattice::dx [private]

physical distance between lattice points in x-direction

Definition at line 67 of file LatticePatch.h.

Referenced by $get_dx()$, setDiscreteDimensions(), and setPhysicalDimensions().

5.8.4.4 dy

```
sunrealtype Lattice::dy [private]
```

physical distance between lattice points in y-direction

Definition at line 69 of file LatticePatch.h.

Referenced by get_dy(), setDiscreteDimensions(), and setPhysicalDimensions().

5.8.4.5 dz

```
sunrealtype Lattice::dz [private]
```

physical distance between lattice points in z-direction

Definition at line 71 of file LatticePatch.h.

Referenced by get_dz(), setDiscreteDimensions(), and setPhysicalDimensions().

5.8.4.6 ghostLayerWidth

```
const int Lattice::ghostLayerWidth [private]
```

required width of ghost layers (depends on the stencil order)

Definition at line 75 of file LatticePatch.h.

Referenced by get_ghostLayerWidth().

5.8.4.7 my_prc

```
int Lattice::my_prc
```

number of MPI process

Definition at line 83 of file LatticePatch.h.

 $Referenced\ by\ initialize Communicator(),\ Simulation::initialize CVODE object(),\ Output Manager::out US tate(),\ and\ Simulation::Simulation().$

5.8 Lattice Class Reference 57

5.8.4.8 n_prc

```
int Lattice::n_prc
```

number of MPI processes

Definition at line 81 of file LatticePatch.h.

Referenced by initializeCommunicator().

5.8.4.9 profobj

```
SUNProfiler Lattice::profobj
```

SUNProfiler object.

Definition at line 94 of file LatticePatch.h.

Referenced by Simulation::initializeCVODEobject().

5.8.4.10 statusFlags

```
unsigned char Lattice::statusFlags [private]
```

char for checking if lattice flags are set

Definition at line 77 of file LatticePatch.h.

Referenced by Lattice(), and setPhysicalDimensions().

5.8.4.11 stencilOrder

```
const int Lattice::stencilOrder [private]
```

stencil order

Definition at line 73 of file LatticePatch.h.

Referenced by get_stencilOrder().

5.8.4.12 sunctx

SUNContext Lattice::sunctx

SUNContext object.

Definition at line 92 of file LatticePatch.h.

Referenced by Simulation::initializeCVODEobject(), Simulation::Simulation(), and Simulation::~Simulation().

5.8.4.13 tot_lx

```
sunrealtype Lattice::tot_lx [private]
```

physical size of the lattice in x-direction

Definition at line 49 of file LatticePatch.h.

 $Referenced \ by \ get_tot_lx(), \ setDiscreteDimensions(), \ and \ setPhysicalDimensions().$

5.8.4.14 tot_ly

```
sunrealtype Lattice::tot_ly [private]
```

physical size of the lattice in y-direction

Definition at line 51 of file LatticePatch.h.

Referenced by get_tot_ly(), setDiscreteDimensions(), and setPhysicalDimensions().

5.8.4.15 tot_lz

```
sunrealtype Lattice::tot_lz [private]
```

physical size of the lattice in z-direction

Definition at line 53 of file LatticePatch.h.

Referenced by get_tot_lz(), setDiscreteDimensions(), and setPhysicalDimensions().

5.8 Lattice Class Reference 59

5.8.4.16 tot_noDP

```
sunindextype Lattice::tot_noDP [private]
```

number of lattice points times data dimension of each point

Definition at line 65 of file LatticePatch.h.

Referenced by get_tot_noDP(), and setDiscreteDimensions().

5.8.4.17 tot_noP

```
sunindextype Lattice::tot_noP [private]
```

total number of lattice points

Definition at line 61 of file LatticePatch.h.

Referenced by get_tot_noP(), and setDiscreteDimensions().

5.8.4.18 tot_nx

```
sunindextype Lattice::tot_nx [private]
```

number of points in x-direction

Definition at line 55 of file LatticePatch.h.

Referenced by get_tot_nx(), setDiscreteDimensions(), and setPhysicalDimensions().

5.8.4.19 tot_ny

```
sunindextype Lattice::tot_ny [private]
```

number of points in y-direction

Definition at line 57 of file LatticePatch.h.

Referenced by get_tot_ny(), setDiscreteDimensions(), and setPhysicalDimensions().

5.8.4.20 tot_nz

```
sunindextype Lattice::tot_nz [private]
```

number of points in z-direction

Definition at line 59 of file LatticePatch.h.

Referenced by get_tot_nz(), setDiscreteDimensions(), and setPhysicalDimensions().

The documentation for this class was generated from the following files:

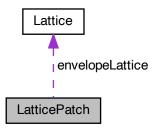
- src/LatticePatch.h
- src/LatticePatch.cpp

5.9 LatticePatch Class Reference

LatticePatch class for the construction of the patches in the enveloping lattice.

```
#include <src/LatticePatch.h>
```

Collaboration diagram for LatticePatch:



Public Member Functions

• LatticePatch ()

constructor setting up a default first lattice patch

∼LatticePatch ()

destructor freeing parallel vectors

• int discreteSize (int dir=0) const

function to get the discrete size of the LatticePatch

• sunrealtype origin (const int dir) const

function to get the origin of the patch

• sunrealtype getDelta (const int dir) const

function to get distance between points

• void generateTranslocationLookup ()

function to fill out the lookup tables for translocation

void rotateIntoEigen (const int dir)

function to rotate u into Z-matrix eigenraum

• void rotateIntoEigen3D ()

function to rotate as in rotateIntoEigen with special 3D halo buffers

• void derotate (int dir, sunrealtype *buffOut)

function to derotate uAux into dudata lattice direction of x

• void initializeGhostLayer ()

initialize ghost cells for halo exchange

• void initializeBuffers ()

initialize buffers to save derivatives

void exchangeGhostCells (const int dir)

function to exchange ghost cells in uAux for the derivative

void exchangeGhostCells3D ()

function to exchange ghost cells using a neighborhood collective operation

void bufferCreator (int li, int mx, int my, int mz, int distToRight)

outsourced convenience function to fill halo buffers with uData for 3D

• void derive (const int dir)

function to derive the centered values in uAux and save them noncentered

void checkFlag (unsigned int flag) const

function to check if a flag has been set and if not abort

Data Fields

• int ID

ID of the LatticePatch, corresponds to process number.

• N Vector u

 $N_{\text{-}}$ Vector for saving field components u=(E,B) in lattice points.

N_Vector du

N_Vector for saving temporal derivatives of the field data.

sunrealtype * uData

pointer to field data

sunrealtype * uAuxData

pointer to auxiliary data vector

sunrealtype * duData

pointer to time-derivative data

array< sunrealtype *, 3 > buffData

- sunrealtype * gCLData
- sunrealtype * gCRData
- sunrealtype * gCBData
- sunrealtype * gCTData
- sunrealtype * gCFData
- sunrealtype * gCAData

Private Member Functions

```
    void rotateToX (sunrealtype *outArray, const sunrealtype *inArray, const vector< int > &lookup)
```

- void rotateToY (sunrealtype *outArray, const sunrealtype *inArray, const vector< int > &lookup)
- void rotateToZ (sunrealtype *outArray, const sunrealtype *inArray, const vector< int > &lookup)

Private Attributes

• sunrealtype x0

origin of the patch in physical space; x-coordinate

• sunrealtype y0

origin of the patch in physical space; y-coordinate

• sunrealtype z0

origin of the patch in physical space; z-coordinate

sunindextype Llx

inner position of lattice-patch in the lattice patchwork; x-points

• sunindextype Lly

inner position of lattice-patch in the lattice patchwork; y-points

sunindextype Llz

inner position of lattice-patch in the lattice patchwork; z-points

• sunrealtype Ix

physical size of the lattice-patch in the x-dimension

sunrealtype ly

physical size of the lattice-patch in the y-dimension

· sunrealtype Iz

physical size of the lattice-patch in the z-dimension

sunindextype nx

number of points in the lattice patch in the x-dimension

· sunindextype ny

number of points in the lattice patch in the y-dimension

sunindextype nz

number of points in the lattice patch in the z-dimension

sunrealtype dx

physical distance between lattice points in x-direction

· sunrealtype dy

physical distance between lattice points in y-direction

sunrealtype dz

physical distance between lattice points in z-direction

const Lattice * envelopeLattice

pointer to the enveloping lattice

- vector< sunrealtype > uAux
- unsigned char statusFlags
- vector< int > uTox
- vector< int > uToy

- vector< int > uToz
- vector< int > xTou
- vector< int > yTou
- vector< int > zTou
- vector< sunrealtype > buffX
- vector< sunrealtype > buffY
- vector< sunrealtype > buffZ
- vector< sunrealtype > ghostCellLeft
- vector< sunrealtype > ghostCellRight
- vector< sunrealtype > ghostCellLeftToSend
- $\bullet \ \ vector < sunreal type > ghost Cell Right To Send \\$
- vector< sunrealtype > ghostCellsToSend
- vector< sunrealtype > ghostCells
- vector< int > lgcTox
- vector< int > rgcTox
- vector< int > lgcToy
- vector< int > rgcToy
- vector< int > lgcToz
- vector< int > rgcToz

Friends

int generatePatchwork (const Lattice &envelopeLattice, LatticePatch &patchToMold, const int DLx, const int DLy, const int DLz)

friend function for creating the patchwork slicing of the overall lattice

5.9.1 Detailed Description

LatticePatch class for the construction of the patches in the enveloping lattice.

Definition at line 137 of file LatticePatch.h.

5.9.2 Constructor & Destructor Documentation

5.9.2.1 LatticePatch()

```
LatticePatch::LatticePatch ( )
```

constructor setting up a default first lattice patch

Construct the lattice patch.

Definition at line 78 of file LatticePatch.cpp.

```
00079
        // set default origin coordinates to (0,0,0)
        x0 = y0 = z0 = 0; 
// set default position in Lattice-Patchwork to (0,0,0)
00080
00081
00082
        LIx = LIy = LIz = 0;
        // set default physical lentgth for lattice patch to (0,0,0)
00084
        1x = 1y = 1z = 0;
        // set default discrete length for lattice patch to (0,1,1)
00085
00086
        /\star This is done in this manner as even in 1D simulations require a 1 point
00087
        * width */
        nx = 0;
00088
00089
        ny = nz = 1;
00090
00091
        \ensuremath{//}\xspace u is not initialized as it wouldn't make any sense before the dimensions
00092
        \ensuremath{//} are set idem for the enveloping lattice
00093
00094
        // set default statusFlags to non set
00095
        statusFlags = 0;
00096 }
```

References Llx, Lly, Llz, lx, ly, lz, nx, ny, nz, statusFlags, x0, y0, and z0.

5.9.2.2 ~LatticePatch()

```
LatticePatch::~LatticePatch ( )
```

destructor freeing parallel vectors

Destruct the patch and thereby destroy the NVectors.

Definition at line 99 of file LatticePatch.cpp.

References du, FLatticePatchSetUp, statusFlags, and u.

5.9.3 Member Function Documentation

5.9.3.1 bufferCreator()

```
void LatticePatch::bufferCreator (
    int li,
    int mx,
    int my,
    int mz,
    int distToRight )
```

outsourced convenience function to fill halo buffers with uData for 3D

Fill the halo buffers for neighborhood collectives.

Definition at line 669 of file LatticePatch.cpp.

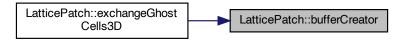
```
00671
          const int dPD = envelopeLattice->get_dataPointDimension();
00672
          // Initialize running index ui for to be transferred uData
00673
         int ui = 0;
00674
00675 // #pragma omp parallel for reduction(+:ui) reduction(+:li) -> don't, probably
00676 // bad idea to parallelize ghost cell exchange Loop over all planes and pick to
00677 // be transferred points (uData indices)
00678 #pragma distribute_point
00679
         for (int iz = 0; iz < mz; iz++)</pre>
            for (int iy = 0; iy < my; iy++) {
   // start index of uData vector halo data to be transferred</pre>
00680
00681
00682
              // Here, in contrast to above, start at right boundary to send to left
00683
              // s.t. updated left values are the first indices (bec of neighborhood
00684
              // collective pattern) with each z-step add the whole xy-plane and with
              // y-step the x-range -> iterate all x-ranges
ui = (iz * nx * ny + iy * nx + distToRight) * dPD;
// copy from uData from right boundary (at each dimension) into buffer,
// halo transfer size is given by x length at each step
// memcpy(&ghostCellsToSend[li], \
00685
00686
00687
00688
00690
                              &uData[ui], \
00691
                              sizeof(sunrealtype)*mx*dPD);
00692
              copy(&uData[ui], &uData[ui + mx * dPD], &ghostCellsToSend[li]);
00693
              // increase li by transferred indices in this loop-step
00694
              li += mx * dPD;
00695
00696
00697
00698 #pragma distribute_point
         for (int iz = 0; iz < mz; iz++) {
  for (int iy = 0; iy < my; iy++) {
    // Now copy from left boundary into buffer</pre>
00699
00700
00701
00702
              ui = (iz * nx * ny + iy * nx) * dPD;
00703
              //memcpy(&ghostCellsToSend[li],
00704
                              &uData[ui], \
00705
                              sizeof(sunrealtype)*mx*dPD);
00706
              copy(&uData[ui], &uData[ui + mx * dPD], &ghostCellsToSend[li]);
00707
              li += mx * dPD;
00708
00709
         }
00710 }
```

References envelopeLattice, Lattice::get_dataPointDimension(), ghostCellsToSend, nx, ny, and uData.

Referenced by exchangeGhostCells3D().



Here is the caller graph for this function:



5.9.3.2 checkFlag()

```
void LatticePatch::checkFlag (
          unsigned int flag ) const
```

function to check if a flag has been set and if not abort

Check if all flags are set.

Definition at line 713 of file LatticePatch.cpp.

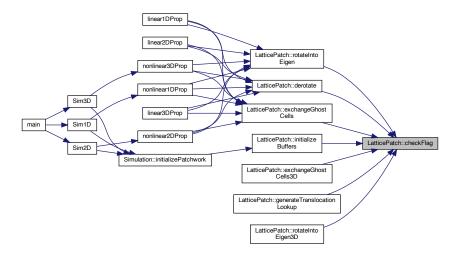
```
00714
      if (!(statusFlags & flag)) {
00715
       string errorMessage;
        switch (flag) {
00717
       case FLatticePatchSetUp:
         errorMessage = "The Lattice patch was not set up please make sure to " "initilize a Lattice topology";
00718
00719
00720
         break:
00721
       case TranslocationLookupSetUp:
00722
         errorMessage = "The translocation lookup tables have not been generated, "
00723
                      "please be sure to run generateTranslocationLookup()";
00724
       00725
00726
00727
00728
00729
       case BuffersInitialized:
         00730
00731
00732
         break:
00733
        default:
00734
         errorMessage = "Uppss, you've made a non-standard error, sadly I can't "
00735
                      "help you there";
00736
00737
00738
        errorKill(errorMessage);
00739
      return;
```

References BuffersInitialized, errorKill(), FLatticePatchSetUp, GhostLayersInitialized, statusFlags, and TranslocationLookupSetUp.

Referenced by derotate(), exchangeGhostCells(), exchangeGhostCells3D(), generateTranslocationLookup(), initializeBuffers(), rotateIntoEigen(), and rotateIntoEigen3D().



Here is the caller graph for this function:



5.9.3.3 derive()

function to derive the centered values in uAux and save them noncentered

Calculate derivatives in the patch (uAux) in the specified direction.

Definition at line 744 of file LatticePatch.cpp.

```
00744
00745
         // ghost layer width
00746
         const int gLW = envelopeLattice->get_ghostLayerWidth();
00747
        // dimensionality of data points \rightarrow 6
        const int dPD = envelopeLattice->get_dataPointDimension();
// total width of patch in given direction including ghost layers at ends
const int dirWidth = discreteSize(dir) + 2 * gLW;
00748
00749
00750
00751
        // width of patch only in given direction
00752
        const int dirWidthO = discreteSize(dir);
00753
         // size of plane perpendicular to given dimension
        const int perpPlainSize = discreteSize() / discreteSize(dir);
00754
        // physical distance between points in that direction
00755
00756
        sunrealtype dxi = NAN;
00757
        switch (dir) {
00758
        case 1:
00759
          dxi = dx;
00760
          break;
00761
        case 2:
00762
          dxi = dv;
00763
          break;
00764
        case 3:
00765
          dxi = dz;
00766
          break;
00767
        default:
00768
          dxi = 1;
00769
           errorKill("Tried to derive in the wrong direction");
00770
00771
00772
         // Derive according to chosen stencil accuracy order (which determines also
00773
        // gLW)
00774
        const int order = envelopeLattice->get_stencilOrder();
00775
        switch (order) {
00776
        case 1:
```

```
for (int i = 0; i < perpPlainSize; i++) {</pre>
                 for (int j = (i * dirWidth + gLW) * dPD;

j < (i * dirWidth + gLW + dirWidthO) * dPD; j += dPD) {
00778
00779
                     uAux[j + 0 - gLW * dPD] = s1b(&uAux[j + 0]) / dxi;
uAux[j + 1 - gLW * dPD] = s1b(&uAux[j + 1]) / dxi;
00780
00781
                     uAux[j + 2 - gLW * dPD] = slf(&uAux[j + 2]) / dxi;

uAux[j + 3 - gLW * dPD] = slf(&uAux[j + 3]) / dxi;

uAux[j + 4 - gLW * dPD] = slf(&uAux[j + 4]) / dxi;
00782
00783
00784
                      uAux[j + 5 - gLW * dPD] = slf(&uAux[j + 5]) / dxi;
00785
00786
00787
               }
00788
               break:
00789
            case 2:
00790
              for (int i = 0; i < perpPlainSize; i++) {</pre>
00791
                   for (int j = (i * dirWidth + gLW) * dPD;
                     j < (i * dirWidth + gLW + dirWidthO) * dPD; j += dPD) {
uAux[j + 0 - gLW * dPD] = s2b(&uAux[j + 0]) / dxi;
uAux[j + 1 - gLW * dPD] = s2b(&uAux[j + 1]) / dxi;
00792
00793
00794
                     uAux[j + 2 - gLW * dPD] = s2f(&uAux[j + 2]) / dxi;
00796
                     uAux[j + 3 - gLW * dPD] = s2f(&uAux[j + 3]) / dxi;
                     uAux[j + 4 - gLW * dPD] = s2c(&uAux[j + 4]) / dxi;

uAux[j + 5 - gLW * dPD] = s2c(&uAux[j + 5]) / dxi;
00797
00798
00799
00800
00801
               break;
            case 3:
00803
              for (int i = 0; i < perpPlainSize; i++) {</pre>
                  for (int j = (i * dirWidth + gLW) * dPD;

j < (i * dirWidth + gLW + dirWidth) * dPD; j += dPD) {

uAux[j + 0 - gLW * dPD] = s3b(&uAux[j + 0]) / dxi;

uAux[j + 1 - gLW * dPD] = s3b(&uAux[j + 1]) / dxi;
00804
00805
00806
00807
00808
                      uAux[j + 2 - gLW * dPD] = s3f(&uAux[j + 2]) / dxi;
                      uAux[j + 3 - gLW * dPD] = s3f(&uAux[j + 3]) / dxi;
uAux[j + 4 - gLW * dPD] = s3f(&uAux[j + 4]) / dxi;
uAux[j + 5 - gLW * dPD] = s3f(&uAux[j + 4]) / dxi;
00809
00810
00811
00812
00813
               break;
00815
            case 4:
00816
              for (int i = 0; i < perpPlainSize; i++) {</pre>
                  for (int j = (i * dirWidth + gLW) * dPD;
    j < (i * dirWidth + gLW + dirWidth) * dPD; j += dPD) {
    uAux[j + 0 - gLW * dPD] = s4b(&uAux[j + 0]) / dxi;
    uAux[j + 1 - gLW * dPD] = s4b(&uAux[j + 1]) / dxi;</pre>
00817
00818
00819
00820
                     uAux[j + 2 - gLW * dPD] = s4f(&uAux[j + 2]) / dxi;
00821
                      uAux[j + 3 - gLW * dPD] = s4f(&uAux[j + 3]) / dxi;
00822
                     uAux[j + 4 - gLW * dPD] = s4c(&uAux[j + 4]) / dxi;

uAux[j + 5 - gLW * dPD] = s4c(&uAux[j + 5]) / dxi;
00823
00824
00825
                  }
00826
00827
               break;
00828
            case 5:
00829
              for (int i = 0; i < perpPlainSize; i++) {</pre>
                  for (int i = 0, i = perpendicular) for (int j = (i * dirWidth + gLW) * dPD; j += dPD) {
    j < (i * dirWidth + gLW + dirWidthO) * dPD; j += dPD) {
00830
00831
                     00832
                      uAux[j + 2 - gLW * dPD] = s5f(&uAux[j + 2]) / dxi;
00834
                     uAux[j + 3 - gLW * dPD] = s5f(&uAux[j + 3]) / dxi;
uAux[j + 4 - gLW * dPD] = s5f(&uAux[j + 4]) / dxi;
uAux[j + 5 - gLW * dPD] = s5f(&uAux[j + 5]) / dxi;
00835
00836
00837
00838
                  }
00839
00840
               break;
            case 6:
00841
              00842
00843
00844
                     uAux[j + 1 - gLW * dPD] = s6b(&uAux[j + 0]) / dxi;
uAux[j + 1 - gLW * dPD] = s6b(&uAux[j + 1]) / dxi;
00845
                     uAux[j + 2 - gLW * dPD] = s6f(&uAux[j + 2]) / dxi;

uAux[j + 3 - gLW * dPD] = s6f(&uAux[j + 3]) / dxi;

uAux[j + 4 - gLW * dPD] = s6c(&uAux[j + 3]) / dxi;

uAux[j + 5 - gLW * dPD] = s6c(&uAux[j + 4]) / dxi;
00847
00848
00849
00850
00851
00852
00853
               break;
00854
            case 7:
               00855
00856
00857
                     uAux[j + 0 - gLW * dPD] = s7b(&uAux[j + 0]) / dxi;
uAux[j + 1 - gLW * dPD] = s7b(&uAux[j + 1]) / dxi;
00859
                      uAux[j + 2 - gLW * dPD] = s7f(&uAux[j + 2]) / dxi;
00860
                     uAux[j + 3 - gLW * dPD] = s7f(&uAux[j + 3]) / dxi;

uAux[j + 4 - gLW * dPD] = s7f(&uAux[j + 4]) / dxi;

uAux[j + 5 - gLW * dPD] = s7f(&uAux[j + 5]) / dxi;
00861
00862
00863
```

```
}
00865
00866
           break;
00867
         case 8:
           00868
00869
                uAux[j + 0 - gLW * dPD] = s8b(&uAux[j + 0]) / dxi;
uAux[j + 1 - gLW * dPD] = s8b(&uAux[j + 1]) / dxi;
uAux[j + 2 - gLW * dPD] = s8f(&uAux[j + 2]) / dxi;
00871
00872
00873
                uAux[j + 3 - gLW * dPD] = s8f(&uAux[j + 3]) / dxi;
uAux[j + 4 - gLW * dPD] = s8c(&uAux[j + 4]) / dxi;
00874
00875
                uAux[j + 5 - gLW * dPD] = s8c(&uAux[j + 5]) / dxi;
00876
00877
00878
00879
           break;
00880
         case 9:
           00881
00883
                uAux[j + 0 - gLW * dPD] = s9b(&uAux[j + 0]) / dxi;

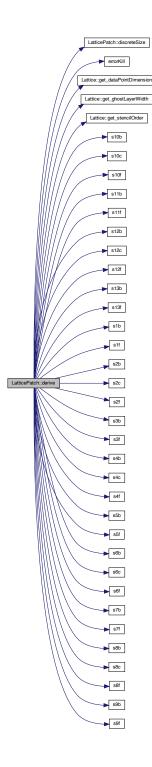
uAux[j + 1 - gLW * dPD] = s9b(&uAux[j + 1]) / dxi;
00884
00885
                uAux[j + 2 - gLW * dPD] = s9f(&uAux[j + 2]) / dxi;
uAux[j + 3 - gLW * dPD] = s9f(&uAux[j + 3]) / dxi;
00886
00887
00888
                uAux[j + 4 - gLW * dPD] = s9f(&uAux[j + 4]) / dxi;
                uAux[j + 5 - gLW * dPD] = s9f(&uAux[j + 5]) / dxi;
00890
00891
00892
           break;
00893
         case 10:
           00894
00895
00896
                uAux[j + 0 - gLW * dPD] = s10b(&uAux[j + 0]) / dxi;

uAux[j + 1 - gLW * dPD] = s10b(&uAux[j + 1]) / dxi;
00897
00898
                uAux[j + 2 - gLW * dPD] = s10f(&uAux[j + 2]) / dxi;
00899
                uAux[j + 3 - gLW * dPD] = slof(&uAux[j + 3]) / dxi;
uAux[j + 4 - gLW * dPD] = sloc(&uAux[j + 4]) / dxi;
00900
00902
                uAux[j + 5 - gLW * dPD] = s10c(&uAux[j + 5]) / dxi;
00903
00904
00905
           break:
00906
         case 11:
00907
           for (int i = 0; i < perpPlainSize; i++) {</pre>
             for (int j = (i * dirWidth + gLW) * dPD;
00908
00909
                    j < (i * dirWidth + gLW + dirWidthO) * dPD; j += dPD) {</pre>
                uAux[j + 0 - gLW * dPD] = sllb(&uAux[j + 0]) / dxi;
uAux[j + 1 - gLW * dPD] = sllb(&uAux[j + 1]) / dxi;
00910
00911
                uAux[j + 2 - gLW * dPD] = s11f(&uAux[j + 2]) / dxi;
00912
                uAux[j + 3 - gLW * dPD] = s11f(&uAux[j + 3]) / dxi;
00913
                uAux[j + 4 - gLW * dPD] = s11f(&uAux[j + 4]) / dxi;
00915
                uAux[j + 5 - gLW * dPD] = s11f(&uAux[j + 5]) / dxi;
00916
00917
00918
           break:
00919
         case 12:
          for (int i = 0; i < perpPlainSize; i++) {</pre>
              for (int j = (i * dirWidth + gLW) * dPD;
    j < (i * dirWidth + gLW + dirWidthO) * dPD; j += dPD) {</pre>
00921
00922
                uAux[j + 0 - gLW * dPD] = s12b(&uAux[j + 0]) / dxi;
uAux[j + 1 - gLW * dPD] = s12b(&uAux[j + 1]) / dxi;
00923
00924
                uAux[j + 2 - gLW * dPD] = s12f(&uAux[j + 2]) / dxi;
00925
                uAux[j + 3 - gLW * dPD] = s12f(&uAux[j + 3]) / dxi;
00926
                uAux[j + 4 - gLW * dPD] = s12c(&uAux[j + 4]) / dxi;
00927
                uAux[j + 5 - gLW * dPD] = s12c(&uAux[j + 5]) / dxi;
00928
00929
             }
00930
00931
           break:
00932
         case 13:
           //#pragma omp parallel for default(none) firstprivate(uAux)
00934
            //shared(dxi,dirWidth,dirWidth0,gLW,dPD) collapse(2) schedule(static,6)
00935
           //#pragma ivdep
00936
            //#pragma distribute_point -> No.
00937
           //#pragma unroll_and_jam
00938
           \ensuremath{//} Iterate through all points in the plane perpendicular to the given
            // direction
00940
            for (int i = 0; i < perpPlainSize; i++) {</pre>
00941
              // stencil functions range over 2*gLW+6 indices, attention to cache-line // false-sharing
00942
              //#pragma omp simd safelen(2*gLW+dPD)
00943
              // Iterate through the direction for each perpendicular plane point for (int j = (i * dirWidth + gLW /*to shift left by gLW below */) * dPD; j < (i * dirWidth + gLW + dirWidthO) * dPD; j += dPD) {
00944
00946
00947
                /\star Compute the stencil derivative for any of the six field components
00948
                 \star with a ghostlayer width adjusted to the order of the finite
00949
                 * difference scheme */
00950
                uAux[j + 0 - qLW * dPD] = s13b(&uAux[j + 0]) / dxi;
```

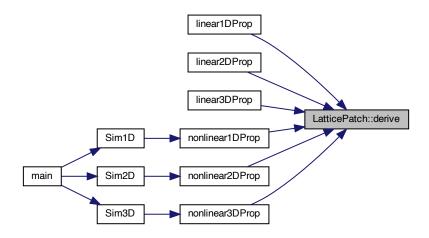
```
uAux[j + 1 - gLW * dPD] = s13b(&uAux[j + 1]) / dxi;
                         uAux[j + 1 - gLW * dPD] = $13b(&uAux[j + 1]) / dxi;
uAux[j + 2 - gLW * dPD] = $13f(&uAux[j + 2]) / dxi;
uAux[j + 3 - gLW * dPD] = $13f(&uAux[j + 3]) / dxi;
uAux[j + 4 - gLW * dPD] = $13f(&uAux[j + 4]) / dxi;
uAux[j + 5 - gLW * dPD] = $13f(&uAux[j + 5]) / dxi;
00952
00953
00954
00955
00956
00958
00959
00960
              default:
                  errorKill("Please set an existing stencil order");
00961
00962
                  break;
00963
00964 }
```

 $References\ discrete Size(),\ dx,\ dy,\ dz,\ envelope Lattice,\ error Kill(),\ Lattice::get_dataPointDimension(),\ Lattice::get_ghostLayerWidth(),\ Lattice::get_stencilOrder(),\ s10b(),\ s10c(),\ s10f(),\ s11b(),\ s11f(),\ s12b(),\ s12c(),\ s12f(),\ s13b(),\ s13f(),\ s13f(),\ s1b(),\ s1f(),\ s2b(),\ s2c(),\ s2f(),\ s3b(),\ s3f(),\ s4b(),\ s4c(),\ s4f(),\ s5b(),\ s5f(),\ s6c(),\ s6c(),\ s6f(),\ s7b(),\ s7f(),\ s8b(),\ s8c(),\ s8f(),\ s9b(),\ s9f(),\ and\ uAux.$

Referenced by linear1DProp(), linear2DProp(), linear3DProp(), nonlinear1DProp(), nonlinear2DProp(), and nonlinear3DProp().



Here is the caller graph for this function:



5.9.3.4 derotate()

```
void LatticePatch::derotate (
          int dir,
           sunrealtype * buffOut )
```

function to derotate uAux into dudata lattice direction of x

Derotate uAux with transposed rotation matrices and write to derivative buffer – normalization is done here by the factor 1/2

Definition at line 426 of file LatticePatch.cpp.

```
00426
           // Check that the lattice as well as the translocation lookups have been set
00427
00428
           // up;
00429
           checkFlag(FLatticePatchSetUp);
00430
           checkFlag(TranslocationLookupSetUp);
           const int dPD = envelopeLattice->get_dataPointDimension();
const int gLW = envelopeLattice->get_ghostLayerWidth();
00431
00432
           const int uSize = discreteSize();
00433
           int ii = 0, target = 0;
00434
00435
           switch (dir) {
00436
           case 1:
00437 #pragma ivdep
00438 #pragma omp simd // safelen(6) - also good
00439 #pragma distribute_point

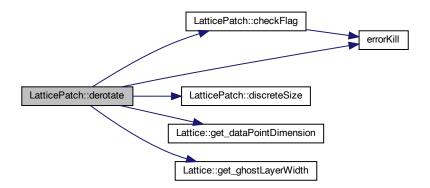
00440 for (int i = 0; i < uSize; i++) {

00441 // get correct indices in u and rotation space
00442
                 target = dPD * i;
00443
                 ii = dPD * (uTox[i] - gLW);
                11 = GED * (HIOX[1] - GLW);
buffOut[target + 0] = uAux[5 + ii];
buffOut[target + 1] = (-uAux[ii] + uAux[2 + ii]) / 2.;
buffOut[target + 2] = (uAux[1 + ii] - uAux[3 + ii]) / 2.;
buffOut[target + 3] = uAux[4 + ii];
buffOut[target + 4] = (uAux[1 + ii] + uAux[3 + ii]) / 2.;
00444
00445
00446
00447
00448
                 buffOut[target + 5] = (uAux[ii] + uAux[2 + ii]) / 2.;
00449
00450
00451
              break;
00452
          case 2:
00453 #pragma omp simd // safelen(6)
00454 #pragma distribute_point
```

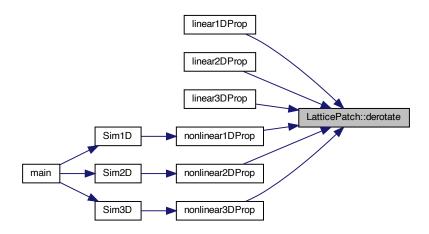
```
for (int i = 0; i < uSize; i++) {</pre>
                target = dPD * i;
00456
00457
                  ii = dPD * (uToy[i] - gLW);
                 buffOut[target + 0] = (uAux[ii] - uAux[2 + ii]) / 2.;
00458
                 buffOut[target + 0] = (uAux[1] - uAux[2 + 11]) / 2.,
buffOut[target + 1] = uAux[5 + ii];
buffOut[target + 2] = (-uAux[1 + ii] + uAux[3 + ii]) / 2.;
buffOut[target + 3] = (uAux[1 + ii] + uAux[3 + ii]) / 2.;
buffOut[target + 4] = uAux[4 + ii];
00459
00460
00461
00462
00463
                 buffOut[target + 5] = (uAux[ii] + uAux[2 + ii]) / 2.;
00464
00465
              break:
00466
           case 3:
00467 #pragma omp simd // safelen(6)
00468 #pragma distribute_point
00469
             for (int i = 0; i < uSize; i++) {</pre>
                 target = dPD * i;
ii = dPD * (uToz[i] - gLW);
00470
00471
                 buffOut[target + 0] = (-uAux[ii] + uAux[2 + ii]) / 2.;
buffOut[target + 1] = (uAux[1 + ii] - uAux[3 + ii]) / 2.;
buffOut[target + 2] = uAux[5 + ii];
00472
00474
                 buffOut[target + 3] = (uAux[1 + ii] + uAux[3 + ii]) / 2.;
buffOut[target + 4] = (uAux[ii] + uAux[2 + ii]) / 2.;
00475
00476
                 buffOut[target + 5] = uAux[4 + ii];
00477
00478
00479
              break;
00480
           default:
00481
              errorKill("Tried to derotate from the wrong direction");
00482
              break;
00483
00484 }
```

References checkFlag(), discreteSize(), envelopeLattice, errorKill(), FLatticePatchSetUp, Lattice::get_dataPointDimension(), Lattice::get_ghostLayerWidth(), TranslocationLookupSetUp, uAux, uTox, uToy, and uToz.

Referenced by linear1DProp(), linear2DProp(), linear3DProp(), nonlinear1DProp(), nonlinear2DProp(), and nonlinear3DProp().



Here is the caller graph for this function:



5.9.3.5 discreteSize()

```
int LatticePatch::discreteSize (
    int dir = 0 ) const
```

function to get the discrete size of the LatticePatch

Return the discrete size of the patch: number of lattice patch points in specified dimension

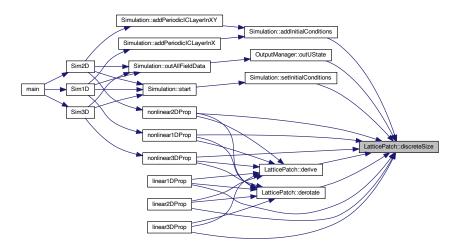
Definition at line 196 of file LatticePatch.cpp.

```
switch (dir) {
00198
        case 0:
00199
         return nx * ny * nz;
00200
       case 1:
00201
         return nx;
00202
        case 2:
00203
         return ny;
00204
        case 3:
       return nz;
// case 4: return uAux.size(); // for debugging
00205
00206
00207
       default:
00208
         return -1;
00209
00210 }
```

References nx, ny, and nz.

 $Referenced \ by \ Simulation:: addInitial Conditions(), \ derive(), \ derotate(), \ linear 1DProp(), \ linear 2DProp(), \ linear 3DProp(), \ nonlinear 2DProp(), \ nonlinear 3DProp(), \ nonlinear 3$

Here is the caller graph for this function:



5.9.3.6 exchangeGhostCells()

```
void LatticePatch::exchangeGhostCells ( {\tt const\ int}\ dir\ )
```

function to exchange ghost cells in uAux for the derivative

Perform the ghost cell exchange in a specified direction.

```
Definition at line 502 of file LatticePatch.cpp.
```

```
00502
00503
         // Check that the lattice has been set up
00504
        checkFlag(FLatticeDimensionSet);
00505
        checkFlag(FLatticePatchSetUp);
00506
        // Variables to per dimension calculate the halo indices, and distance to
        // other side halo boundary
int mx = 1, my = 1, mz = 1, distToRight = 1;
const int gLW = envelopeLattice->get_ghostLayerWidth();
00507
00508
00509
00510
        // In the chosen direction m is set to ghost layer width while the others
00511
         // remain to form the plane
00512
         switch (dir) {
00513
        case 1:
00514
          mx = gLW;
          my = ny;

mz = nz;
00515
00516
00517
           distToRight = (nx - gLW);
00518
          break;
00519
        case 2:
00520
          mx = nx;
          my = gLW;

mz = nz;
00521
00522
00523
           distToRight = nx * (ny - gLW);
00524
          break;
00525
         case 3:
00526
          mx = nx;
          my = ny;

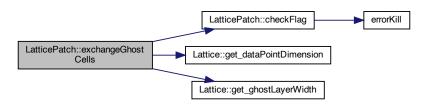
mz = gLW;
00527
00528
00529
           distToRight = nx * ny * (nz - gLW);
00530
00531
00532
        \ensuremath{//} total number of exchanged points
00533
        const int dPD = envelopeLattice->get_dataPointDimension();
00534
        const int exchangeSize = mx * my * mz * dPD;
00535
        // provide size of the halos for ghost cells
```

```
ghostCellLeft.resize(exchangeSize);
        ghostCellRight.resize(ghostCellLeft.size());
00537
00538
        ghostCellLeftToSend.resize(ghostCellLeft.size());
00539
        ghostCellRightToSend.resize(ghostCellLeft.size());
00540
        gCLData = &ghostCellLeft[0];
        gCRData = &ghostCellRight[0];
00541
00542
        statusFlags |= GhostLayersInitialized;
00543
00544
        // Initialize running index li for the halo buffers, and index ui of uData for
00545
        // data transfer
00546
        int 1i = 0, ui = 0;
00547
00548 // #pragma omp parallel for reduction(+:ui) reduction(+:li) -> don't probably
00549 // bad idea to parallelize ghost cell exchange Loop over to be copied points in
00550 // z and y direction
00551 #pragma distribute_point
        for (int iz = 0; iz < mz; iz++) {
  for (int iy = 0; iy < my; iy++) {
    // uData vector start index of halo data to be transferred</pre>
00552
00553
00555
             // with each z-step add the whole xy-plane and with y-step the x-range ->
00556
             // iterate all x-ranges
00557
             ui = (iz * nx * ny + iy * nx) * dPD;
             // copy left halo data from uData to buffer, transfer size is given by
00558
             // x-length (not x-range) perhaps faster but more fragile C lib copy
00559
00560
            // operation (contained in cstring header)
00561
            memcpy(&ghostCellLeftToSend[li],
00562
00563
                    &uData[ui],
                    sizeof(sunrealtype)*mx*dPD);
00564
            // increase ui by the distance to vis-a-vis boundary and copy right halo
00565
            data to buffer ui+=distToRight*dPD; memcpy(&ghostCellRightToSend[li],
00566
00567
                    &uData[ui],
00568
                    sizeof(sunrealtype)*mx*dPD);
00569
            // perhaps more safe but slower copy operation (contained in algorithm // header) performance highly system dependent copy(&uData[ui], &uData[ui + mx * dPD], &ghostCellLeftToSend[li]); ui += distToRight * dPD;
00570
00571
00572
00574
            copy(&uData[ui], &uData[ui + mx * dPD], &ghostCellRightToSend[li]);
00575
00576
             \ensuremath{//} increase halo index by transferred items per y-iteration step
00577
             // (x-length)
00578
            li += mx * dPD:
00579
          }
00580
00581
00582
        /\star Send and receive the data to and from neighboring latticePatches \star/
00583
        // Adjust direction to cartesian communicator
00584
        int dim = 2; // default for dir==1
00585
        if (dir == 2) {
        dim = 1;
} else if (dir == 3) {
00586
00587
00588
          dim = 0;
00589
00590
        int rank_source = 0, rank_dest = 0;
00591
        MPI_Cart_shift (envelopeLattice->comm, dim, -1, &rank_source,
00592
                        &rank_dest); // s.t. rank_dest is left & v.v.
00593
00594
        // nonblocking Isend/Irecv
00595
00596
        MPI Request requests[4];
        MPI_Irecv(&ghostCellRight[0], exchangeSize, MPI_SUNREALTYPE, rank_source, 1,
00597
00598
        envelopeLattice->comm, &requests[0]);
00599
        MPI_Isend(&ghostCellLeftToSend[0], exchangeSize, MPI_SUNREALTYPE, rank_dest,
00600
        1, envelopeLattice->comm, &requests[1]);
00601
        MPI_Irecv(&ghostCellLeft[0], exchangeSize, MPI_SUNREALTYPE, rank_dest, 2,
00602
        envelopeLattice->comm, &requests[2]);
        MPI_Isend(&ghostCellRightToSend[0], exchangeSize, MPI_SUNREALTYPE, rank_source, 2, envelopeLattice->comm, &requests[3]);
00603
00604
        MPI_Waitall(4, requests, MPI_STATUS_IGNORE);
00605
00606
00607
00608
        // blocking Sendrecv:
00609
        MPI_Sendrecv(&ghostCellLeftToSend[0], exchangeSize, MPI_SUNREALTYPE,
00610
                      rank_dest, 1, &ghostCellRight[0], exchangeSize, MPI_SUNREALTYPE,
00611
                       rank_source, 1, envelopeLattice->comm, MPI_STATUS_IGNORE);
00612
        00613
00614
00615
                      rank_dest, 2, envelopeLattice->comm, MPI_STATUS_IGNORE);
00616
00617 }
```

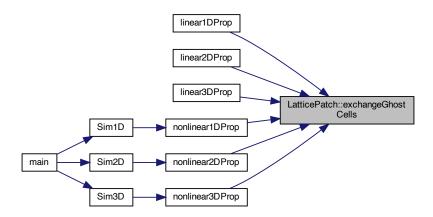
References checkFlag(), Lattice::comm, envelopeLattice, FLatticeDimensionSet, FLatticePatchSetUp, gCLData, gCRData, Lattice::get_dataPointDimension(), Lattice::get_ghostLayerWidth(), ghostCellLeft, ghostCellLeftToSend, ghostCellRight, ghostCellRightToSend, GhostLayersInitialized, nx, ny, nz, statusFlags, and uData.

Referenced by linear1DProp(), linear2DProp(), linear3DProp(), nonlinear1DProp(), nonlinear2DProp(), and nonlinear3DProp().

Here is the call graph for this function:



Here is the caller graph for this function:



5.9.3.7 exchangeGhostCells3D()

```
void LatticePatch::exchangeGhostCells3D ( )
```

function to exchange ghost cells using a neighborhood collective operation

Exchange ghost cells with a neighborhood collective operation.

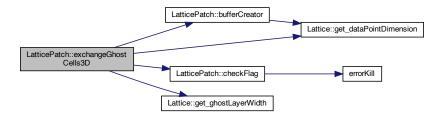
Definition at line 620 of file LatticePatch.cpp.

```
00620
00621
        // Check that the lattice has been set up
00622
        checkFlag(FLatticeDimensionSet);
00623
        // ghostlayerwidth
00624
        const int gLW = envelopeLattice->get_ghostLayerWidth();
        // datapoint dimension
const int dPD = envelopeLattice->get_dataPointDimension();
00625
00626
00627
        // total number of exchanged points per halo
00628
        const int n = nx; // only cubic patches allowed -> use general length n
```

```
const int exchangeSize = n * n * gLW * dPD;
00630
                    // Give ghostCells the total size of the ghost layers (the six halos)
00631
                    const int tot_exchangeSize = 6 * exchangeSize;
00632
                    ghostCells.resize(tot_exchangeSize);
00633
                    ghostCellsToSend.resize(ghostCells.size());
                    // ghost cell data in all directions: left,right,bottom,top,front,abaft; but // with MPI dim order "lefts" are the first receivers and "rights" are the
00634
00635
00636
                    // first senders -> see buffer creator below
00637
                    gCFData = &ghostCells[0];
00638
                    gCAData = &ghostCells[exchangeSize];
                    gCBData = &ghostCells[2 * exchangeSize];
gCTData = &ghostCells[3 * exchangeSize];
00639
00640
00641
                    gCLData = &ghostCells[4 * exchangeSize];
00642
                    gCRData = &ghostCells[5 * exchangeSize];
00643
                    statusFlags |= GhostLayersInitialized;
00644
00645
                    checkFlag(FLatticePatchSetUp);
                    // variables to set to ghost layer width and point distance to next // communication point -> depends on direction
00646
00647
00648
                    int li = 0; // running index for buffers int distToRight = 0; // distance to vis-a-vis halo data, varies per dim
00649
00650
                    // filling buffers along the MPI \operatorname{dim} order
00651
                    00652
00653
00654
00655
                    distToRight = n * (n - gLW);
bufferCreator(li, n, gLW, n, distToRight);
00656
00657
                    li += 2 * exchangeSize;
00658
00659
00660
                    distToRight = (n - gLW);
00661
                    bufferCreator(li, gLW, n, n, distToRight);
00662
00663
                    {\tt MPI\_Neighbor\_alltoall(\&ghostCellsToSend[0], exchangeSize, MPI\_SUNREALTYPE, and the property of the proper
00664
                                                                              &ghostCells[0], exchangeSize, MPI_SUNREALTYPE,
00665
                                                                              envelopeLattice->comm);
00666 }
```

References bufferCreator(), checkFlag(), Lattice::comm, envelopeLattice, FLatticeDimensionSet, FLatticePatchSetUp, gCAData, gCFData, gCFData, gCFData, gCTData, Lattice::get_dataPointDimension(), Lattice::get_ghostLayerWidth(), ghostCells, ghostCellsToSend, GhostLayersInitialized, nx, and statusFlags.

Here is the call graph for this function:



5.9.3.8 generateTranslocationLookup()

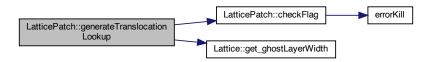
```
void LatticePatch::generateTranslocationLookup ( )
```

function to fill out the lookup tables for translocation

To avoid cache misses: create vectors to translate u vector into space coordinates and vice versa and same for left and right ghost layers to space

```
Definition at line 246 of file LatticePatch.cpp.
00247
         // Check that the lattice has been set up
00248
        checkFlag(FLatticeDimensionSet);
00249
        // lenghts for auxilliary layers, including ghost layers
00250
        const int gLW = envelopeLattice->get_ghostLayerWidth();
        const int mx = nx + 2 * gLW;
00252
        const int my = ny + 2 * gLW;
00253
        const int mz = nz + 2 * gLW;
00254
        // sizes for lookup vectors
        // generate u->uAux
00255
00256
        uTox.resize(nx * ny * nz);
00257
        uToy.resize(nx * ny * nz);
00258
        uToz.resize(nx * ny * nz);
00259
        // generate uAux->u with length including halo
00260
        xTou.resize(mx * ny * nz);
00261
        yTou.resize(nx * my * nz);
        zTou.resize(nx * ny * mz);
00262
00263
        // variables for cartesian position in the 3D discrete lattice
        int px = 0, py = 0, pz = 0;
for (unsigned int i = 0; i < uToy.size(); i++) { // loop over all points in the patch
00264
00265
00266
          // calulate cartesian coordinates
          px = i % nx;
py = (i / nx) % ny;
pz = (i / nx) / ny;
00267
00268
00269
00270
           ^{\prime\prime} // fill lookups extended by halos (useful for y and z direction)
          00271
00272
          xTou[px + py * mx + pz * mx * ny] =
00273
          i; // match cartesian point to u location
uToy[i] = (py + gLW) + pz * my + px * my * nz;
yTou[py + pz * my + px * my * nz] = i;
00274
00275
00276
00277
           uToz[i] = (pz + gLW) + px * mz + py * mz * nx;
00278
           zTou[pz + px * mz + py * mz * nx] = i;
00279
        // same for ghost layer lookup tables
00280
        lgcTox.resize(gLW * ny * nz);
rgcTox.resize(gLW * ny * nz);
00281
00283
        for (unsigned int i = 0; i < lgcTox.size(); i++) {</pre>
00284
         px = i % gLW;
          py = (i / gLW) % ny;
pz = (i / gLW) / ny;
00285
00286
           lgcTox[i] = px + py * mx + pz * mx * ny;
00287
          rgcTox[i] = px + nx + gLW + py * mx + pz * mx * ny;
00288
00289
00290
        lgcToy.resize(gLW * nx * nz);
00291
        rgcToy.resize(gLW * nx * nz);
00292
        for (unsigned int i = 0; i < lgcToy.size(); i++) {</pre>
00293
          px = i % nx;
00294
          py = (i / nx) % gLW;
          pz = (i / nx) / gLW;
00295
00296
           lgcToy[i] = py + pz * my + px * my * nz;
00297
           rgcToy[i] = py + ny + gLW + pz * my + px * my * nz;
00298
00299
        lgcToz.resize(gLW * nx * ny);
        rgcToz.resize(gLW * nx * ny);
00300
        for (unsigned int i = 0; i < lgcToz.size(); i++) {</pre>
00302
          px = i % nx;
00303
          py = (i / nx) % ny;
          pz = (i / nx) / ny;
00304
           \frac{1}{gcToz}[i] = pz + px * mz + py * mz * nx;
00305
00306
          rgcToz[i] = pz + nz + gLW + px * mz + py * mz * nx;
00307
        statusFlags |= TranslocationLookupSetUp;
00309 }
```

References checkFlag(), envelopeLattice, FLatticeDimensionSet, Lattice::get_ghostLayerWidth(), lgcTox, lgcToy, lgcToz, nx, ny, nz, rgcTox, rgcToy, rgcToz, statusFlags, TranslocationLookupSetUp, uTox, uToy, uToz, xTou, yTou, and zTou.



5.9.3.9 getDelta()

```
sunrealtype LatticePatch::getDelta ( const int dir ) const
```

function to get distance between points

Return the distance between points in the patch in a dimension.

Definition at line 228 of file LatticePatch.cpp.

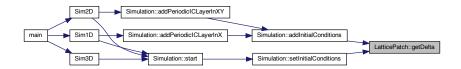
```
00228
00229
        switch (dir) {
00230
       case 1:
00231
          return dx;
00232
       case 2:
00233
         return dy;
00234
       case 3:
00235
         return dz;
00236
       default:
        errorKill(
"LatticePatch::getDelta function called with wrong dir parameter");
00237
00238
00239
         return -1;
00240
00241 }
```

References dx, dy, dz, and errorKill().

Referenced by Simulation::addInitialConditions(), and Simulation::setInitialConditions().

Here is the call graph for this function:





5.9.3.10 initializeBuffers()

```
void LatticePatch::initializeBuffers ( )
```

initialize buffers to save derivatives

Create buffers to save derivative values, optimizing computational load.

Definition at line 487 of file LatticePatch.cpp.

```
00488
            // Check that the lattice has been set up
00489
           checkFlag(FLatticeDimensionSet);
          const int dPD = envelopeLattice->get_dataPointDimension();
buffX.resize(nx * ny * nz * dPD);
buffY.resize(nx * ny * nz * dPD);
buffZ.resize(nx * ny * nz * dPD);
00490
00491
00492
00493
00494
           // Set pointers used for propagation functions
          buffData[0] = &buffX[0];
buffData[1] = &buffY[0];
00495
00496
           buffData[2] = &buffZ[0];
00497
          statusFlags |= BuffersInitialized;
00498
00499 }
```

References buffData, BuffersInitialized, buffY, buffY, buffZ, checkFlag(), envelopeLattice, FLatticeDimensionSet, Lattice::get_dataPointDimension(), nx, ny, nz, and statusFlags.

Referenced by Simulation::initializePatchwork().

Here is the call graph for this function:



Here is the caller graph for this function:



5.9.3.11 initializeGhostLayer()

```
void LatticePatch::initializeGhostLayer ( )
```

initialize ghost cells for halo exchange

5.9.3.12 origin()

```
sunrealtype LatticePatch::origin ( {\tt const\ int}\ dir\ )\ {\tt const}
```

function to get the origin of the patch

Return the physical origin of the patch in a dimension.

Definition at line 213 of file LatticePatch.cpp.

```
00214
        switch (dir) {
00215
        case 1:
       return x0; case 2:
00216
00217
00218
         return y0;
00219
        case 3:
00220
         return z0;
00221
        default:
00222
        errorKill("LatticePatch::origin function called with wrong dir parameter");
00223
          return -1;
00224
00225 }
```

References errorKill(), x0, y0, and z0.

Referenced by Simulation::addInitialConditions(), and Simulation::setInitialConditions().

Here is the call graph for this function:





5.9.3.13 rotateIntoEigen()

function to rotate u into Z-matrix eigenraum

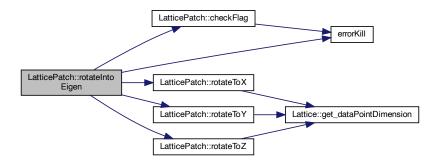
Rotate into eigenraum along R matrices of paper using below rotation functions -> uAuxData gets the rotated left-halo-, inner-patch-, right-halo-data

Definition at line 314 of file LatticePatch.cpp.

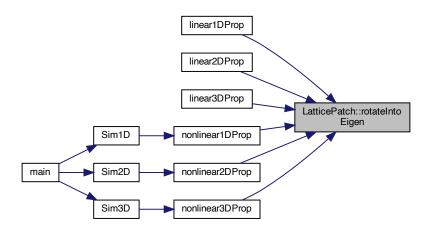
```
00315
       // Check that the lattice, ghost layers as well as the translocation lookups
00316
       // have been set up;
00317
       checkFlag(FLatticePatchSetUp);
00318
       checkFlag(TranslocationLookupSetUp);
      00319
00320
00321
       switch (dir) {
00322
00323
       rotateToX(uAuxData, gCLData, lgcTox);
00324
         rotateToX(uAuxData, uData, uTox);
00325
        rotateToX(uAuxData, gCRData, rgcTox);
00326
        break;
00327
      case 2:
        rotateToY(uAuxData, gCLData, lgcToy);
00329
        rotateToY(uAuxData, uData, uToy);
00330
        rotateToY(uAuxData, gCRData, rgcToy);
        break;
00331
00332
      case 3:
00333
       rotateToZ(uAuxData, gCLData, lgcToz);
00334
        rotateToZ(uAuxData, uData, uToz);
00335
        rotateToZ(uAuxData, gCRData, rgcToz);
00336
00337
      default:
00338
       errorKill("Tried to rotate into the wrong direction");
00339
        break:
00340
00341 }
```

References checkFlag(), errorKill(), FLatticePatchSetUp, gCLData, gCRData, GhostLayersInitialized, IgcTox, IgcToy, IgcToz, rgcTox, rgcToy, rgcToz, rotateToX(), rotateToY(), rotateToZ(), TranslocationLookupSetUp, uAuxData, uData, uTox, uToy, and uToz.

Referenced by linear1DProp(), linear2DProp(), linear3DProp(), nonlinear1DProp(), nonlinear2DProp(), and nonlinear3DProp().



Here is the caller graph for this function:



5.9.3.14 rotateIntoEigen3D()

```
void LatticePatch::rotateIntoEigen3D ( )
```

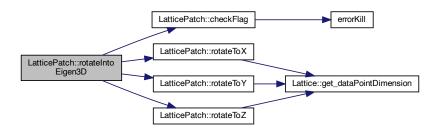
function to rotate as in rotateIntoEigen with special 3D halo buffers

Same as ${\tt rotateIntoEigen}$ but for neighborhood 3D halo buffers.

Definition at line 344 of file LatticePatch.cpp.

```
00344
00345
         checkFlag(FLatticePatchSetUp);
00346
         checkFlag(TranslocationLookupSetUp);
00347
         checkFlag(GhostLayersInitialized);
00348
         rotateToX(uAuxData, gCLData, lgcTox);
00349
         rotateToX(uAuxData, uData, uTox);
         rotateToX(uAuxData, gCRData, rgcTox);
rotateToY(uAuxData, gCBData, lgcToy);
rotateToY(uAuxData, uData, uToy);
00350
00351
00353
         rotateToY(uAuxData, gCTData, rgcToy);
00354
         rotateToZ(uAuxData, gCFData, lgcToz);
00355
         rotateToZ(uAuxData, uData, uToz);
00356
         rotateToZ(uAuxData, gCAData, rgcToz);
00357 }
```

References checkFlag(), FLatticePatchSetUp, gCAData, gCBData, gCFData, gCRData, gCRData, gCTData, GCRData, gCRD



5.9.3.15 rotateToX()

rotate and translocate an input array according to a lookup into an output array

Rotate halo and inner-patch data vectors with rotation matrix Rx into eigenspace of Z matrix and write to auxiliary vector

Definition at line 361 of file LatticePatch.cpp.

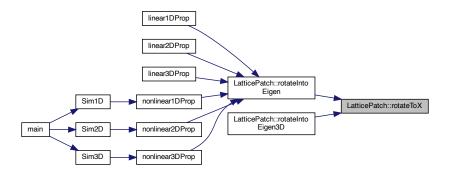
```
00363
                                                                                                                                        {
               int ii = 0, target = 0;
00364
00365 #pragma ivdep
00366 #pragma omp simd // safelen(6) - also good
00367 #pragma distribute_point
00368
             for (unsigned int i = 0; i < lookup.size(); i++) {</pre>
                 // get correct u-vector and spatial indices along previously defined lookup // tables
00369
00370
                  target = envelopeLattice->get_dataPointDimension() * lookup[i];
ii = envelopeLattice->get_dataPointDimension() * i;
00371
00372
                  11 = envelopeLattice->get_dataPointDimension() * i;
  outArray[target + 0] = -inArray[1 + ii] + inArray[5 + ii];
  outArray[target + 1] = inArray[2 + ii] + inArray[4 + ii];
  outArray[target + 2] = inArray[1 + ii] + inArray[5 + ii];
  outArray[target + 3] = -inArray[2 + ii] + inArray[4 + ii];
  outArray[target + 4] = inArray[3 + ii];
  outArray[target + 5] = inArray[ii];
00373
00374
00375
00376
00377
00378
00379
00380 }
```

References envelopeLattice, and Lattice::get_dataPointDimension().

Referenced by rotateIntoEigen(), and rotateIntoEigen3D().

Here is the call graph for this function:





5.9.3.16 rotateToY()

Rotate halo and inner-patch data vectors with rotation matrix Ry into eigenspace of Z matrix and write to auxiliary vector

Definition at line 384 of file LatticePatch.cpp.

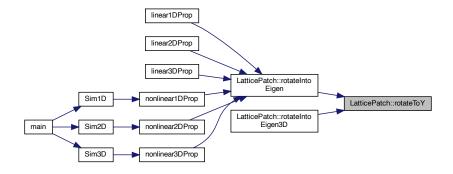
```
00386
00387
                int ii = 0, target = 0;
00388 #pragma ivdep
00389 #pragma omp simd // safelen(6)
00390 #pragma distribute_point
                for (unsigned int i = 0; i < lookup.size(); i++) {</pre>
00391
                   target = envelopeLattice->get_dataPointDimension() * lookup[i];
ii = envelopeLattice->get_dataPointDimension() * i;
outArray[target + 0] = inArray[ii] + inArray[5 + ii];
outArray[target + 1] = -inArray[2 + ii] + inArray[3 + ii];
00392
00393
00394
00395
                   outArray[target + 1] = -inArray[2 + ii] + inArray[5 + ii];
outArray[target + 2] = -inArray[ii] + inArray[5 + ii];
outArray[target + 3] = inArray[2 + ii] + inArray[3 + ii];
outArray[target + 4] = inArray[4 + ii];
outArray[target + 5] = inArray[1 + ii];
00396
00397
00398
00399
00400
00401 }
```

References envelopeLattice, and Lattice::get_dataPointDimension().

Referenced by rotateIntoEigen(), and rotateIntoEigen3D().

Here is the call graph for this function:





5.9.3.17 rotateToZ()

Rotate halo and inner-patch data vectors with rotation matrix Rz into eigenspace of Z matrix and write to auxiliary vector

Definition at line 405 of file LatticePatch.cpp.

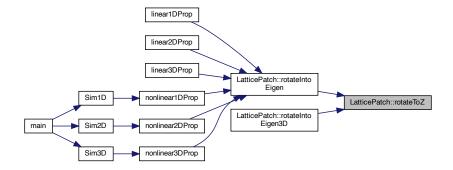
```
00408
                int ii = 0, target = 0;
00409 #pragma ivdep
00410 #pragma omp simd // safelen(6)
00411 #pragma distribute_point
00412 for (unsigned int i = 0; i < lookup.size(); i++) {
                    target = envelopeLattice->get_dataPointDimension() * lookup[i];
00414
                    ii = envelopeLattice->get_dataPointDimension() * i;
                   11 = envelopeLattice->get_dataPointDimension() * 1;
outArray[target + 0] = -inArray[ii] + inArray[4 + ii];
outArray[target + 1] = inArray[1 + ii] + inArray[3 + ii];
outArray[target + 2] = inArray[ii] + inArray[4 + ii];
outArray[target + 3] = -inArray[1 + ii] + inArray[3 + ii];
outArray[target + 4] = inArray[5 + ii];
outArray[target + 5] = inArray[2 + ii];
00415
00416
00417
00418
00419
00420
00421
00422 }
```

References envelopeLattice, and Lattice::get dataPointDimension().

Referenced by rotateIntoEigen(), and rotateIntoEigen3D().

Here is the call graph for this function:





5.9.4 Friends And Related Function Documentation

5.9.4.1 generatePatchwork

friend function for creating the patchwork slicing of the overall lattice

```
Definition at line 109 of file LatticePatch.cpp.
```

```
00110
00111
         // Retrieve the ghost laver depth
00112
        const int gLW = envelopeLattice.get_ghostLayerWidth();
00113
        // Retrieve the data point dimension
00114
        const int dPD = envelopeLattice.get_dataPointDimension();
00115
        // MPI process/patch
        const int my_prc = envelopeLattice.my_prc;
00116
        // Determine thicknes of the slice
00117
00118
        const sunindextype tot_NOXP = envelopeLattice.get_tot_nx(); // total points of lattice
00119
        const sunindextype tot_NOYP = envelopeLattice.get_tot_ny();
00120
        const sunindextype tot_NOZP = envelopeLattice.get_tot_nz();
00121
        // position of the patch in the lattice of patches \rightarrow process associated to
        // position
00122
        const sunindextype LIx = my_prc % DLx;
00123
        const sunindextype LIy = (my_prc / DLx) % DLy;
const sunindextype LIz = (my_prc / DLx) / DLy;
00124
00125
00126
        // Determine the number of points in the patch and first absolute points in
00127
        // each dimension
        const sunindextype local_NOXP = tot_NOXP / DLx;
const sunindextype local_NOYP = tot_NOYP / DLy;
00128
00129
        const sunindextype local_NOZP = tot_NOZP / DLz;
00130
        // absolute positions of the first point in each dimension
        const sunindextype firstXPoint = local_NOXP * LIx;
const sunindextype firstYPoint = local_NOYP * LIy;
00132
00133
        const sunindextype firstZPoint = local_NOZP * LIz;
00134
00135
        // total number of points in the patch
00136
        const sunindextype local_NODP = dPD * local_NOXP * local_NOYP * local_NOZP;
00137
00138
        // Set patch up with above derived quantities
00139
        // Experiment: Resolution can be adapted for each process/patch
00140
        const int Scaler=4; // Better hand over as parameter via `initializePatchwork`
if(my_prc==0){patchToMold.dx=envelopeLattice.get_dx();}
00141
00142
00143
        else if (my_prc==1) {patchToMold.dx=envelopeLattice.get_dx() *Scaler;}
00144
        else{errorKill("Only do this resolution barrier test with 2 processes.");}
00145
00146
        patchToMold.dx = envelopeLattice.get_dx();
        patchToMold.dy = envelopeLattice.get_dy();
00147
        patchToMold.dz = envelopeLattice.get_dz();
00148
        patchToMold.x0 = firstXPoint * patchToMold.dx;
00149
        patchToMold.y0 = firstYPoint * patchToMold.dy;
00150
00151
        patchToMold.z0 = firstZPoint * patchToMold.dz;
        patchToMold.LIx = LIx;
00152
        patchToMold.LIy = LIy;
00153
        patchToMold.LIz = LIz;
00154
00155
        patchToMold.nx = local_NOXP;
        patchToMold.ny = local_NOYP;
00156
        patchToMold.nz = local_NOZP;
00157
00158
        patchToMold.lx = patchToMold.nx * patchToMold.dx;
        patchToMold.ly = patchToMold.ny * patchToMold.dy;
patchToMold.lz = patchToMold.nz * patchToMold.dz;
00159
00160
00161
        /* // Check name of lattice communicator
00162
        char lattice_comm_name[MPI_MAX_OBJECT_NAME];
00163
        int lattice_namelen;
        MPI_Comm_get_name(envelopeLattice.comm, lattice_comm_name, &lattice_namelen); cout«"envelopeLattice.comm gives "« lattice_comm_name « endl;
00164
00165
00166
00167
        /* Create and allocate memory for parallel vectors with defined local and
00168
         * global lenghts *
00169
          * (-> CVode problem sizes Nlocal and N)
```

```
\star for field data and temporal derivatives and set extra pointers to them \star/
         patchToMold.u =
00171
00172
               N_VNew_Parallel(envelopeLattice.comm, local_NODP,
00173
                                   envelopeLattice.get_tot_noDP(), envelopeLattice.sunctx);
         patchToMold.uData = NV_DATA_P (patchToMold.u);
00174
00175
         patchToMold.du =
00176
               N_VNew_Parallel(envelopeLattice.comm, local_NODP,
00177
                                   envelopeLattice.get_tot_noDP(), envelopeLattice.sunctx);
00178
         patchToMold.duData = NV_DATA_P(patchToMold.du);
         // Allocate space for auxiliary uAux so that the lattice and all possible // directions of ghost Layers fit
00179
00180
         const int s1 = patchToMold.nx, s2 = patchToMold.ny, s3 = patchToMold.nz;
const int s_min = min(s1, min(s2, s3));
patchToMold.uAux.resize(s1 * s2 * s3 / s_min * (s_min + 2 * gLW) * dPD);
00181
00182
00183
00184
          patchToMold.uAuxData = &patchToMold.uAux[0];
         patchToMold.envelopeLattice = &envelopeLattice;
// Set patch "name" to process number -> only for debugging
// patchToMold.ID=my_prc;
// set flag
00185
00186
00187
00188
         patchToMold.statusFlags = FLatticePatchSetUp;
00189
00190
         patchToMold.generateTranslocationLookup();
00191
          return 0;
00192 }
```

5.9.5 Field Documentation

5.9.5.1 buffData

```
array<sunrealtype *, 3> LatticePatch::buffData
```

pointer to spatial derivative data buffers

Definition at line 221 of file LatticePatch.h.

Referenced by initializeBuffers(), linear1DProp(), linear2DProp(), linear3DProp(), nonlinear1DProp(), nonlinear2DProp(), and nonlinear3DProp().

5.9.5.2 buffX

```
vector<sunrealtype> LatticePatch::buffX [private]
```

buffer to save spatial derivative values

Definition at line 179 of file LatticePatch.h.

Referenced by initializeBuffers().

5.9.5.3 buffY

```
vector<sunrealtype> LatticePatch::buffY [private]
```

buffer to save spatial derivative values

Definition at line 179 of file LatticePatch.h.

Referenced by initializeBuffers().

5.9.5.4 buffZ

```
vector<sunrealtype> LatticePatch::buffZ [private]
```

buffer to save spatial derivative values

Definition at line 179 of file LatticePatch.h.

Referenced by initializeBuffers().

5.9.5.5 du

```
N_Vector LatticePatch::du
```

N_Vector for saving temporal derivatives of the field data.

Definition at line 209 of file LatticePatch.h.

Referenced by \sim LatticePatch().

5.9.5.6 duData

```
sunrealtype* LatticePatch::duData
```

pointer to time-derivative data

Definition at line 215 of file LatticePatch.h.

Referenced by TimeEvolution::f(), linear1DProp(), linear2DProp(), and linear3DProp().

5.9.5.7 dx

```
sunrealtype LatticePatch::dx [private]
```

physical distance between lattice points in x-direction

Definition at line 164 of file LatticePatch.h.

Referenced by derive(), and getDelta().

5.9.5.8 dy

```
sunrealtype LatticePatch::dy [private]
```

physical distance between lattice points in y-direction

Definition at line 166 of file LatticePatch.h.

Referenced by derive(), and getDelta().

5.9.5.9 dz

```
sunrealtype LatticePatch::dz [private]
```

physical distance between lattice points in z-direction

Definition at line 168 of file LatticePatch.h.

Referenced by derive(), and getDelta().

5.9.5.10 envelopeLattice

```
const Lattice* LatticePatch::envelopeLattice [private]
```

pointer to the enveloping lattice

Definition at line 170 of file LatticePatch.h.

Referenced by bufferCreator(), derive(), derotate(), exchangeGhostCells(), exchangeGhostCells3D(), generateTranslocationLookup(), initializeBuffers(), rotateToX(), rotateToY(), and rotateToZ().

5.9.5.11 gCAData

```
sunrealtype * LatticePatch::gCAData
```

pointer to halo data

Definition at line 218 of file LatticePatch.h.

Referenced by exchangeGhostCells3D(), and rotateIntoEigen3D().

5.9.5.12 gCBData

```
sunrealtype * LatticePatch::gCBData
```

pointer to halo data

Definition at line 218 of file LatticePatch.h.

Referenced by exchangeGhostCells3D(), and rotateIntoEigen3D().

5.9.5.13 gCFData

```
sunrealtype * LatticePatch::gCFData
```

pointer to halo data

Definition at line 218 of file LatticePatch.h.

Referenced by exchangeGhostCells3D(), and rotateIntoEigen3D().

5.9.5.14 gCLData

```
sunrealtype* LatticePatch::gCLData
```

pointer to halo data

Definition at line 218 of file LatticePatch.h.

Referenced by exchangeGhostCells(), exchangeGhostCells3D(), rotateIntoEigen(), and rotateIntoEigen3D().

5.9.5.15 gCRData

```
sunrealtype * LatticePatch::gCRData
```

pointer to halo data

Definition at line 218 of file LatticePatch.h.

Referenced by exchangeGhostCells(), exchangeGhostCells3D(), rotateIntoEigen(), and rotateIntoEigen3D().

5.9.5.16 gCTData

```
sunrealtype * LatticePatch::gCTData
```

pointer to halo data

Definition at line 218 of file LatticePatch.h.

Referenced by exchangeGhostCells3D(), and rotateIntoEigen3D().

5.9.5.17 ghostCellLeft

```
vector<sunrealtype> LatticePatch::ghostCellLeft [private]
```

buffer for passing ghost cell data

Definition at line 183 of file LatticePatch.h.

Referenced by exchangeGhostCells().

5.9.5.18 ghostCellLeftToSend

```
vector<sunrealtype> LatticePatch::ghostCellLeftToSend [private]
```

buffer for passing ghost cell data

Definition at line 183 of file LatticePatch.h.

Referenced by exchangeGhostCells().

5.9.5.19 ghostCellRight

```
vector<sunrealtype> LatticePatch::ghostCellRight [private]
```

buffer for passing ghost cell data

Definition at line 183 of file LatticePatch.h.

Referenced by exchangeGhostCells().

5.9.5.20 ghostCellRightToSend

vector<sunrealtype> LatticePatch::ghostCellRightToSend [private]

buffer for passing ghost cell data

Definition at line 184 of file LatticePatch.h.

Referenced by exchangeGhostCells().

5.9.5.21 ghostCells

```
vector<sunrealtype> LatticePatch::ghostCells [private]
```

buffer for passing ghost cell data

Definition at line 184 of file LatticePatch.h.

Referenced by exchangeGhostCells3D().

5.9.5.22 ghostCellsToSend

```
vector<sunrealtype> LatticePatch::ghostCellsToSend [private]
```

buffer for passing ghost cell data

Definition at line 184 of file LatticePatch.h.

Referenced by bufferCreator(), and exchangeGhostCells3D().

5.9.5.23 ID

int LatticePatch::ID

ID of the LatticePatch, corresponds to process number.

Definition at line 205 of file LatticePatch.h.

5.9.5.24 IgcTox

```
vector<int> LatticePatch::lgcTox [private]
```

ghost cell translocation lookup table

Definition at line 188 of file LatticePatch.h.

Referenced by generateTranslocationLookup(), rotateIntoEigen(), and rotateIntoEigen3D().

5.9.5.25 IgcToy

```
vector<int> LatticePatch::lgcToy [private]
```

ghost cell translocation lookup table

Definition at line 188 of file LatticePatch.h.

Referenced by generateTranslocationLookup(), rotateIntoEigen(), and rotateIntoEigen3D().

5.9.5.26 IgcToz

```
vector<int> LatticePatch::lgcToz [private]
```

ghost cell translocation lookup table

Definition at line 188 of file LatticePatch.h.

Referenced by generateTranslocationLookup(), rotateIntoEigen(), and rotateIntoEigen3D().

5.9.5.27 Llx

```
sunindextype LatticePatch::LIx [private]
```

inner position of lattice-patch in the lattice patchwork; x-points

Definition at line 146 of file LatticePatch.h.

Referenced by LatticePatch().

5.9.5.28 Lly

```
sunindextype LatticePatch::LIy [private]
```

inner position of lattice-patch in the lattice patchwork; y-points

Definition at line 148 of file LatticePatch.h.

Referenced by LatticePatch().

5.9.5.29 LIz

```
sunindextype LatticePatch::LIz [private]
```

inner position of lattice-patch in the lattice patchwork; z-points

Definition at line 150 of file LatticePatch.h.

Referenced by LatticePatch().

5.9.5.30 lx

```
sunrealtype LatticePatch::lx [private]
```

physical size of the lattice-patch in the x-dimension

Definition at line 152 of file LatticePatch.h.

Referenced by LatticePatch().

5.9.5.31 ly

```
sunrealtype LatticePatch::ly [private]
```

physical size of the lattice-patch in the y-dimension

Definition at line 154 of file LatticePatch.h.

Referenced by LatticePatch().

5.9.5.32 lz

```
sunrealtype LatticePatch::lz [private]
```

physical size of the lattice-patch in the z-dimension

Definition at line 156 of file LatticePatch.h.

Referenced by LatticePatch().

5.9.5.33 nx

```
sunindextype LatticePatch::nx [private]
```

number of points in the lattice patch in the x-dimension

Definition at line 158 of file LatticePatch.h.

Referenced by bufferCreator(), discreteSize(), exchangeGhostCells(), exchangeGhostCells3D(), generateTranslocationLookup(), initializeBuffers(), and LatticePatch().

5.9.5.34 ny

```
sunindextype LatticePatch::ny [private]
```

number of points in the lattice patch in the y-dimension

Definition at line 160 of file LatticePatch.h.

Referenced by bufferCreator(), discreteSize(), exchangeGhostCells(), generateTranslocationLookup(), initializeBuffers(), and LatticePatch().

5.9.5.35 nz

```
sunindextype LatticePatch::nz [private]
```

number of points in the lattice patch in the z-dimension

Definition at line 162 of file LatticePatch.h.

Referenced by discreteSize(), exchangeGhostCells(), generateTranslocationLookup(), initializeBuffers(), and LatticePatch().

5.9.5.36 rgcTox

```
vector<int> LatticePatch::rgcTox [private]
```

ghost cell translocation lookup table

Definition at line 188 of file LatticePatch.h.

Referenced by generateTranslocationLookup(), rotateIntoEigen(), and rotateIntoEigen3D().

5.9.5.37 rgcToy

```
vector<int> LatticePatch::rgcToy [private]
```

ghost cell translocation lookup table

Definition at line 188 of file LatticePatch.h.

Referenced by generateTranslocationLookup(), rotateIntoEigen(), and rotateIntoEigen3D().

5.9.5.38 rgcToz

```
vector<int> LatticePatch::rgcToz [private]
```

ghost cell translocation lookup table

Definition at line 188 of file LatticePatch.h.

Referenced by generateTranslocationLookup(), rotateIntoEigen(), and rotateIntoEigen3D().

5.9.5.39 statusFlags

```
unsigned char LatticePatch::statusFlags [private]
```

char for checking flags

Definition at line 191 of file LatticePatch.h.

Referenced by checkFlag(), exchangeGhostCells(), exchangeGhostCells3D(), generateTranslocationLookup(), initializeBuffers(), LatticePatch(), and \sim LatticePatch().

5.9.5.40 u

N_Vector LatticePatch::u

N_Vector for saving field components u=(E,B) in lattice points.

Definition at line 207 of file LatticePatch.h.

Referenced by Simulation::advanceToTime(), Simulation::initializeCVODEobject(), and ~LatticePatch().

5.9.5.41 uAux

vector<sunrealtype> LatticePatch::uAux [private]

aid (auxilliarly) vector including ghost cells to compute the derivatives

Definition at line 176 of file LatticePatch.h.

Referenced by derive(), and derotate().

5.9.5.42 uAuxData

sunrealtype* LatticePatch::uAuxData

pointer to auxiliary data vector

Definition at line 213 of file LatticePatch.h.

Referenced by rotateIntoEigen(), and rotateIntoEigen3D().

5.9.5.43 uData

sunrealtype* LatticePatch::uData

pointer to field data

Definition at line 211 of file LatticePatch.h.

Referenced by Simulation::addInitialConditions(), bufferCreator(), exchangeGhostCells(), TimeEvolution::f(), OutputManager::outUState(), rotateIntoEigen(), rotateIntoEigen3D(), and Simulation::setInitialConditions().

5.9.5.44 uTox

```
vector<int> LatticePatch::uTox [private]
```

translocation lookup table

Definition at line 173 of file LatticePatch.h.

Referenced by derotate(), generateTranslocationLookup(), rotateIntoEigen(), and rotateIntoEigen3D().

5.9.5.45 uToy

```
vector<int> LatticePatch::uToy [private]
```

translocation lookup table

Definition at line 173 of file LatticePatch.h.

Referenced by derotate(), generateTranslocationLookup(), rotateIntoEigen(), and rotateIntoEigen3D().

5.9.5.46 uToz

```
vector<int> LatticePatch::uToz [private]
```

translocation lookup table

Definition at line 173 of file LatticePatch.h.

Referenced by derotate(), generateTranslocationLookup(), rotateIntoEigen(), and rotateIntoEigen3D().

5.9.5.47 x0

```
sunrealtype LatticePatch::x0 [private]
```

origin of the patch in physical space; x-coordinate

Definition at line 140 of file LatticePatch.h.

Referenced by LatticePatch(), and origin().

5.9.5.48 xTou

```
vector<int> LatticePatch::xTou [private]
```

translocation lookup table

Definition at line 173 of file LatticePatch.h.

Referenced by generateTranslocationLookup().

5.9.5.49 y0

```
sunrealtype LatticePatch::y0 [private]
```

origin of the patch in physical space; y-coordinate

Definition at line 142 of file LatticePatch.h.

Referenced by LatticePatch(), and origin().

5.9.5.50 yTou

```
vector<int> LatticePatch::yTou [private]
```

translocation lookup table

Definition at line 173 of file LatticePatch.h.

Referenced by generateTranslocationLookup().

5.9.5.51 z0

```
sunrealtype LatticePatch::z0 [private]
```

origin of the patch in physical space; z-coordinate

Definition at line 144 of file LatticePatch.h.

Referenced by LatticePatch(), and origin().

5.9.5.52 zTou

```
vector<int> LatticePatch::zTou [private]
```

translocation lookup table

Definition at line 173 of file LatticePatch.h.

Referenced by generateTranslocationLookup().

The documentation for this class was generated from the following files:

- src/LatticePatch.h
- src/LatticePatch.cpp

5.10 OutputManager Class Reference

Output Manager class to generate and coordinate output writing to disk.

```
#include <src/Outputters.h>
```

Public Member Functions

• OutputManager ()

default constructor

• void generateOutputFolder (const string &dir)

function that creates folder to save simulation data

void set_outputStyle (const char _outputStyle)

set the output style

• void outUState (const int &state, const Lattice &lattice, const LatticePatch &latticePatch)

function to write data to disk in specified way

const string & getSimCode () const

simCode getter function

Static Private Member Functions

• static string SimCodeGenerator ()

function to create the Code of the Simulations

Private Attributes

string simCode

varible to safe the SimCode generated at execution

string Path

variable for the path to the output folder

· char outputStyle

output style; csv or binary

5.10.1 Detailed Description

Output Manager class to generate and coordinate output writing to disk.

Definition at line 25 of file Outputters.h.

5.10.2 Constructor & Destructor Documentation

5.10.2.1 OutputManager()

```
OutputManager::OutputManager ( )
```

default constructor

Directly generate the simCode at construction.

Definition at line 9 of file Outputters.cpp.

```
00009 {
00010 simCode = SimCodeGenerator();
00011 outputStyle = 'c';
00012 }
```

References outputStyle, simCode, and SimCodeGenerator().

Here is the call graph for this function:



5.10.3 Member Function Documentation

5.10.3.1 generateOutputFolder()

```
void OutputManager::generateOutputFolder ( {\tt const\ string\ \&\ dir\ )}
```

function that creates folder to save simulation data

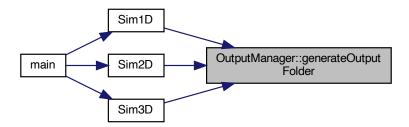
Generate the folder to save the data to by one process: In the given directory it creates a directory "SimResults" and a directory with the simCode. The relevant part of the main file is written to a "config.txt" file in that directory to log the settings.

Definition at line 40 of file Outputters.cpp.

```
// Do this only once for the first process
00041
00042
          int myPrc;
00043
          MPI_Comm_rank(MPI_COMM_WORLD, &myPrc);
00044
         if (myPrc == 0) {
00045
           if (!fs::is_directory(dir))
           fs::create_directory(dir);
if (!fs::is_directory(dir + "/SimResults"))
fs::create_directory(dir + "/SimResults");
if (!fs::is_directory(dir + "/SimResults/" + simCode))
00046
00047
00048
00049
00050
               fs::create_directory(dir + "/SimResults/" + simCode);
00051
         // path variable for the output generation
Path = dir + "/SimResults/" + simCode + "/";
00052
00053
00054
00055
          // Logging configurations from main.cpp
         ifstream fin("main.cpp");
ofstream fout(Path + "config.txt");
00056
00057
00058
          string line;
00059
          int begin=1000;
         for (int i = 1; !fin.eof(); i++) {
  getline(fin, line);
00060
00061
00062
            if (line.starts_with("
                                              //---- B")) {
00063
                 begin=i;
00064
            if (i < begin) {</pre>
00065
00066
              continue;
00067
            fout « line « endl;
00068
            if (line.starts_with("
00070
                 break;
00071
            }
00072
          }
00073
          return;
00074 }
```

References Path, and simCode.

Referenced by Sim1D(), Sim2D(), and Sim3D().



5.10.3.2 getSimCode()

```
const string & OutputManager::getSimCode ( ) const [inline]
```

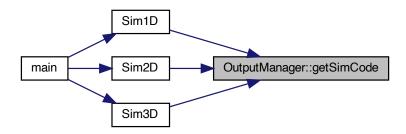
simCode getter function

Definition at line 45 of file Outputters.h. 00045 { return simCode; }

References simCode.

Referenced by Sim1D(), Sim2D(), and Sim3D().

Here is the caller graph for this function:



5.10.3.3 outUState()

function to write data to disk in specified way

Write the field data either in csv format to one file per each process (patch) or in binary form to a single file. Files are stores inthe simCode directory. For csv files the state (simulation step) denotes the prefix and the suffix after an underscore is given by the process/patch number. Binary files are simply named after the step number.

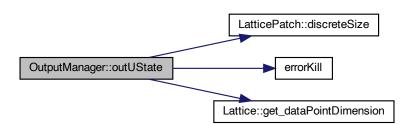
Definition at line 85 of file Outputters.cpp.

```
00086
00087
         switch(outputStyle){
00088
             case 'c': { // one csv file per process
00089
         ofstream ofs:
        ofs.open(Path + to_string(state) + "_" + to_string(lattice.my_prc) + ".csv");
// Precision of sunrealtype in significant decimal digits; 15 for IEEE double
ofs « setprecision(numeric_limits<sunrealtype>::digits10);
00090
00091
00092
00093
00094
         // Walk through each lattice point
        00095
00096
00097
00098
00099
                « latticePatch.uData[i + 4] « "," « latticePatch.uData[i + 5]
```

```
00100
               « endl;
00101
00102
        ofs.close();
00103
        break;
00104
00105
             case 'b': { // a single binary file
00106
00107
        // Open the output file
00108
        MPI_File fh;
        const string filename = Path+to_string(state);
MPI_File_open(lattice.comm,&filename[0],MPI_MODE_WRONLY|MPI_MODE_CREATE,
00109
00110
00111
        \label{eq:MPI_INFO_NULL,&fh);} $$// \ number \ of \ datapoints \ in \ the patch \ with \ process \ offset
00112
00113
        const int count = latticePatch.discreteSize()*lattice.get_dataPointDimension();
00114
        MPI_Offset offset = lattice.my_prc*count*sizeof(MPI_SUNREALTYPE);
        // Go to offset in file and write data to it; maximal precision in // "native" representation
00115
00116
00117
        MPI_File_set_view(fh, offset, MPI_SUNREALTYPE, MPI_SUNREALTYPE, "native",
00118
                 MPI_INFO_NULL);
00119
        MPI_File_write_all(fh,latticePatch.uData,count,MPI_SUNREALTYPE,MPI_STATUS_IGNORE);
00120
00121
        MPI_Request write_request;
        MPI_File_iwrite_all(fh,latticePatch.uData,count,MPI_SUNREALTYPE,&write_request);
00122
00123
        MPI_Wait(&write_request,MPI_STATUS_IGNORE);
00124
00125
00126
        MPI_File_write_at_all(fh,offset,latticePatch.uData,count,MPI_SUNREALTYPE,
00127
                 MPI_STATUS_IGNORE);
00128
                 */
00129
        break:
00130
00131
             default: {
00132
        errorKill("No valid output style defined.\
00133
                 Choose between (c): one csv file per process, (b) one binary file");
00134
00135
00136
        return;
00137
00138 }
```

References Lattice::comm, LatticePatch::discreteSize(), errorKill(), Lattice::get_dataPointDimension(), Lattice::my_prc, outputStyle, Path, and LatticePatch::uData.

 $Referenced \ by \ Simulation::outAllFieldData().$



Here is the caller graph for this function:



5.10.3.4 set_outputStyle()

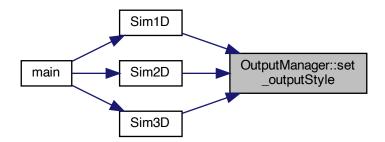
set the output style

Definition at line 76 of file Outputters.cpp.

```
00076
00077 outputStyle = _outputStyle;
00078 }
```

References outputStyle.

Referenced by Sim1D(), Sim2D(), and Sim3D().



5.10.3.5 SimCodeGenerator()

```
string OutputManager::SimCodeGenerator ( ) [static], [private]
```

function to create the Code of the Simulations

Generate the identifier number reverse from year to minute in the format yy-mm-dd hh-MM-ss

Definition at line 16 of file Outputters.cpp.

```
00017
           const chrono::time_point<chrono::system_clock> now{
00018
          chrono::system_clock::now();;
const chrono::year_month_day ymd{chrono::floor<chrono::days>(now)};
00019
00020
          const auto tod = now - chrono::floor<chrono::days>(now);
00021
          const chrono::hh_mm_ss hms{tod};
00022
          stringstream temp;
00023
          temp \ll setfill('0') \ll set (2) 
00024
                  « static_cast<int>(ymd.year() - chrono::years(2000)) « "-"
« setfill('0') « setw(2) « static_cast<unsigned>(ymd.month()) « "-"
« setfill('0') « setw(2) « static_cast<unsigned>(ymd.day()) « "_"
00025
00026
00027
00028
                  « setfill('0') « setw(2) « hms.hours().count() « "-" « setfill('0')
« setw(2) « hms.minutes().count() « "-" « setfill('0') « setw(2)
00029
                 « hms.seconds().count();
//« "_" « hms.subseconds().count(); // subseconds render the filename
00030
00031
00032
                  // too large
          return temp.str();
00034 }
```

Referenced by OutputManager().

Here is the caller graph for this function:



5.10.4 Field Documentation

5.10.4.1 outputStyle

```
char OutputManager::outputStyle [private]
```

output style; csv or binary

Definition at line 34 of file Outputters.h.

 $Referenced \ by \ Output Manager(), \ out UState(), \ and \ set_output Style().$

5.10.4.2 Path

string OutputManager::Path [private]

variable for the path to the output folder

Definition at line 32 of file Outputters.h.

Referenced by generateOutputFolder(), and outUState().

5.10.4.3 simCode

```
string OutputManager::simCode [private]
```

varible to safe the SimCode generated at execution

Definition at line 30 of file Outputters.h.

Referenced by generateOutputFolder(), getSimCode(), and OutputManager().

The documentation for this class was generated from the following files:

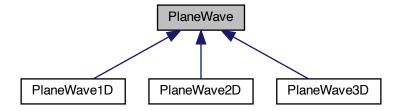
- src/Outputters.h
- src/Outputters.cpp

5.11 PlaneWave Class Reference

super-class for plane waves

#include <src/ICSetters.h>

Inheritance diagram for PlaneWave:



Protected Attributes

```
    sunrealtype kx

      wavenumber k_x
· sunrealtype ky
      wavenumber k_y

    sunrealtype kz

      wavenumber k_z
• sunrealtype px
      polarization & amplitude in x-direction, p_x

    sunrealtype py

      polarization & amplitude in y-direction, p_y
• sunrealtype pz
      polarization & amplitude in z-direction, p_z

    sunrealtype phix

      phase shift in x-direction, \phi_x
· sunrealtype phiy
      phase shift in y-direction, \phi_y

    sunrealtype phiz

      phase shift in z-direction, \phi_z
```

5.11.1 Detailed Description

```
super-class for plane waves
```

They are given in the form $ec{E}=ec{E}_0~\cos\left(ec{k}\cdotec{x}-ec{\phi}
ight)$

Definition at line 23 of file ICSetters.h.

5.11.2 Field Documentation

5.11.2.1 kx

```
sunrealtype PlaneWave::kx [protected]
```

wavenumber k_x

Definition at line 26 of file ICSetters.h.

Referenced by PlaneWave1D::addToSpace(), PlaneWave2D::addToSpace(), PlaneWave3D::addToSpace(), PlaneWave1D::PlaneWave1D(), PlaneWave2D(), and PlaneWave3D::PlaneWave3D().

5.11.2.2 ky

```
sunrealtype PlaneWave::ky [protected]
```

wavenumber k_u

Definition at line 28 of file ICSetters.h.

Referenced by PlaneWave1D::addToSpace(), PlaneWave2D::addToSpace(), PlaneWave3D::addToSpace(), PlaneWave1D::PlaneWave1D(), PlaneWave2D(), and PlaneWave3D::PlaneWave3D().

5.11.2.3 kz

```
sunrealtype PlaneWave::kz [protected]
```

wavenumber k_z

Definition at line 30 of file ICSetters.h.

Referenced by PlaneWave1D::addToSpace(), PlaneWave2D::addToSpace(), PlaneWave3D::addToSpace(), PlaneWave1D::PlaneWave1D(), PlaneWave2D(), and PlaneWave3D::PlaneWave3D().

5.11.2.4 phix

```
sunrealtype PlaneWave::phix [protected]
```

phase shift in x-direction, ϕ_x

Definition at line 38 of file ICSetters.h.

5.11.2.5 phiy

```
sunrealtype PlaneWave::phiy [protected]
```

phase shift in y-direction, ϕ_y

Definition at line 40 of file ICSetters.h.

Referenced by PlaneWave1D::addToSpace(), PlaneWave2D::addToSpace(), PlaneWave3D::addToSpace(), PlaneWave1D::PlaneWave1D(), PlaneWave2D(), and PlaneWave3D::PlaneWave3D().

5.11.2.6 phiz

```
sunrealtype PlaneWave::phiz [protected]
```

phase shift in z-direction, ϕ_z

Definition at line 42 of file ICSetters.h.

Referenced by PlaneWave1D::addToSpace(), PlaneWave2D::addToSpace(), PlaneWave3D::addToSpace(), PlaneWave1D::PlaneWave1D(), PlaneWave2D(), and PlaneWave3D::PlaneWave3D().

5.11.2.7 px

```
sunrealtype PlaneWave::px [protected]
```

polarization & amplitude in x-direction, p_x

Definition at line 32 of file ICSetters.h.

Referenced by PlaneWave1D::addToSpace(), PlaneWave2D::addToSpace(), PlaneWave3D::addToSpace(), PlaneWave1D::PlaneWave1D(), PlaneWave2D(), and PlaneWave3D::PlaneWave3D().

5.11.2.8 py

```
sunrealtype PlaneWave::py [protected]
```

polarization & amplitude in y-direction, p_y

Definition at line 34 of file ICSetters.h.

Referenced by PlaneWave1D::addToSpace(), PlaneWave2D::addToSpace(), PlaneWave3D::addToSpace(), PlaneWave1D::PlaneWave1D(), PlaneWave2D(), and PlaneWave3D::PlaneWave3D().

5.11.2.9 pz

```
sunrealtype PlaneWave::pz [protected]
```

polarization & amplitude in z-direction, p_z

Definition at line 36 of file ICSetters.h.

Referenced by PlaneWave1D::addToSpace(), PlaneWave2D::addToSpace(), PlaneWave3D::addToSpace(), PlaneWave1D::PlaneWave1D(), PlaneWave2D(), and PlaneWave3D::PlaneWave3D().

The documentation for this class was generated from the following file:

• src/ICSetters.h

5.12 planewave Struct Reference

plane wave structure

#include <src/SimulationFunctions.h>

Data Fields

- vector< sunrealtype > k
- vector< sunrealtype > p
- vector< sunrealtype > phi

5.12.1 Detailed Description

plane wave structure

Definition at line 20 of file SimulationFunctions.h.

5.12.2 Field Documentation

5.12.2.1 k

```
vector < sunrealtype > planewave::k
```

wavevector (normalized to $1/\lambda$)

Definition at line 21 of file SimulationFunctions.h.

Referenced by main().

5.12.2.2 p

vector<sunrealtype> planewave::p

amplitde & polarization vector

Definition at line 22 of file SimulationFunctions.h.

Referenced by main().

5.12.2.3 phi

vector<sunrealtype> planewave::phi

phase shift

Definition at line 23 of file SimulationFunctions.h.

Referenced by main().

The documentation for this struct was generated from the following file:

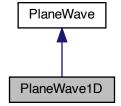
• src/SimulationFunctions.h

5.13 PlaneWave1D Class Reference

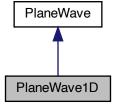
class for plane waves in 1D

#include <src/ICSetters.h>

Inheritance diagram for PlaneWave1D:



Collaboration diagram for PlaneWave1D:



Public Member Functions

- PlaneWave1D (vector< sunrealtype > k={1, 0, 0}, vector< sunrealtype > p={0, 0, 1}, vector< sunrealtype > phi={0, 0, 0})
 - construction with default parameters
- void addToSpace (sunrealtype x, sunrealtype y, sunrealtype z, sunrealtype *pTo6Space) const function for the actual implementation in the lattice

Additional Inherited Members

5.13.1 Detailed Description

class for plane waves in 1D

Definition at line 46 of file ICSetters.h.

5.13.2 Constructor & Destructor Documentation

5.13.2.1 PlaneWave1D()

```
PlaneWave1D::PlaneWave1D (  \mbox{vector} < \mbox{sunrealtype} > k = \{1, 0, 0\}, \\ \mbox{vector} < \mbox{sunrealtype} > p = \{0, 0, 1\}, \\ \mbox{vector} < \mbox{sunrealtype} > phi = \{0, 0, 0\} \ )
```

construction with default parameters

PlaneWave1D construction with

- wavevectors k_x
- k_y
- k_z normalized to $1/\lambda$
- amplitude (polarization) in x-direction p_x
- amplitude (polarization) in y-direction $p_{\boldsymbol{y}}$
- amplitude (polarization) in z-direction p_z
- phase shift in x-direction ϕ_x
- phase shift in y-direction ϕ_y
- phase shift in z-direction ϕ_z

Definition at line 12 of file ICSetters.cpp.

```
00014
          kx = k[0]; /** - wavevectors <math>f k_x \ f */
         ky = k[1]; /** - \f$ k_y \f$ */
kz = k[2]; /** - \f$ k_z \f$ normalized to \f$ 1/\lambda \f$ */
00015
00016
         // Amplitude bug: lower by factor 3
00017
         00019
00020
         pz = p[2] / 3; /** - amplitude (polarization) in z-direction <math>f p_z f */
         phix = phi[0]; /** - phase shift in x-direction \f$ \phi_x \f$ */
phiy = phi[1]; /** - phase shift in y-direction \f$ \phi_y \f$ */
phiz = phi[2]; /** - phase shift in z-direction \f$ \phi_z \f$ */
00021
00022
00023
00024 }
```

References PlaneWave::kx, PlaneWave::ky, PlaneWave::kz, PlaneWave::phix, PlaneWave::phiy, PlaneWave::phiy, PlaneWave::phiz, PlaneWave::px, PlaneWave::px, PlaneWave::px.

5.13.3 Member Function Documentation

5.13.3.1 addToSpace()

function for the actual implementation in the lattice

PlaneWave1D implementation in space

Definition at line 28 of file ICSetters.cpp.

```
00029
       00030
00032
00033
       // Plane wave definition
00034
00035 const array<sunrealtype, 3> E{{
                                                                    /* E-field vector */
                                00036
00037
00038
       // Put E-field into space
00039
00040 pTo6Space[0] += E[0];
00041 pTo6Space[1] += E[1];
       pTo6Space[2] += E[2];
00042
00043
       // and B-field
       pTo6Space[3] += (ky * E[2] - kz * E[1]) / wavelength;
pTo6Space[4] += (kz * E[0] - kx * E[2]) / wavelength;
pTo6Space[5] += (kx * E[1] - ky * E[0]) / wavelength;
00045
00046
00047 }
```

References PlaneWave::kx, PlaneWave::ky, PlaneWave::kz, PlaneWave::phix, PlaneWave::phiy, PlaneWave::phiz, PlaneWave::px, PlaneWave::px, PlaneWave::px, PlaneWave::px, PlaneWave::px.

The documentation for this class was generated from the following files:

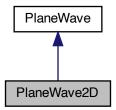
- · src/ICSetters.h
- src/ICSetters.cpp

5.14 PlaneWave2D Class Reference

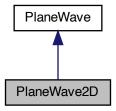
class for plane waves in 2D

```
#include <src/ICSetters.h>
```

Inheritance diagram for PlaneWave2D:



Collaboration diagram for PlaneWave2D:



Public Member Functions

- PlaneWave2D (vector< sunrealtype > k={1, 0, 0}, vector< sunrealtype > p={0, 0, 1}, vector< sunrealtype > phi={0, 0, 0})
 - construction with default parameters
- void addToSpace (sunrealtype x, sunrealtype y, sunrealtype z, sunrealtype *pTo6Space) const function for the actual implementation in the lattice

Additional Inherited Members

5.14.1 Detailed Description

class for plane waves in 2D

Definition at line 58 of file ICSetters.h.

5.14.2 Constructor & Destructor Documentation

5.14.2.1 PlaneWave2D()

```
PlaneWave2D::PlaneWave2D (  \mbox{vector} < \mbox{sunrealtype} > k = \{1, 0, 0\}, \\ \mbox{vector} < \mbox{sunrealtype} > p = \{0, 0, 1\}, \\ \mbox{vector} < \mbox{sunrealtype} > phi = \{0, 0, 0\} \ )
```

construction with default parameters

PlaneWave2D construction with

- wavevectors k_x
- k_y
- k_z normalized to $1/\lambda$
- amplitude (polarization) in x-direction p_x
- amplitude (polarization) in y-direction p_y
- amplitude (polarization) in z-direction p_z
- phase shift in x-direction ϕ_x
- phase shift in y-direction ϕ_y
- phase shift in z-direction ϕ_z

Definition at line 50 of file ICSetters.cpp.

References PlaneWave::kx, PlaneWave::ky, PlaneWave::kz, PlaneWave::phix, PlaneWave::phiy, PlaneWave::phiz, PlaneWave::px, Plan

5.14.3 Member Function Documentation

5.14.3.1 addToSpace()

function for the actual implementation in the lattice

PlaneWave2D implementation in space

Definition at line 66 of file ICSetters.cpp.

```
00067
00068
     00069
00071
                     numbers::pi; /* \f$ 2\pi \ \vec{k} \cdot \vec{x} \f$ */
00072
     // Plane wave definition
00073
     const array<sunrealtype, 3> E{{
                                                /* E-field vector */
                      00074
00075
00076
00077
     // Put E-field into space
00078
     pTo6Space[0] += E[0];
00079
     pTo6Space[1] += E[1];
     pTo6Space[2] += E[2];
// and B-field
08000
00081
     00082
00083
00084
00085 }
```

References PlaneWave::kx, PlaneWave::ky, PlaneWave::kz, PlaneWave::phix, PlaneWave::phiy, PlaneWave::phiz, PlaneWave::px, PlaneWave::px, PlaneWave::px, PlaneWave::px, PlaneWave::px.

The documentation for this class was generated from the following files:

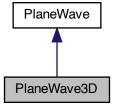
- src/ICSetters.h
- src/ICSetters.cpp

5.15 PlaneWave3D Class Reference

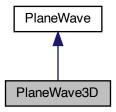
class for plane waves in 3D

```
#include <src/ICSetters.h>
```

Inheritance diagram for PlaneWave3D:



Collaboration diagram for PlaneWave3D:



Public Member Functions

• PlaneWave3D (vector< sunrealtype > k={1, 0, 0}, vector< sunrealtype > p={0, 0, 1}, vector< sunrealtype > phi={0, 0, 0})

construction with default parameters

• void addToSpace (sunrealtype x, sunrealtype y, sunrealtype z, sunrealtype *pTo6Space) const function for the actual implementation in space

Additional Inherited Members

5.15.1 Detailed Description

class for plane waves in 3D

Definition at line 70 of file ICSetters.h.

5.15.2 Constructor & Destructor Documentation

5.15.2.1 PlaneWave3D()

```
PlaneWave3D::PlaneWave3D (  \mbox{vector} < \mbox{sunrealtype} > k = \{1, 0, 0\}, \\ \mbox{vector} < \mbox{sunrealtype} > p = \{0, 0, 1\}, \\ \mbox{vector} < \mbox{sunrealtype} > phi = \{0, 0, 0, 0\} \ )
```

construction with default parameters

PlaneWave3D construction with

• wavevectors k_x

- k_y
- k_z normalized to $1/\lambda$
- amplitude (polarization) in x-direction p_x
- amplitude (polarization) in y-direction p_y
- amplitude (polarization) in z-direction p_z
- phase shift in x-direction ϕ_x
- phase shift in y-direction ϕ_y
- phase shift in z-direction ϕ_z

Definition at line 88 of file ICSetters.cpp.

```
/** - wavevectors \f \ k_x \f \ */
00090
                                           kx = k[0];
                                                                                                                        00091
                                          ky = k[1];
                                          kz = k[2];
00092
                                                                                                                        /** - \lambda \lambda
00093
                                          ;[0]q = xq
00094
                                         py = p[1];
                                                                                                                          /** - amplitude (polarization) in z-direction \f$ p_z \f$ */
                                         pz = p[2];
                                        phix = phi[0]; /** - phase shift in x-direction \f\$ \phiix \f\$ */
phiy = phi[1]; /** - phase shift in y-direction \f\$ \phi_x \f\$ */
00096
00097
00098 phiz = phi[2]; /** - phase shift in z-direction \f$ \phi_z \f$ */
00099 }
```

References PlaneWave::kx, PlaneWave::ky, PlaneWave::kz, PlaneWave::phix, PlaneWave::phiy, PlaneWave::phiz, PlaneWave::px, Plan

5.15.3 Member Function Documentation

5.15.3.1 addToSpace()

function for the actual implementation in space

PlaneWave3D implementation in space

Definition at line 103 of file ICSetters.cpp.

```
00104
00105
     const sunrealtype wavelength =
     00106
00107
                      numbers::pi; /* \f$ 2\pi \ \ec{k} \cdot \vec{x} \f$ */
00108
00109
     // Plane wave definition
00110
     const array<sunrealtype, 3> E\{{/* E-field vector f\$ \vec{E}}\f$*/
                       00111
00112
                        pz * cos(kScalarX - phiz)}}; /* \f$ E_z \f$ */
00113
00114
     // Put E-field into space
00115
     pTo6Space[0] += E[0];
00116
     pTo6Space[1] += E[1];
00117
     pTo6Space[2] += E[2];
00118
     // and B-field
     00119
00120
00121
00122 }
```

References PlaneWave::kx, PlaneWave::kx, PlaneWave::phix, PlaneWave::phix, PlaneWave::phix, PlaneWave::phix, PlaneWave::px, Pl

The documentation for this class was generated from the following files:

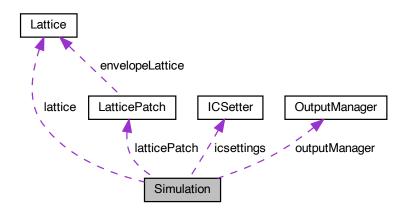
- · src/ICSetters.h
- src/ICSetters.cpp

5.16 Simulation Class Reference

Simulation class to instantiate the whole walkthrough of a Simulation.

#include <src/SimulationClass.h>

Collaboration diagram for Simulation:



Public Member Functions

- Simulation (const int nx, const int ny, const int nz, const int StencilOrder, const bool periodicity)
 - constructor function for the creation of the cartesian communicator
- ∼Simulation ()
 - destructor function freeing CVode memory and Sundials context
- MPI_Comm * get_cart_comm ()
 - Reference to the cartesian communicator of the lattice -> for debugging.
- void setDiscreteDimensionsOfLattice (const sunindextype _tot_nx, const sunindextype _tot_ny, const sunindextype _tot_nz)

function to set discrete dimensions of the lattice

- void setPhysicalDimensionsOfLattice (const sunrealtype lx, const sunrealtype ly, const sunrealtype lz)
 - function to set physical dimensions of the lattice
- void initializePatchwork (const int nx, const int ny, const int nz)
 - function to initialize the Patchwork
- void initializeCVODEobject (const sunrealtype reltol, const sunrealtype abstol)
 - function to initialize the CVODE object with all requirements
- void start ()
 - function to start the simulation for time iteration
- void setInitialConditions ()
 - functions to set the initial field configuration onto the lattice

void addInitialConditions (const int xm, const int ym, const int zm=0)

functions to add initial periodic field configurations

· void addPeriodicICLayerInX ()

function to add a periodic IC Layer in one dimension

void addPeriodicICLayerInXY ()

function to add periodic IC Layers in two dimensions

• void advanceToTime (const sunrealtype &tEnd)

function to advance solution in time with CVODE

void outAllFieldData (const int &state)

function to generate Output of the whole field at a given time

· void checkFlag (unsigned int flag) const

function to check that a flag has been set and if not print an error

• void checkNoFlag (unsigned int flag) const

function to check that if flag has not been set and if print an error

Data Fields

ICSetter icsettings

IC Setter object.

OutputManager outputManager

Output Manager object.

void * cvode_mem

Pointer to CVode memory object – public to avoid cross library errors.

Private Attributes

· Lattice lattice

Lattice object.

· LatticePatch latticePatch

LatticePatch object.

· sunrealtype t

current time of the simulation

unsigned char statusFlags

char for checking simulation flags

5.16.1 Detailed Description

Simulation class to instantiate the whole walkthrough of a Simulation.

Definition at line 37 of file SimulationClass.h.

5.16.2 Constructor & Destructor Documentation

5.16.2.1 Simulation()

constructor function for the creation of the cartesian communicator

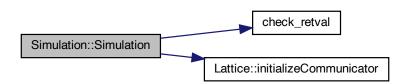
Along with the simulation object, create the cartesian communicator and SUNContext object

Definition at line 14 of file SimulationClass.cpp.

```
00016
           lattice(StencilOrder) {
00017
        statusFlags = 0;
        t = 0;
// Initialize the cartesian communicator
00018
00019
00020
        lattice.initializeCommunicator(nx, ny, nz, periodicity);
00021
00022
        // Create the SUNContext object associated with the thread of execution
00023
00024
        retval = SUNContext_Create(&lattice.comm, &lattice.sunctx);
        if (check_retval(&retval, "SUNContext_Create", 1, lattice.my_prc))
    MPI_Abort(lattice.comm, 1);
00025
00026
        // if (flag != CV_SUCCESS) { printf("SUNContext_Create failed, flag=%d.\n",
00028
        // flag);
00029
                MPI_Abort(lattice.comm, 1); }
00030 }
```

References check_retval(), Lattice::comm, Lattice::initializeCommunicator(), lattice, Lattice::my_prc, statusFlags, Lattice::sunctx, and t.

Here is the call graph for this function:



5.16.2.2 \sim Simulation()

```
Simulation::~Simulation ()
```

destructor function freeing CVode memory and Sundials context

Free the CVode solver memory and Sundials context object with the finish of the simulation

Definition at line 34 of file SimulationClass.cpp.

References cvode_mem, CvodeObjectSetUp, lattice, statusFlags, and Lattice::sunctx.

5.16.3 Member Function Documentation

5.16.3.1 addInitialConditions()

functions to add initial periodic field configurations

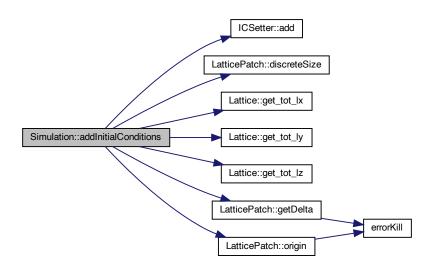
Use parameters to add periodic IC layers.

Definition at line 185 of file SimulationClass.cpp.

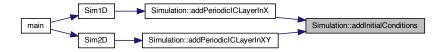
```
00186
         const sunrealtype dx = latticePatch.getDelta(1);
00187
         const sunrealtype dy = latticePatch.getDelta(2);
const sunrealtype dz = latticePatch.getDelta(3);
00188
00189
         const int nx = latticePatch.discreteSize(1);
const int ny = latticePatch.discreteSize(2);
00190
00191
         // Correct for demanded displacement, rest as for setInitialConditions
00192
00193
         const sunrealtype x0 = latticePatch.origin(1) + xm*lattice.get_tot_lx();
         const sunrealtype y0 = latticePatch.origin(2) + ym*lattice.get_tot_ly();
00194
00195
         const sunrealtype z0 = latticePatch.origin(3) + zm*lattice.get_tot_lz();
00196
         int px = 0, py = 0, pz = 0;
         for (int i = 0; i < latticePatch.discreteSize() * 6; i += 6) {
    px = (i / 6) % nx;
    py = ((i / 6) / nx) % ny;
    pz = ((i / 6) / nx) / ny;
00197
00198
00199
00200
           icsettings.add(static_cast<sunrealtype>(px) * dx + x0,
00202
                     static_cast<sunrealtype>(py) * dy + y0,
00203
                     static_cast<sunrealtype>(pz) * dz + z0, &latticePatch.uData[i]);
00204
00205
         return;
00206 }
```

References ICSetter::add(), LatticePatch::discreteSize(), Lattice::get_tot_lx(), Lattice::get_tot_ly(), Lattice::get_tot_lz(), LatticePatch::getDelta(), icsettings, latticePatch.:discreteSize(), LatticePatch::getDelta(), icsettings, latticePatch.:discreteSize(), LatticePatch::getDelta(), icsettings, latticePatch::discreteSize(), LatticePatch::getDelta(), icsettings, latti

Referenced by addPeriodicICLayerInX(), and addPeriodicICLayerInXY().



Here is the caller graph for this function:



5.16.3.2 addPeriodiclCLayerInX()

```
void Simulation::addPeriodicICLayerInX ( )
```

function to add a periodic IC Layer in one dimension

Add initial conditions in one dimension.

Definition at line 209 of file SimulationClass.cpp.

```
00209

00210 addInitialConditions(-1, 0, 0);

00211 addInitialConditions(1, 0, 0);

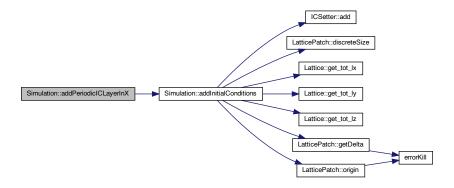
00212 return;

00213 }
```

References addInitialConditions().

Referenced by Sim1D().

Here is the call graph for this function:





5.16.3.3 addPeriodicICLayerInXY()

```
void Simulation::addPeriodicICLayerInXY ( )
```

function to add periodic IC Layers in two dimensions

Add initial conditions in two dimensions.

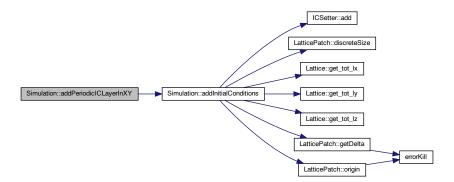
Definition at line 216 of file SimulationClass.cpp.

```
00216
00217 addInitialConditions(-1, -1, 0);
00218 addInitialConditions(-1, 0, 0);
00219 addInitialConditions(-1, 1, 0);
00220 addInitialConditions(0, 1, 0);
00221 addInitialConditions(0, -1, 0);
00222 addInitialConditions(1, -1, 0);
00223 addInitialConditions(1, 0, 0);
00224 addInitialConditions(1, 1, 0);
00225 return;
00226 }
```

References addInitialConditions().

Referenced by Sim2D().

Here is the call graph for this function:





5.16.3.4 advanceToTime()

```
void Simulation::advanceToTime ( {\tt const\ sunrealtype\ \&\ \it tEnd}\ )
```

function to advance solution in time with CVODE

Advance the solution in time -> integrate the ODE over an interval t.

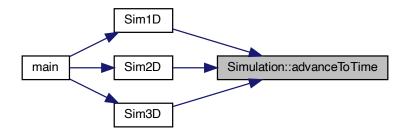
Definition at line 229 of file SimulationClass.cpp.

References checkFlag(), cvode_mem, latticePatch, SimulationStarted, t, and LatticePatch::u.

Referenced by Sim1D(), Sim2D(), and Sim3D().

Here is the call graph for this function:





5.16.3.5 checkFlag()

```
void Simulation::checkFlag (
          unsigned int flag ) const
```

function to check that a flag has been set and if not print an error

Check the presence configuration flags.

Definition at line 247 of file SimulationClass.cpp.

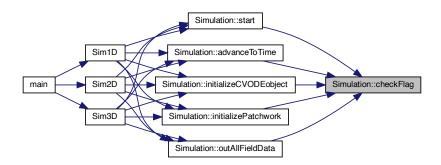
```
00248
        if (!(statusFlags & flag)) {
00249
         string errorMessage;
00250
         switch (flag) {
00251
         case LatticeDiscreteSetUp:
           errorMessage = "The discrete size of the Simulation has not been set up";
00252
00254
         case LatticePhysicalSetUp:
00255
          errorMessage = "The physical size of the Simulation has not been set up";
00256
         case LatticePatchworkSetUp:
00257
00258
           errorMessage = "The patchwork for the Simulation has not been set up";
00259
           break;
00260
         case CvodeObjectSetUp:
          errorMessage = "The CVODE object has not been initialized";
00261
00262
           break;
         case SimulationStarted:
  errorMessage = "The Simulation has not been started";
00263
00264
00265
            break;
00266
00267
           errorMessage = "Uppss, you've made a non-standard error, sadly I can't "
00268
                           "help you there";
00269
           break:
00270
00271
         errorKill(errorMessage);
00272
00273
        return;
00274 }
```

References CvodeObjectSetUp, errorKill(), LatticeDiscreteSetUp, LatticePatchworkSetUp, LatticePhysicalSetUp, SimulationStarted, and statusFlags.

Referenced by advanceToTime(), initializeCVODEobject(), initializePatchwork(), outAllFieldData(), and start().



Here is the caller graph for this function:



5.16.3.6 checkNoFlag()

```
void Simulation::checkNoFlag (  \mbox{unsigned int } \mathit{flag} \ ) \ \mbox{const}
```

function to check that if flag has not been set and if print an error

Check the absence of configuration flags.

```
Definition at line 277 of file SimulationClass.cpp.
```

```
00278
        if ((statusFlags & flag)) {
00279
          string errorMessage;
00280
          switch (flag) {
00281
         case LatticeDiscreteSetUp:
00282
          errorMessage =
                "The discrete size of the Simulation has already been set up";
           break;
00284
00285
        case LatticePhysicalSetUp:
          errorMessage =
00286
                "The physical size of the Simulation has already been set up";
00287
00288
           break;
00289
         case LatticePatchworkSetUp:
00290
          errorMessage = "The patchwork for the Simulation has already been set up";
00291
         case CvodeObjectSetUp:
  errorMessage = "The CVODE object has already been initialized";
00292
00293
00294
00295
         case SimulationStarted:
           errorMessage = "The simulation has already started, some changes are no "
"longer possible";
00296
00297
00298
           break;
         default:
00299
           errorMessage = "Uppss, you've made a non-standard error, sadly I can't "
00300
00301
                            "help you there";
00302
00303
00304
          errorKill(errorMessage);
00305
00306
        return;
00307 }
```

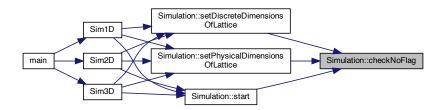
References CvodeObjectSetUp, errorKill(), LatticeDiscreteSetUp, LatticePatchworkSetUp, LatticePhysicalSetUp, SimulationStarted, and statusFlags.

Referenced by setDiscreteDimensionsOfLattice(), setPhysicalDimensionsOfLattice(), and start().

Here is the call graph for this function:



Here is the caller graph for this function:



5.16.3.7 get_cart_comm()

```
MPI_Comm * Simulation::get_cart_comm ( ) [inline]
```

Reference to the cartesian communicator of the lattice -> for debugging.

```
Definition at line 61 of file SimulationClass.h. 00061 { return &lattice.comm; };
```

References Lattice::comm, and lattice.

5.16.3.8 initializeCVODEobject()

function to initialize the CVODE object with all requirements

Configure CVODE.

```
Definition at line 74 of file SimulationClass.cpp.

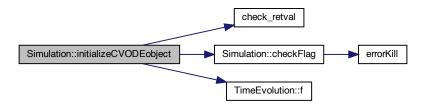
00075
00076 checkFlag(SimulationStarted);
```

```
00078
         // CVode settings return value
00079
        int retval = 0;
08000
00081
00082
        retval = SUNContext_GetProfiler(lattice.sunctx, &lattice.profobj);
        if (check_retval(&retval, "SUNContext_GetProfiler", 1, lattice.my_prc))
00084
           MPI_Abort(lattice.comm, 1);
        // if (flag != CV_SUCCESS) { printf("SUNContext_GetProfiler failed,
// flag=%d.\n", flag);
00085
00086
00087
                MPI_Abort(lattice.comm, 1); }
00088
00089
        // SUNDIALS_MARK_FUNCTION_BEGIN(profobj);
00090
00091
         // Create CVODE object \operatorname{\mathsf{--}} returns a pointer to the cvode memory structure
00092
         // with Adams method (Adams-Moulton formula) solver chosen for non-stiff ODE
00093
        cvode mem = CVodeCreate(CV ADAMS, lattice.sunctx);
00094
00095
        // Specify user data and attach it to the main cvode memory block
00096
        retval = CVodeSetUserData(
00097
             cvode_mem,
00098
             &latticePatch); // patch contains the user data as used in CVRhsFn
          f (check_retval(&retval, "CVodeSetUserData", 1, lattice.my_prc))
MPI_Abort(lattice.comm, 1);
00099
00100
        // if (flag != CV_SUCCESS) { printf("CVodeSetUserData failed, flag=%d.\n",
00101
         // flag);
00103
                 MPI_Abort(lattice.comm, 1); }
00104
        // Initialize CVODE solver \rightarrow can only be called after start of simulation to
00105
00106
        // have data ready Provide required problem and solution specifications,
00107
         \ensuremath{//} allocate internal memory, and initialize cvode
00108
        retval = CVodeInit(cvode_mem, TimeEvolution::f, 0,
00109
                              latticePatch.u); // allocate memory, CVRhsFn f, t_i=0, u
00110
                                                  // contains the initial values
        if (check_retval(&retval, "CVodeInit", 1, lattice.my_prc))
   MPI_Abort(lattice.comm, 1);
// if (flag != CV_SUCCESS) { printf("CVodeInit failed, flag=%d.\n", flag);
00111
00112
00113
                MPI_Abort(lattice.comm, 1); }
00115
00116
         // Create fixed point nonlinear solver object (suitable for non-stiff ODE) and
00117
         // attach it to CVode
        SUNNonlinearSolver NLS =
00118
            SUNNonlinSol_FixedPoint(latticePatch.u, 0, lattice.sunctx);
00119
00120
         retval = CVodeSetNonlinearSolver(cvode_mem, NLS);
        if (check_retval(&retval, "CVodeSetNonlinearSolver", 1, lattice.my_prc))
00121
00122
          MPI_Abort(lattice.comm, 1);
        // if (flag != CV_SUCCESS) {printf("CVodeSetNonlinearSolver failed,
// flag=%d.\n", flag);
// MPI_Abort(lattice.comm, 1); }
00123
00124
00125
00126
        // Specify the maximum number of steps to be taken by the solver in its
00128
         // attempt to reach the next output time
00129
         retval = CVodeSetMaxNumSteps(cvode_mem, 10000);
        if (check_retval(&retval, "CVodeSetMaxNumSteps", 1, lattice.my_prc))
    MPI_Abort(lattice.comm, 1);
00130
00131
         // if (flag != CV_SUCCESS) { printf("CVodeSetMaxNumSteps failed, flag=%d.\n",
00132
        // flag);
00134
                MPI Abort (lattice.comm, 1); }
00135
00136
        // Specify integration tolerances -- a scalar relative tolerance and scalar
00137
        // absolute tolerance
        retval = CVodeSStolerances(cvode_mem, reltol, abstol);
if (check_retval(&retval, "CVodeSStolerances", 1, lattice.my_prc))
    MPI_Abort(lattice.comm, 1);
00138
00139
00140
00141
        // if (flag != CV_SUCCESS) { printf("CVodeSStolerances failed, flag=%d.\n",
00142
00143
                MPI Abort (lattice.comm, 1); }
00144
00145
        statusFlags |= CvodeObjectSetUp;
00146 }
```

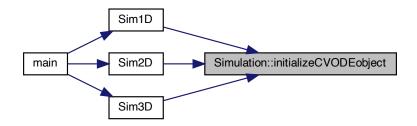
References check_retval(), checkFlag(), Lattice::comm, cvode_mem, CvodeObjectSetUp, TimeEvolution::f(), lattice, latticePatch, Lattice::my_prc, Lattice::profobj, SimulationStarted, statusFlags, Lattice::sunctx, and LatticePatch::u.

Referenced by Sim1D(), Sim2D(), and Sim3D().

Here is the call graph for this function:



Here is the caller graph for this function:



5.16.3.9 initializePatchwork()

function to initialize the Patchwork

Check that the lattice dimensions are set up and generate the patchwork.

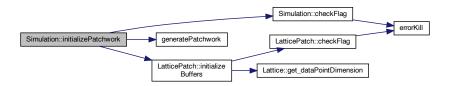
Definition at line 61 of file SimulationClass.cpp.

```
00062
        checkFlag(LatticeDiscreteSetUp);
00063
00064
       checkFlag(LatticePhysicalSetUp);
00065
00066
       // Generate the patchwork
00067
       generatePatchwork(lattice, latticePatch, nx, ny, nz);
00068
        latticePatch.initializeBuffers();
00069
00070
       statusFlags |= LatticePatchworkSetUp;
00071 }
```

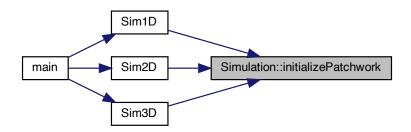
References checkFlag(), generatePatchwork(), LatticePatch::initializeBuffers(), lattice, LatticeDiscreteSetUp, latticePatch, LatticePatchworkSetUp, LatticePhysicalSetUp, and statusFlags.

Referenced by Sim1D(), Sim2D(), and Sim3D().

Here is the call graph for this function:



Here is the caller graph for this function:



5.16.3.10 outAllFieldData()

function to generate Output of the whole field at a given time

Write specified simulations steps to disk.

```
Definition at line 241 of file SimulationClass.cpp.
```

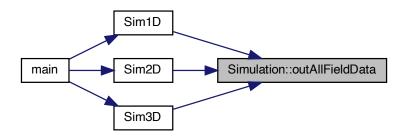
References checkFlag(), lattice, latticePatch, outputManager, OutputManager::outUState(), and SimulationStarted.

Referenced by Sim1D(), Sim2D(), and Sim3D().

Here is the call graph for this function:



Here is the caller graph for this function:



5.16.3.11 setDiscreteDimensionsOfLattice()

function to set discrete dimensions of the lattice

Set the discrete dimensions, the number of points per dimension.

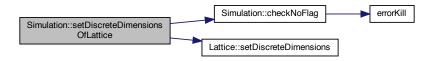
```
Definition at line 45 of file SimulationClass.cpp.
```

```
00046
00047 checkNoFlag(LatticePatchworkSetUp);
00048 lattice.setDiscreteDimensions(nx, ny, nz);
00049 statusFlags |= LatticeDiscreteSetUp;
00050 }
```

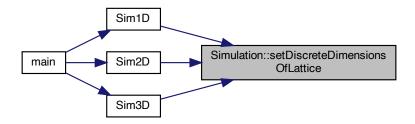
References checkNoFlag(), lattice, LatticeDiscreteSetUp, LatticePatchworkSetUp, Lattice::setDiscreteDimensions(), and statusFlags.

Referenced by Sim1D(), Sim2D(), and Sim3D().

Here is the call graph for this function:



Here is the caller graph for this function:



5.16.3.12 setInitialConditions()

```
void Simulation::setInitialConditions ( )
```

functions to set the initial field configuration onto the lattice

Set initial conditions: Fill the lattice points with the initial field values

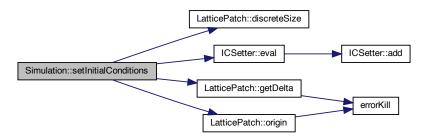
Definition at line 161 of file SimulationClass.cpp.

```
00161
00162
           const sunrealtype dx = latticePatch.getDelta(1);
           const sunrealtype dy = latticePatch.getDelta(2);
const sunrealtype dz = latticePatch.getDelta(3);
00163
00164
           const int nx = latticePatch.discreteSize(1);
const int ny = latticePatch.discreteSize(2);
00165
00166
           const sunrealtype x0 = latticePatch.origin(1);
00167
           const sunrealtype y0 = latticePatch.origin(2);
00168
           const sunrealtype z0 = latticePatch.origin(3);
00169
00170
            int px = 0, py = 0, pz = 0;
00171
            // space coordinates
           for (int i = 0; i < latticePatch.discreteSize() * 6; i += 6) {
   px = (i / 6) % nx;
   py = ((i / 6) / nx) % ny;
   pz = ((i / 6) / nx) / ny;
   // Call the 'eval' function to fill the lattice points with the field data</pre>
00172
00173
00174
00175
00176
00177
              icsettings.eval(static_cast<sunrealtype>(px) \star dx + x0,
                         static_cast<sunrealtype>(py) * dy + y0,
static_cast<sunrealtype>(pz) * dz + z0, &latticePatch.uData[i]);
00178
00179
00180
00181
           return;
00182 }
```

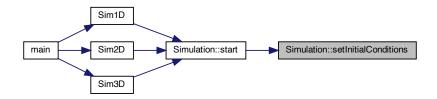
References LatticePatch::discreteSize(), ICSetter::eval(), LatticePatch::getDelta(), icsettings, latticePatch, LatticePatch::uData.

Referenced by start().

Here is the call graph for this function:



Here is the caller graph for this function:



5.16.3.13 setPhysicalDimensionsOfLattice()

function to set physical dimensions of the lattice

Set the physical dimensions with lenghts in micro meters.

```
Definition at line 53 of file SimulationClass.cpp.

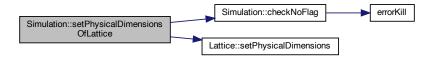
00054
00055 checkNoFlag(LatticePatchworkSetUp);
```

00055 checkNoFlag(LatticePatchworkSetUp);
00056 lattice.setPhysicalDimensions(lx, ly, lz);
00057 statusFlags |= LatticePhysicalSetUp;
00058 }

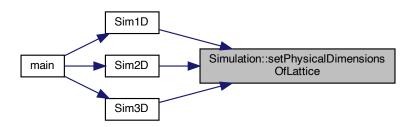
References checkNoFlag(), lattice, LatticePatchworkSetUp, LatticePhysicalSetUp, Lattice::setPhysicalDimensions(), and statusFlags.

Referenced by Sim1D(), Sim2D(), and Sim3D().

Here is the call graph for this function:



Here is the caller graph for this function:



5.16.3.14 start()

```
void Simulation::start ( )
```

function to start the simulation for time iteration

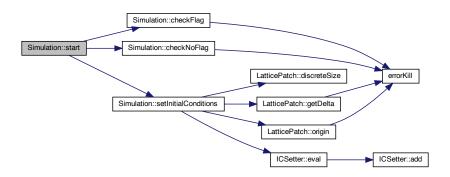
Check if the lattice patchwork is set up and set the initial conditions.

Definition at line 149 of file SimulationClass.cpp.

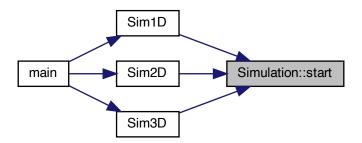
References checkFlag(), checkNoFlag(), CvodeObjectSetUp, LatticeDiscreteSetUp, LatticePatchworkSetUp, LatticePhysicalSetUp, setInitialConditions(), SimulationStarted, and statusFlags.

Referenced by Sim1D(), Sim2D(), and Sim3D().

Here is the call graph for this function:



Here is the caller graph for this function:



5.16.4 Field Documentation

5.16.4.1 cvode_mem

void* Simulation::cvode_mem

Pointer to CVode memory object – public to avoid cross library errors.

Definition at line 54 of file SimulationClass.h.

Referenced by advanceToTime(), initializeCVODEobject(), and \sim Simulation().

5.16.4.2 icsettings

ICSetter Simulation::icsettings

IC Setter object.

Definition at line 50 of file SimulationClass.h.

Referenced by addInitialConditions(), setInitialConditions(), Sim1D(), Sim2D(), and Sim3D().

5.16.4.3 lattice

Lattice Simulation::lattice [private]

Lattice object.

Definition at line 40 of file SimulationClass.h.

Referenced by addInitialConditions(), $get_cart_comm()$, initializeCVODEobject(), initializePatchwork(), outAllFieldData(), setDiscreteDimensionsOfLattice(), setPhysicalDimensionsOfLattice(), setPhysicalD

5.16.4.4 latticePatch

LatticePatch Simulation::latticePatch [private]

LatticePatch object.

Definition at line 42 of file SimulationClass.h.

 $Referenced \ by \ add Initial Conditions (), \ advance To Time (), \ initialize CVODE object (), \ initialize Patchwork (), \ out All Field Data (), \ and \ set Initial Conditions ().$

5.16.4.5 outputManager

OutputManager Simulation::outputManager

Output Manager object.

Definition at line 52 of file SimulationClass.h.

Referenced by outAllFieldData(), Sim1D(), Sim2D(), and Sim3D().

5.16.4.6 statusFlags

```
unsigned char Simulation::statusFlags [private]
```

char for checking simulation flags

Definition at line 46 of file SimulationClass.h.

Referenced by checkFlag(), checkNoFlag(), initializeCVODEobject(), initializePatchwork(), setDiscreteDimensionsOfLattice(), setPhysicalDimensionsOfLattice(), Simulation(), start(), and ~Simulation().

5.16.4.7 t

```
sunrealtype Simulation::t [private]
```

current time of the simulation

Definition at line 44 of file SimulationClass.h.

Referenced by advanceToTime(), and Simulation().

The documentation for this class was generated from the following files:

- src/SimulationClass.h
- src/SimulationClass.cpp

5.17 TimeEvolution Class Reference

monostate TimeEvolution Class to propagate the field data in time in a given order of the HE weak-field expansion

```
#include <src/TimeEvolutionFunctions.h>
```

Static Public Member Functions

• static int f (sunrealtype t, N_Vector u, N_Vector udot, void *data_loc)

CVODE right hand side function (CVRhsFn) to provide IVP of the ODE.

Static Public Attributes

- static int * c = nullptr
 - choice which processes of the weak field expansion are included
- static void(* TimeEvolver)(LatticePatch *, N_Vector, N_Vector, int *) = nonlinear1DProp

 Pointer to functions for differentiation and time evolution.

5.17.1 Detailed Description

monostate TimeEvolution Class to propagate the field data in time in a given order of the HE weak-field expansion Definition at line 15 of file TimeEvolutionFunctions.h.

5.17.2 Member Function Documentation

5.17.2.1 f()

CVODE right hand side function (CVRhsFn) to provide IVP of the ODE.

CVode right-hand-side function (CVRhsFn)

Definition at line 13 of file TimeEvolutionFunctions.cpp.

```
00014
        // Set recover pointer to provided lattice patch where the data resides
00015
        LatticePatch *data = nullptr;
00016
        data = static_cast<LatticePatch *>(data_loc);
00017
00018
       // pointers for update circle
00019
        sunrealtype *udata = nullptr, *dudata = nullptr;
00020
       sunrealtype *originaluData = nullptr, *originalduData = nullptr;
00021
00022
        // Access NVECTOR_PARALLEL argument data with pointers
       udata = NV DATA P(u);
00023
00024
       dudata = NV_DATA_P (udot);
00025
00026
       // Store original data location of the patch
00027
        originaluData = data->uData;
00028
        originalduData = data->duData;
        // Point patch data to arguments of f
00029
00030
       data->uData = udata;
00031
       data->duData = dudata;
00032
00033
        // Time-evolve these arguments (the field data) with specific propagator below
00034
       TimeEvolver(data, u, udot, c);
00035
00036
       // Refer patch data back to original location
00037
       data->uData = originaluData;
00038
       data->duData = originalduData;
00039
00040
        return (0);
00041 }
```

References c, LatticePatch::duData, TimeEvolver, and LatticePatch::uData.

Referenced by Simulation::initializeCVODEobject().



5.17.3 Field Documentation

5.17.3.1 c

```
int * TimeEvolution::c = nullptr [static]
```

choice which processes of the weak field expansion are included

Definition at line 18 of file TimeEvolutionFunctions.h.

Referenced by f(), Sim1D(), Sim2D(), and Sim3D().

5.17.3.2 TimeEvolver

```
void(* TimeEvolution::TimeEvolver)(LatticePatch *, N_Vector, N_Vector, int *) = nonlinear1DProp
[static]
```

Pointer to functions for differentiation and time evolution.

Definition at line 21 of file TimeEvolutionFunctions.h.

Referenced by f(), Sim1D(), Sim2D(), and Sim3D().

The documentation for this class was generated from the following files:

- src/TimeEvolutionFunctions.h
- src/SimulationFunctions.cpp
- src/TimeEvolutionFunctions.cpp

Chapter 6

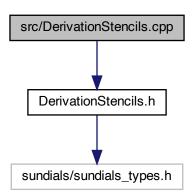
File Documentation

6.1 README.md File Reference

6.2 src/DerivationStencils.cpp File Reference

Empty. All definitions in the header.

#include "DerivationStencils.h"
Include dependency graph for DerivationStencils.cpp:



6.2.1 Detailed Description

Empty. All definitions in the header.

Definition in file DerivationStencils.cpp.

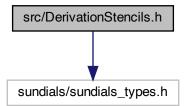
6.3 DerivationStencils.cpp

Go to the documentation of this file.

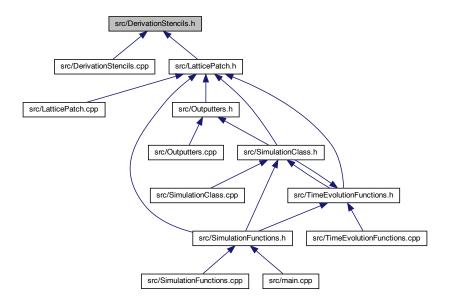
6.4 src/DerivationStencils.h File Reference

Definition of derivation stencils from order 1 to 13.

#include <sundials/sundials_types.h>
Include dependency graph for DerivationStencils.h:



This graph shows which files directly or indirectly include this file:



Functions

 sunrealtype s1f (sunrealtype *udata, int nx) sunrealtype s1b (sunrealtype *udata, int nx) • sunrealtype s2f (const sunrealtype *udata, int nx) sunrealtype s2c (const sunrealtype *udata, int nx) sunrealtype s2b (const sunrealtype *udata, int nx) sunrealtype s3f (const sunrealtype *udata, int nx) sunrealtype s3b (sunrealtype *udata, int nx) sunrealtype s4f (const sunrealtype *udata, int nx) sunrealtype s4c (const sunrealtype *udata, int nx) sunrealtype s4b (const sunrealtype *udata, int nx) sunrealtype s5f (const sunrealtype *udata, int nx) sunrealtype s5b (sunrealtype *udata, int nx) sunrealtype s6f (const sunrealtype *udata, int nx) • sunrealtype s6c (const sunrealtype *udata, int nx) sunrealtype s6b (const sunrealtype *udata, int nx) sunrealtype s7f (const sunrealtype *udata, int nx) sunrealtype s7b (sunrealtype *udata, int nx) sunrealtype s8f (const sunrealtype *udata, int nx) • sunrealtype s8c (const sunrealtype *udata, int nx) sunrealtype s8b (const sunrealtype *udata, int nx) • sunrealtype s9f (const sunrealtype *udata, int nx) sunrealtype s9b (sunrealtype *udata, int nx) sunrealtype s10f (const sunrealtype *udata, int nx) sunrealtype s10c (const sunrealtype *udata, int nx) sunrealtype s10b (const sunrealtype *udata, int nx) sunrealtype s11f (const sunrealtype *udata, int nx) sunrealtype s11b (sunrealtype *udata, int nx) sunrealtype s12f (const sunrealtype *udata, int nx) sunrealtype s12c (const sunrealtype *udata, int nx) sunrealtype s12b (const sunrealtype *udata, int nx) • sunrealtype s13f (const sunrealtype *udata, int nx) sunrealtype s13b (sunrealtype *udata, int nx) • sunrealtype s1f (sunrealtype *udata) sunrealtype s1b (sunrealtype *udata) sunrealtype s2f (sunrealtype *udata) sunrealtype s2c (sunrealtype *udata) sunrealtype s2b (sunrealtype *udata) sunrealtype s3f (sunrealtype *udata) sunrealtype s3b (sunrealtype *udata) sunrealtype s4f (sunrealtype *udata) sunrealtype s4c (sunrealtype *udata) sunrealtype s4b (sunrealtype *udata) • sunrealtype s5f (sunrealtype *udata) sunrealtype s5b (sunrealtype *udata) sunrealtype s6f (sunrealtype *udata) sunrealtype s6c (sunrealtype *udata) • sunrealtype s6b (sunrealtype *udata) • sunrealtype s7f (sunrealtype *udata) sunrealtype s7b (sunrealtype *udata) sunrealtype s8f (sunrealtype *udata) sunrealtype s8c (sunrealtype *udata) sunrealtype s8b (sunrealtype *udata) sunrealtype s9f (sunrealtype *udata)

- sunrealtype s9b (sunrealtype *udata)
- sunrealtype s10f (sunrealtype *udata)
- sunrealtype s10c (sunrealtype *udata)
- sunrealtype s10b (sunrealtype *udata)
- sunrealtype s11f (sunrealtype *udata)
- sunrealtype s11b (sunrealtype *udata)
- sunrealtype s12f (sunrealtype *udata)
- sunrealtype s12c (sunrealtype *udata)
- sunrealtype s12b (sunrealtype *udata)
- sunrealtype s13f (sunrealtype *udata)
- sunrealtype s13b (sunrealtype *udata)

6.4.1 Detailed Description

Definition of derivation stencils from order 1 to 13.

Definition in file DerivationStencils.h.

6.4.2 Function Documentation

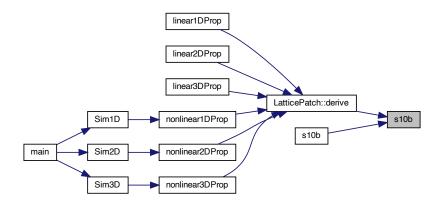
6.4.2.1 s10b() [1/2]

```
sunrealtype s10b (  {\rm const\ sunrealtype\ *\ udata,}  int nx ) [inline]
```

Definition at line 144 of file DerivationStencils.h.

```
00144
00145
return 1.0 / 840.0 * udata[-4 * nx] - 1.0 / 63.0 * udata[-3 * nx] +
00146
00147
11.0 / 30.0 * udata[-2 * nx] - 4.0 / 7.0 * udata[-1 * nx] -
00148
11.0 / 30.0 * udata[0] + 6.0 / 5.0 * udata[1 * nx] -
00149
3.0 / 56.0 * udata[2 * nx] + 4.0 / 21.0 * udata[3 * nx] -
00150
1.0 / 1260.0 * udata[4 * nx] + 1.0 / 105.0 * udata[5 * nx] -
00151 }
```

Referenced by LatticePatch::derive(), and s10b().



6.4.2.2 s10b() [2/2]

References s10b().

Here is the call graph for this function:

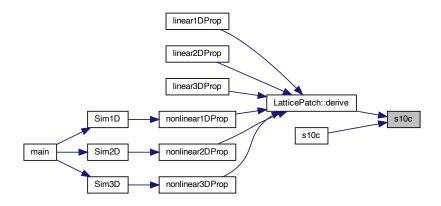


6.4.2.3 s10c() [1/2]

```
sunrealtype s10c ( {\rm const~sunrealtype~*~} udata, \\ {\rm int~} nx~) ~ [{\rm inline}]
```

Definition at line 137 of file DerivationStencils.h.

Referenced by LatticePatch::derive(), and s10c().



6.4.2.4 s10c() [2/2]

Definition at line 243 of file DerivationStencils.h.

```
00243 { return s10c(udata, 6); }
```

References s10c().

Here is the call graph for this function:

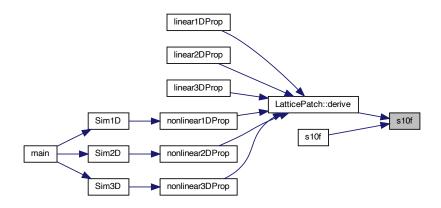


6.4.2.5 s10f() [1/2]

```
sunrealtype s10f (  {\rm const\ sunrealtype\ *\ udata,}  int nx ) [inline]
```

Definition at line 129 of file DerivationStencils.h.

Referenced by LatticePatch::derive(), and s10f().



6.4.2.6 s10f() [2/2]

```
sunrealtype s10f (
            sunrealtype * udata ) [inline]
```

Definition at line 242 of file DerivationStencils.h. 00242 { return sl0f(udata, 6); }

References s10f().

Here is the call graph for this function:



6.4.2.7 s11b() [1/2]

```
sunrealtype s11b (
            sunrealtype * udata ) [inline]
```

Definition at line 246 of file DerivationStencils.h.

```
00246 { return s11b(udata, 6); }
```

References s11b().

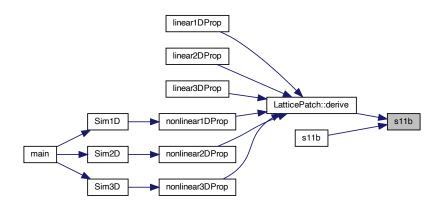


6.4.2.8 s11b() [2/2]

Definition at line 160 of file DerivationStencils.h.

Referenced by LatticePatch::derive(), and s11b().

Here is the caller graph for this function:



6.4.2.9 s11f() [1/2]

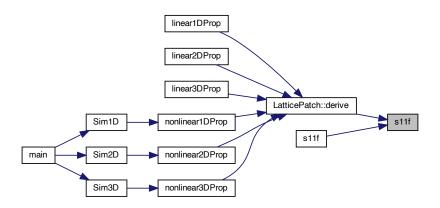
```
sunrealtype s11f (  \mbox{const sunrealtype * } udata, \\ \mbox{int } nx \; ) \; \mbox{[inline]}
```

Definition at line 152 of file DerivationStencils.h.

```
00152
00153
return 1.0 / 2772.0 * udata[-6 * nx] - 1.0 / 210.0 * udata[-5 * nx] + 00154
00155
5.0 / 168.0 * udata[-4 * nx] - 5.0 / 42.0 * udata[-3 * nx] + 00155
00156
1.0 / 6.0 * udata[-2 * nx] - 1.0 / 1.0 * udata[-1 * nx] + 00157
00157
5.0 / 28.0 * udata[0] + 5.0 / 7.0 * udata[1 * nx] - 00158
1.0 / 168.0 * udata[2 * nx] + 5.0 / 126.0 * udata[3 * nx] - 00158
00159 }
```

Referenced by LatticePatch::derive(), and s11f().

Here is the caller graph for this function:



6.4.2.10 s11f() [2/2]

```
sunrealtype s11f (
            sunrealtype * udata ) [inline]
```

Definition at line 245 of file DerivationStencils.h.

00245 { return s11f(udata, 6); }

References s11f().

Here is the call graph for this function:



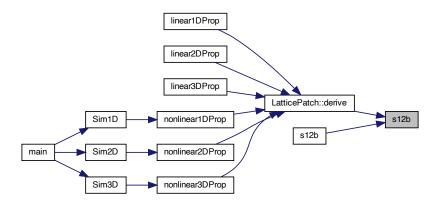
6.4.2.11 s12b() [1/2]

```
sunrealtype s12b (
            const sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 185 of file DerivationStencils.h.

Referenced by LatticePatch::derive(), and s12b().

Here is the caller graph for this function:



6.4.2.12 s12b() [2/2]

Definition at line 249 of file DerivationStencils.h.

```
00249 { return s12b(udata, 6); }
```

References s12b().

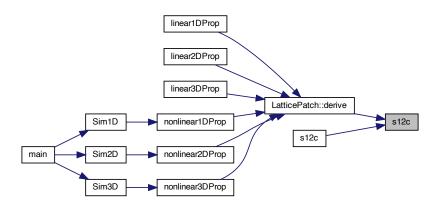


6.4.2.13 s12c() [1/2]

```
sunrealtype s12c (
                                const sunrealtype * udata,
                                 int nx ) [inline]
Definition at line 177 of file DerivationStencils.h.
                  return 1.0 / 5544.0 * udata[-6 * nx] - 1.0 / 385.0 * udata[-5 * nx] + 1.0 / 56.0 * udata[-4 * nx] - 5.0 / 63.0 * udata[-3 * nx] + 15.0 / 56.0 * udata[-2 * nx] - 6.0 / 7.0 * udata[-1 * nx] + 0 + 6.0 / 7.0 * udata[1 * nx] - 15.0 / 56.0 * udata[2 * nx] + 5.0 / 63.0 * udata[3 * nx] - 1.0 / 56.0 * udata[4 * nx] + 1.0 / 385.0 * udata[5 * nx] - 1.0 / 5544.0 * udata[6 * nx];
00178
00179
00180
00181
00182
00183
00184 }
```

Referenced by LatticePatch::derive(), and s12c().

Here is the caller graph for this function:



6.4.2.14 s12c() [2/2]

```
sunrealtype s12c (
            sunrealtype * udata ) [inline]
```

Definition at line 248 of file DerivationStencils.h.

00248 { return s12c(udata, 6); }

References s12c().



6.4.2.15 s12f() [1/2]

```
sunrealtype s12f ( {\tt const\ sunrealtype\ *\ udata,} {\tt int\ nx\ )\ [inline]}
```

Definition at line 168 of file DerivationStencils.h.

```
00168

return -1.0 / 5544.0 * udata[-7 * nx] + 1.0 / 396.0 * udata[-6 * nx] -

00170

1.0 / 60.0 * udata[-5 * nx] + 5.0 / 72.0 * udata[-4 * nx] -

00171

5.0 / 24.0 * udata[-3 * nx] + 1.0 / 2.0 * udata[-2 * nx] -

00172

7.0 / 6.0 * udata[-1 * nx] + 13.0 / 42.0 * udata[0] +

00173

5.0 / 8.0 * udata[1 * nx] - 5.0 / 36.0 * udata[2 * nx] +

00174

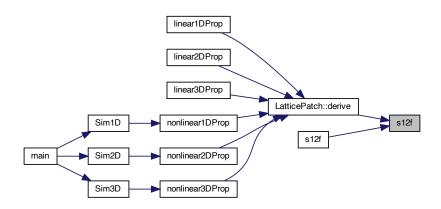
1.0 / 36.0 * udata[3 * nx] - 1.0 / 264.0 * udata[4 * nx] +

00175

1.0 / 3960.0 * udata[5 * nx];
```

Referenced by LatticePatch::derive(), and s12f().

Here is the caller graph for this function:



6.4.2.16 s12f() [2/2]

Definition at line 247 of file DerivationStencils.h.

00247 { return s12f(udata, 6); }

References s12f().



6.4.2.17 s13b() [1/2]

References s13b().

Here is the call graph for this function:



6.4.2.18 s13b() [2/2]

Definition at line 206 of file DerivationStencils.h.

```
00206

00207 return 1.0 / 10296.0 * udata[-6 * nx] - 1.0 / 660.0 * udata[-5 * nx] +

00208 1.0 / 88.0 * udata[-4 * nx] - 1.0 / 18.0 * udata[-3 * nx] +

00209 5.0 / 24.0 * udata[-2 * nx] - 3.0 / 4.0 * udata[-1 * nx] -

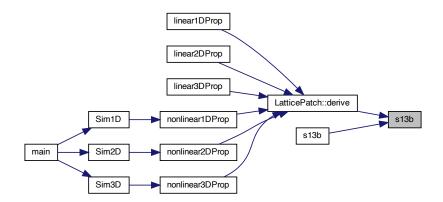
00210 1.0 / 7.0 * udata[0] + udata[1 * nx] - 3.0 / 8.0 * udata[2 * nx] +

00211 5.0 / 36.0 * udata[3 * nx] - 1.0 / 24.0 * udata[4 * nx] +

00212 1.0 / 110.0 * udata[5 * nx] - 1.0 / 792.0 * udata[6 * nx] +

00213 1.0 / 12012.0 * udata[7 * nx];
```

Referenced by LatticePatch::derive(), and s13b().



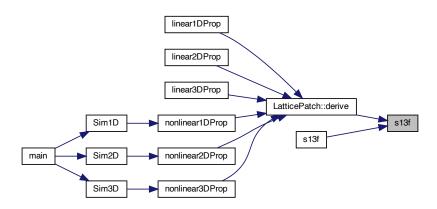
6.4.2.19 s13f() [1/2]

```
sunrealtype s13f (  {\rm const\ sunrealtype\ *\ udata,}  int nx ) [inline]
```

Definition at line 196 of file DerivationStencils.h.

Referenced by LatticePatch::derive(), and s13f().

Here is the caller graph for this function:



6.4.2.20 s13f() [2/2]

Definition at line 250 of file DerivationStencils.h.

00250 { return s13f(udata, 6); }

References s13f().



6.4.2.21 s1b() [1/2]

References s1b().

Here is the call graph for this function:

00221 { return s1b(udata, 6); }



6.4.2.22 s1b() [2/2]

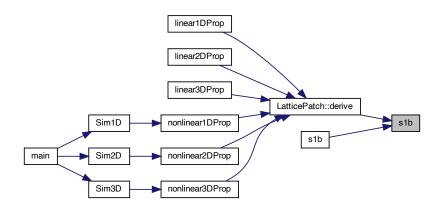
Definition at line 19 of file DerivationStencils.h.

```
00019

00020 return -1.0 / 1.0 * udata[0] + udata[1 * nx];

00021 }
```

Referenced by LatticePatch::derive(), and s1b().



6.4.2.23 s1f() [1/2]

References s1f().

```
sunrealtype s1f ( sunrealtype \ * \ udata \ ) \quad [inline]
```

Definition at line 220 of file DerivationStencils.h. 00220 { return slf(udata, 6); }

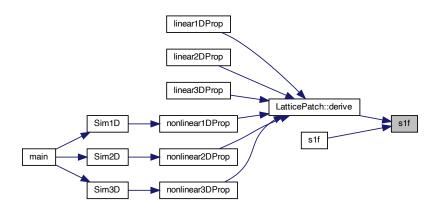
Here is the call graph for this function:



6.4.2.24 s1f() [2/2]

Definition at line 15 of file DerivationStencils.h.

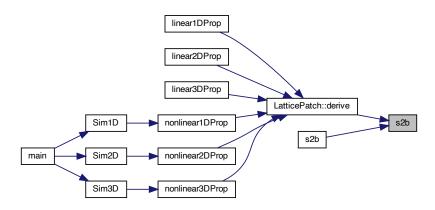
Referenced by LatticePatch::derive(), and s1f().



6.4.2.25 s2b() [1/2]

Referenced by LatticePatch::derive(), and s2b().

Here is the caller graph for this function:



6.4.2.26 s2b() [2/2]

Definition at line 224 of file DerivationStencils.h.

00224 { return s2b(udata, 6); }

References s2b().

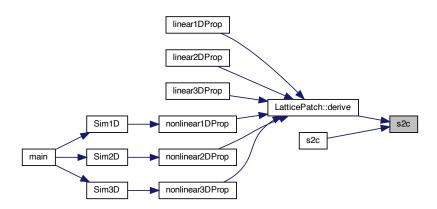


6.4.2.27 s2c() [1/2]

00029 }

Referenced by LatticePatch::derive(), and s2c().

Here is the caller graph for this function:



6.4.2.28 s2c() [2/2]

Definition at line 223 of file DerivationStencils.h.

```
00223 { return s2c(udata, 6); }
```

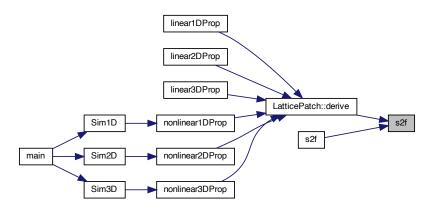
References s2c().



6.4.2.29 s2f() [1/2]

Referenced by LatticePatch::derive(), and s2f().

Here is the caller graph for this function:



6.4.2.30 s2f() [2/2]

Definition at line 222 of file DerivationStencils.h.

```
00222 { return s2f(udata, 6); }
```

References s2f().



6.4.2.31 s3b() [1/2]

```
sunrealtype s3b (
            sunrealtype * udata ) [inline]
```

Definition at line 226 of file DerivationStencils.h.

00226 { return s3b(udata, 6); }

References s3b().

Here is the call graph for this function:



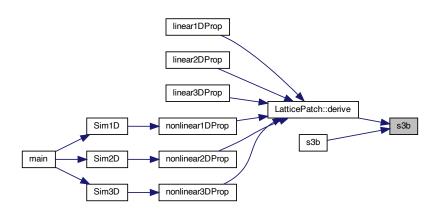
6.4.2.32 s3b() [2/2]

```
sunrealtype s3b (
            sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 38 of file DerivationStencils.h.

```
00038
00039
          return -1.0 / 3.0 * udata[-1 * nx] - 1.0 / 2.0 * udata[0] + udata[1 * nx] - 1.0 / 6.0 * udata[2 * nx];
00040
00041 }
```

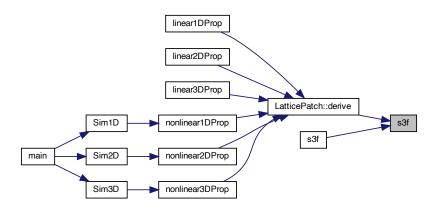
Referenced by LatticePatch::derive(), and s3b().



6.4.2.33 s3f() [1/2]

Referenced by LatticePatch::derive(), and s3f().

Here is the caller graph for this function:



6.4.2.34 s3f() [2/2]

Definition at line 225 of file DerivationStencils.h.

```
00225 { return s3f(udata, 6); }
```

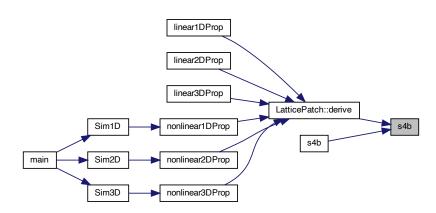
References s3f().



6.4.2.35 s4b() [1/2]

Referenced by LatticePatch::derive(), and s4b().

Here is the caller graph for this function:



6.4.2.36 s4b() [2/2]

Definition at line 229 of file DerivationStencils.h.

```
00229 { return s4b(udata, 6); }
```

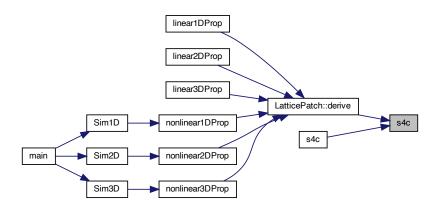
References s4b().



6.4.2.37 s4c() [1/2]

Referenced by LatticePatch::derive(), and s4c().

Here is the caller graph for this function:



6.4.2.38 s4c() [2/2]

Definition at line 228 of file DerivationStencils.h.

```
00228 { return s4c(udata, 6); }
```

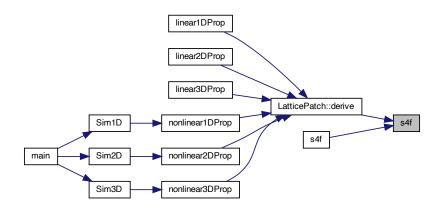
References s4c().



6.4.2.39 s4f() [1/2]

Referenced by LatticePatch::derive(), and s4f().

Here is the caller graph for this function:



6.4.2.40 s4f() [2/2]

Definition at line 227 of file DerivationStencils.h.

```
00227 { return s4f(udata, 6); }
```

References s4f().



6.4.2.41 s5b() [1/2]

References s5b().

Here is the call graph for this function:

00231 { return s5b(udata, 6); }



6.4.2.42 s5b() [2/2]

Definition at line 61 of file DerivationStencils.h.

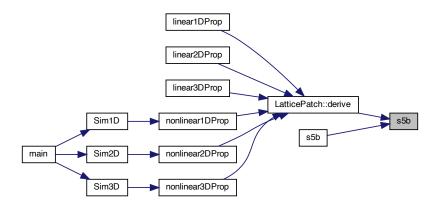
```
00061

00062 return 1.0 / 20.0 * udata[-2 * nx] - 1.0 / 2.0 * udata[-1 * nx] - 00063

1.0 / 3.0 * udata[0] + udata[1 * nx] - 1.0 / 4.0 * udata[2 * nx] + 00064

1.0 / 30.0 * udata[3 * nx];
```

Referenced by LatticePatch::derive(), and s5b().

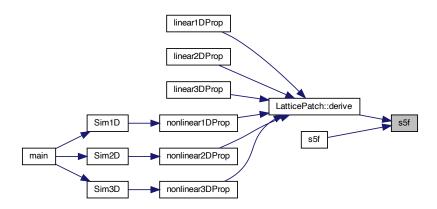


6.4.2.43 s5f() [1/2]

Definition at line 56 of file DerivationStencils.h.

Referenced by LatticePatch::derive(), and s5f().

Here is the caller graph for this function:



6.4.2.44 s5f() [2/2]

Definition at line 230 of file DerivationStencils.h.

```
00230 { return s5f(udata, 6); }
```

References s5f().



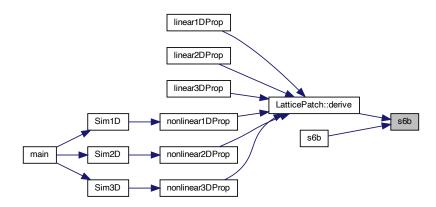
6.4.2.45 s6b() [1/2]

```
sunrealtype s6b ( {\tt const\ sunrealtype\ *\ udata,} {\tt int\ nx\ )\ [inline]}
```

Definition at line 77 of file DerivationStencils.h.

Referenced by LatticePatch::derive(), and s6b().

Here is the caller graph for this function:



6.4.2.46 s6b() [2/2]

```
sunrealtype s6b ( sunrealtype * udata ) \quad [inline]
```

Definition at line 234 of file DerivationStencils.h.

```
00234 { return s6b(udata, 6); }
```

References s6b().



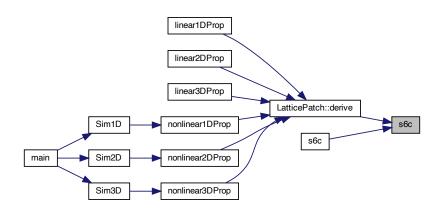
6.4.2.47 s6c() [1/2]

```
sunrealtype s6c ( {\tt const\ sunrealtype\ *\ udata,} {\tt int\ nx\ )\ [inline]}
```

Definition at line 72 of file DerivationStencils.h.

Referenced by LatticePatch::derive(), and s6c().

Here is the caller graph for this function:



6.4.2.48 s6c() [2/2]

Definition at line 233 of file DerivationStencils.h.

```
00233 { return s6c(udata, 6); }
```

References s6c().



6.4.2.49 s6f() [1/2]

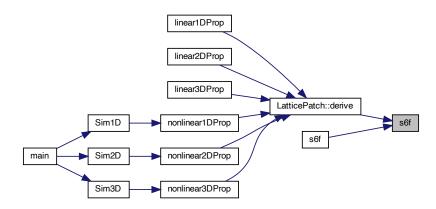
```
sunrealtype s6f (
            const sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 66 of file DerivationStencils.h.

```
00066
00067
                   return 1.0 / 60.0 * udata[-4 * nx] - 2.0 / 15.0 * udata[-3 * nx] + 1.0 / 2.0 * udata[-2 * nx] - 4.0 / 3.0 * udata[-1 * nx] + 7.0 / 12.0 * udata[0] + 2.0 / 5.0 * udata[1 * nx] - 1.0 / 30.0 * udata[2 * nx];
00068
00069
00070
00071 }
```

Referenced by LatticePatch::derive(), and s6f().

Here is the caller graph for this function:



6.4.2.50 s6f() [2/2]

```
sunrealtype s6f (
            sunrealtype * udata ) [inline]
```

Definition at line 232 of file DerivationStencils.h.

00232 { return s6f(udata, 6); }

References s6f().



6.4.2.51 s7b() [1/2]

```
sunrealtype s7b (
            sunrealtype * udata ) [inline]
```

Definition at line 236 of file DerivationStencils.h.

```
00236 { return s7b(udata, 6); }
```

References s7b().

Here is the call graph for this function:



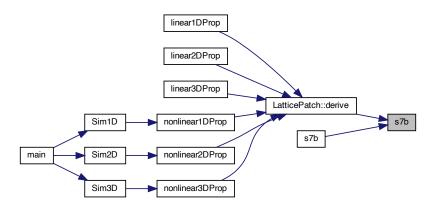
6.4.2.52 s7b() [2/2]

```
sunrealtype s7b (
            sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 89 of file DerivationStencils.h.

```
return -1.0 / 105.0 * udata[-3 * nx] + 1.0 / 10.0 * udata[-2 * nx] - 3.0 / 5.0 * udata[-1 * nx] - 1.0 / 4.0 * udata[0] + udata[1 * nx] - 3.0 / 10.0 * udata[2 * nx] + 1.0 / 15.0 * udata[3 * nx] - 1.0 / 140.0 * udata[4 * nx];
00089
00090
00091
00092
00093
00094 }
```

Referenced by LatticePatch::derive(), and s7b().



6.4.2.53 s7f() [1/2]

```
sunrealtype s7f (  {\rm const\ sunrealtype\ *\ udata,}  int nx ) [inline]
```

Definition at line 83 of file DerivationStencils.h.

```
00083

00084 return 1.0 / 140.0 * udata[-4 * nx] - 1.0 / 15.0 * udata[-3 * nx] +

00085 3.0 / 10.0 * udata[-2 * nx] - 1.0 / 1.0 * udata[-1 * nx] +

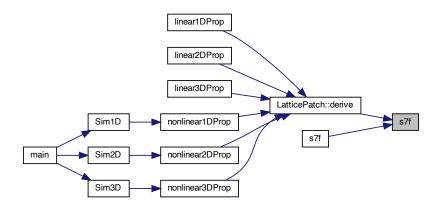
00086 1.0 / 4.0 * udata[0] + 3.0 / 5.0 * udata[1 * nx] -

00087 1.0 / 10.0 * udata[2 * nx] + 1.0 / 105.0 * udata[3 * nx];

00088 }
```

Referenced by LatticePatch::derive(), and s7f().

Here is the caller graph for this function:



6.4.2.54 s7f() [2/2]

Definition at line 235 of file DerivationStencils.h.

```
00235 { return s7f(udata, 6); }
```

References s7f().



6.4.2.55 s8b() [1/2]

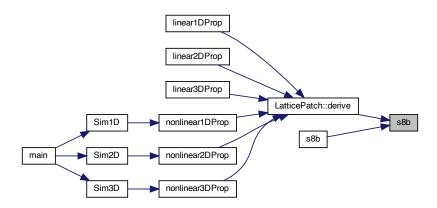
```
sunrealtype s8b (  {\rm const\ sunrealtype\ *\ udata,}  int nx ) [inline]
```

Definition at line 108 of file DerivationStencils.h.

```
00108
00109
return -1.0 / 168.0 * udata[-3 * nx] + 1.0 / 14.0 * udata[-2 * nx] -
00110
1.0 / 2.0 * udata[-1 * nx] - 9.0 / 20.0 * udata[0] +
00111
5.0 / 4.0 * udata[1 * nx] - 1.0 / 2.0 * udata[2 * nx] +
00112
1.0 / 6.0 * udata[3 * nx] - 1.0 / 28.0 * udata[4 * nx] +
00113
1.0 / 280.0 * udata[5 * nx];
```

Referenced by LatticePatch::derive(), and s8b().

Here is the caller graph for this function:



6.4.2.56 s8b() [2/2]

Definition at line 239 of file DerivationStencils.h. 00239 { return s8b(udata, 6); }

References s8b().



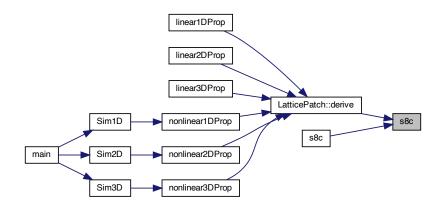
6.4.2.57 s8c() [1/2]

```
sunrealtype s8c (  {\rm const\ sunrealtype\ *\ udata,}  int nx ) [inline]
```

Definition at line 102 of file DerivationStencils.h.

Referenced by LatticePatch::derive(), and s8c().

Here is the caller graph for this function:



6.4.2.58 s8c() [2/2]

```
sunrealtype s8c ( sunrealtype * udata ) \quad [inline]
```

Definition at line 238 of file DerivationStencils.h.

```
00238 { return s8c(udata, 6); }
```

References s8c().

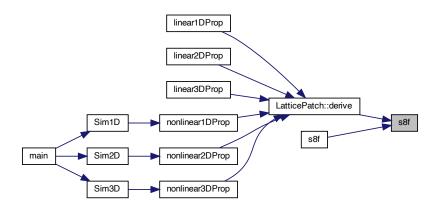


6.4.2.59 s8f() [1/2]

Definition at line 95 of file DerivationStencils.h.

Referenced by LatticePatch::derive(), and s8f().

Here is the caller graph for this function:



6.4.2.60 s8f() [2/2]

Definition at line 237 of file DerivationStencils.h. 00237 { return s8f(udata, 6); }

References s8f().



6.4.2.61 s9b() [1/2]

00241 { return s9b(udata, 6); }

References s9b().

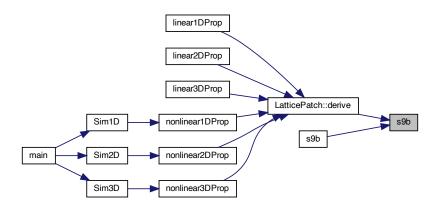
Here is the call graph for this function:



6.4.2.62 s9b() [2/2]

Definition at line 122 of file DerivationStencils.h.

Referenced by LatticePatch::derive(), and s9b().



6.4.2.63 s9f() [1/2]

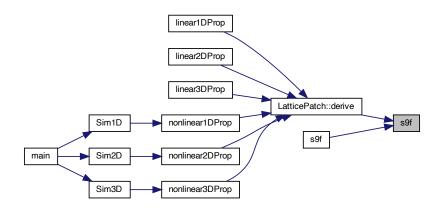
```
sunrealtype s9f (  {\rm const\ sunrealtype\ *\ udata,}  int nx ) [inline]
```

Definition at line 115 of file DerivationStencils.h.

```
00115
00116
return -1.0 / 630.0 * udata[-5 * nx] + 1.0 / 56.0 * udata[-4 * nx] -
00117
2.0 / 21.0 * udata[-3 * nx] + 1.0 / 3.0 * udata[-2 * nx] -
00118
1.0 / 1.0 * udata[-1 * nx] + 1.0 / 5.0 * udata[0] +
00119
2.0 / 3.0 * udata[1 * nx] - 1.0 / 7.0 * udata[2 * nx] +
00120
1.0 / 42.0 * udata[3 * nx] - 1.0 / 504.0 * udata[4 * nx];
00121 }
```

Referenced by LatticePatch::derive(), and s9f().

Here is the caller graph for this function:



6.4.2.64 s9f() [2/2]

```
sunrealtype s9f ( sunrealtype * udata ) \quad [inline]
```

Definition at line 240 of file DerivationStencils.h.

```
00240 { return s9f(udata, 6); }
```

References s9f().



6.5 DerivationStencils.h

6.5 DerivationStencils.h

```
Go to the documentation of this file.
00003 /// @brief Definition of derivation stencils from order 1 to 13
00006 #pragma once
00007
00008 #include <sundials/sundials types.h> /* definition of type sunrealtype */
00009
00011 // Stencils with variable nx -- data point dimension /,
00013
00014 // Downwind (forward) dfferentiating
00015 inline sunrealtype s1f(sunrealtype *udata, int nx) {
      return -1.0 / 1.0 * udata[-1 * nx] + udata[0];
00017 }
00018 // Upwind (backward) differentiating
00019 inline sunrealtype s1b(sunrealtype *udata, int nx) {
     return -1.0 / 1.0 * udata[0] + udata[1 * nx];
00020
00021 }
00023 inline sunrealtype s2f(const sunrealtype *udata, int nx) {
    return 1.0 / 2.0 * udata[-2 * nx] - 2.0 / 1.0 * udata[-1 * nx] + 3.0 / 2.0 * udata[0];
00024
00025
00026 }
00027 inline sunrealtype s2c(const sunrealtype *udata, int nx) { 00028    return -1.0 / 2.0 * udata[-1 * nx] + 0 + 1.0 / 2.0 * udata[1 * nx]; 00029 }
00030 inline sunrealtype s2b(const sunrealtype *udata, int nx) {
00031 return -3.0 / 2.0 * udata[0] + 2.0 / 1.0 * udata[1 * nx] - 00032 1.0 / 2.0 * udata[2 * nx];
00033 }
00037 }
00040
00042 inline sunrealtype s4f(const sunrealtype *udata, int nx) {
00046 }
00047 inline sunrealtype s4c(const sunrealtype *udata, int nx) {
00048 return 1.0 / 12.0 * udata[-2 * nx] - 2.0 / 3.0 * udata[-1 * nx] + 0 + 00049 2.0 / 3.0 * udata[1 * nx] - 1.0 / 12.0 * udata[2 * nx];
00050 }
00054
            1.0 / 12.0 * udata[3 * nx];
00055 }
00056 inline sunrealtype s5f(const sunrealtype *udata, int nx) {
00060 }
00061 inline sunrealtype s5b(sunrealtype *udata, int nx) {
00065 }
00066 inline sunrealtype s6f(const sunrealtype *udata, int nx) {
00067 return 1.0 / 60.0 * udata[-4 * nx] - 2.0 / 15.0 * udata[-3 * nx] + 00068 1.0 / 2.0 * udata[-2 * nx] - 4.0 / 3.0 * udata[-1 * nx] +
            7.0 / 12.0 * udata[0] + 2.0 / 5.0 * udata[1 * nx] - 1.0 / 30.0 * udata[2 * nx];
00069
00070
00071 }
00072 inline sunrealtype s6c(const sunrealtype *udata, int nx) {
00075
            3.0 / 20.0 * udata[2 * nx] + 1.0 / 60.0 * udata[3 * nx];
00076 }
00077 inline sunrealtype s6b(const sunrealtype *udata, int nx) {
00078 return 1.0 / 30.0 * udata[-2 * nx] - 2.0 / 5.0 * udata[-1 * nx] - 00079 7.0 / 12.0 * udata[0] + 4.0 / 3.0 * udata[1 * nx] -
            1.0 / 2.0 * udata[2 * nx] + 2.0 / 15.0 * udata[3 * nx] -
08000
            1.0 / 60.0 * udata[4 * nx];
00081
00082 }
```

```
00083 inline sunrealtype s7f(const sunrealtype *udata, int nx) {
00088 }
00089 inline sunrealtype s7b(sunrealtype *udata, int nx) {
                          105.0 * udata[-3 * nx] + 1.0 / 10.0 * udata[-2 * nx] -
00090
        return -1.0 /
                  3.0 / 5.0 * udata[-1 * nx] - 1.0 / 4.0 * udata[0] + udata[1 * nx] - 3.0 / 10.0 * udata[2 * nx] + 1.0 / 15.0 * udata[3 * nx] -
00091
00092
                  1.0 / 140.0 * udata[4 * nx];
00093
00094 }
00095 inline sunrealtype s8f(const sunrealtype *udata, int nx) {}
       return -1.0 / 280.0 * udata[-5 * nx] + 1.0 / 28.0 * udata[-4 * nx] -
00096
                  1.0 / 6.0 * udata[-3 * nx] + 1.0 / 2.0 * udata[-2 * nx] - 5.0 / 4.0 * udata[-1 * nx] + 9.0 / 20.0 * udata[0] + 1.0 / 2.0 * udata[1 * nx] - 1.0 / 14.0 * udata[2 * nx] +
00097
00098
00099
                  1.0 / 168.0 * udata[3 * nx];
00100
00102 inline sunrealtype s8c(const sunrealtype *udata, int nx) {
4.0 / 105.0 * udata[3 * nx] - 1.0 / 280.0 * udata[4 * nx];
00106
00107 }
00108 inline sunrealtype s8b(const sunrealtype *udata, int nx) {
                          168.0 * udata[-3 * nx] + 1.0 / 14.0 * udata[-2 * nx] -
00109
         return -1.0 /
                 1.0 / 2.0 * udata[-1 * nx] - 9.0 / 20.0 * udata[0] + 5.0 / 4.0 * udata[1 * nx] - 1.0 / 2.0 * udata[2 * nx] + 1.0 / 6.0 * udata[3 * nx] - 1.0 / 28.0 * udata[4 * nx] +
00110
00111
00112
00113
                 1.0 / 280.0 * udata[5 * nx];
00114 }
00115 inline sunrealtype s9f(const sunrealtype *udata, int nx) {
00116    return -1.0 / 630.0 * udata[-5 * nx] + 1.0 / 56.0 * udata[-4 * nx] -
                 2.0 / 21.0 * udata[-3 * nx] + 1.0 / 3.0 * udata[-2 * nx] - 1.0 / 1.0 * udata[-1 * nx] + 1.0 / 5.0 * udata[0] + 2.0 / 3.0 * udata[1 * nx] - 1.0 / 7.0 * udata[2 * nx] +
00117
00118
00119
                  1.0 / 42.0 * udata[3 * nx] - 1.0 / 504.0 * udata[4 * nx];
00121 }
00122 inline sunrealtype s9b(sunrealtype *udata, int nx) {
2.0 / 21.0 * udata[3 * nx] - 1.0 / 56.0 * udata[4 * nx] +
00126
                 1.0 / 630.0 * udata[5 * nx];
00127
00128 }
00129 inline sunrealtype s10f(const sunrealtype *udata, int nx) {
11.0 / 30.0 * udata[0] + 4.0 / 7.0 * udata[1 * nx] -
00133
                 3.0 / 28.0 * udata[2 * nx] + 1.0 / 63.0 * udata[3 * nx] - 1.0 / 840.0 * udata[4 * nx];
00134
00135
00136 }
00137 inline sunrealtype s10c(const sunrealtype *udata, int nx) {
        return -1.0 / 1260.0 * udata[-5 * nx] + 5.0 / 504.0 * udata[-4 * nx] - 5.0 / 84.0 * udata[-3 * nx] + 5.0 / 21.0 * udata[-2 * nx] -
00138
                  5.0 / 6.0 * udata[-1 * nx] + 0 + 5.0 / 6.0 * udata[1 * nx] - 5.0 / 21.0 * udata[2 * nx] + 5.0 / 84.0 * udata[3 * nx] - 5.0 / 504.0 * udata[4 * nx] + 1.0 / 1260.0 * udata[5 * nx];
00140
00141
00142
00143 }
00144 inline sunrealtype s10b(const sunrealtype *udata, int nx)
        return 1.0 / 840.0 * udata[-4 * nx] - 1.0 / 63.0 * udata[-3 * nx] + 3.0 / 28.0 * udata[-2 * nx] - 4.0 / 7.0 * udata[-1 * nx] -
00146
                  11.0 / 30.0 * udata[0] + 6.0 / 5.0 * udata[1 * nx] -
00147
                 1.0 / 2.0 * udata[2 * nx] + 4.0 / 21.0 * udata[3 * nx] - 3.0 / 56.0 * udata[4 * nx] + 1.0 / 105.0 * udata[5 * nx] -
00148
00149
                  1.0 / 1260.0 * udata[6 * nx];
00150
00151 }
00152 inline sunrealtype s11f(const sunrealtype *udata, int nx) {
1.0 / 168.0 * udata[4 * nx] + 1.0 / 2310.0 * udata[5 * nx];
00159 }
00160 inline sunrealtype s11b(sunrealtype *udata, int nx)
        return -1.0 / 2310.0 * udata[-5 * nx] + 1.0 / 168.0 * udata[-4 * nx] -
5.0 / 126.0 * udata[-3 * nx] + 5.0 / 28.0 * udata[-2 * nx] -
5.0 / 7.0 * udata[-1 * nx] - 1.0 / 6.0 * udata[0] + udata[1 * nx] -
5.0 / 14.0 * udata[2 * nx] + 5.0 / 42.0 * udata[3 * nx] -
00161
00162
00163
00164
                  5.0 / 168.0 * udata[4 * nx] + 1.0 / 210.0 * udata[5 * nx] - 1.0 / 2772.0 * udata[6 * nx];
00165
00166
00167 }
00168 inline sunrealtype s12f(const sunrealtype *udata, int nx) {
00169    return -1.0 / 5544.0 * udata[-7 * nx] + 1.0 / 396.0 * udata[-6 * nx] -
```

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```
1.0 / 60.0 * udata[-5 * nx] + 5.0 / 72.0 * udata[-4 * nx] -
                        1.0 / 60.0 * udata[-5 * nx] + 5.0 / /2.0 * udata[-4 * nx] 

5.0 / 24.0 * udata[-3 * nx] + 1.0 / 2.0 * udata[-2 * nx] - 

7.0 / 6.0 * udata[-1 * nx] + 13.0 / 42.0 * udata[0] + 

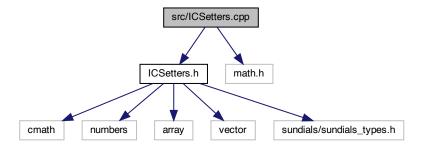
5.0 / 8.0 * udata[1 * nx] - 5.0 / 36.0 * udata[2 * nx] + 

1.0 / 36.0 * udata[3 * nx] - 1.0 / 264.0 * udata[4 * nx] +
00171
00172
00173
00174
                        1.0 / 3960.0 * udata[5 * nx];
00175
00177 inline sunrealtype s12c(const sunrealtype *udata, int nx) {
00178 return 1.0 / 5544.0 * udata[-6 * nx] - 1.0 / 385.0 * udata[-5 * nx] + 00179 1.0 / 56.0 * udata[-4 * nx] - 5.0 / 63.0 * udata[-3 * nx] +
                        15.0 / 56.0 * udata[-2 * nx] - 6.0 / 7.0 * udata[-1 * nx] + 0 +
00180
                        6.0 \ / \ 7.0 \ * \ udata[1 \ * \ nx] \ - \ 15.0 \ / \ 56.0 \ * \ udata[2 \ * \ nx] \ + \ 5.0 \ / \ 63.0 \ * \ udata[3 \ * \ nx] \ - \ 1.0 \ / \ 56.0 \ * \ udata[4 \ * \ nx] \ + \ 
00181
00182
                        1.0 / 385.0 * udata[5 * nx] - 1.0 / 5544.0 * udata[6 * nx];
00183
00184 }
00185 inline sunrealtype s12b(const sunrealtype *udata, int nx) {
                                   3960.0 * udata[-5 * nx] + 1.0 / 264.0 * udata[-4 * nx] -
00186 return -1.0 /
                        1.0 / 36.0 * udata[-3 * nx] + 5.0 / 36.0 * udata[-2 * nx] - 5.0 / 8.0 * udata[-1 * nx] - 13.0 / 42.0 * udata[0] +
00187
                        7.0 / 6.0 * udata[1 * nx] - 1.0 / 2.0 * udata[2 * nx] +
00189
                        5.0 / 24.0 * udata[3 * nx] - 5.0 / 72.0 * udata[4 * nx] + 1.0 / 60.0 * udata[5 * nx] - 1.0 / 396.0 * udata[6 * nx] +
00190
00191
                        1.0 / 5544.0 * udata[7 * nx];
00192
00193 }
00194 //#pragma omp declare simd notinbranch uniform(nx) simdlen(13) // Is this safe
00195 //here? Do I need critical or atomic?
00196 inline sunrealtype s13f(const sunrealtype *udata, int nx) {
00197 return -1.0 / 12012.0 * udata[-7 * nx] + 1.0 / 792.0 * udata[-6 * nx] -
                        1.0 / 110.0 * udata[-5 * nx] + 1.0 / 24.0 * udata[-4 * nx] -
00198
                        1.0 / 110.0 * udata[-3 * nx] + 1.0 / 24.0 * udata[-4 * nx] + 3.0 / 36.0 * udata[-3 * nx] + 3.0 / 8.0 * udata[-2 * nx] - 1.0 / 1.0 * udata[-1 * nx] + 1.0 / 7.0 * udata[0] + 3.0 / 4.0 * udata[1 * nx] - 5.0 / 24.0 * udata[2 * nx] + 1.0 / 18.0 * udata[3 * nx] - 1.0 / 88.0 * udata[4 * nx] + 1.0 / 18.0 * udata[7 * nx] - 1.0 / 18.0 * udata[8 * nx] - 1.0 / 18.0 * udata[
00199
00200
00201
00202
00203
                        1.0 / 660.0 * udata[5 * nx] - 1.0 / 10296.0 * udata[6 * nx];
00204 }
00205 //#pragma omp declare simd notinbranch uniform(nx) simdlen(13)
00206 inline sunrealtype s13b(sunrealtype *udata, int nx) {
00207    return 1.0 / 10296.0 * udata[-6 * nx] - 1.0 / 660.0 * udata[-5 * nx] +
                        1.0 / 88.0 * udata[-4 * nx] - 1.0 / 18.0 * udata[-3 * nx] + 5.0 / 24.0 * udata[-2 * nx] - 3.0 / 4.0 * udata[-1 * nx] -
00208
00209
00210
                        1.0 \ / \ 7.0 \ * \ udata[0] \ + \ udata[1 \ * \ nx] \ - \ 3.0 \ / \ 8.0 \ * \ udata[2 \ * \ nx] \ +
                        5.0 / 36.0 * udata[3 * nx] - 1.0 / 24.0 * udata[4 * nx] + 1.0 / 110.0 * udata[5 * nx] - 1.0 / 792.0 * udata[6 * nx] + 1.0 / 12012.0 * udata[7 * nx];
00211
00212
00213
00214 }
00215
00217 // Stencils with nx fixed to 6//
00219
00220 inline sunrealtype slf(sunrealtype *udata) { return slf(udata, 6); }
00221 inline sunrealtype s1b(sunrealtype *udata) {
                                                                                   return s1b(udata, 6);
00222 inline sunrealtype s2f(sunrealtype *udata)
                                                                                   return s2f(udata, 6);
00223 inline sunrealtype s2c(sunrealtype *udata) {
                                                                                    return s2c(udata, 6);
00224 inline sunrealtype s2b(sunrealtype *udata)
                                                                                    return s2b (udata, 6);
00225 inline sunrealtype s3f(sunrealtype *udata) {
                                                                                    return s3f(udata, 6);
                                                                                    return s3b(udata, 6);
00226 inline sunrealtype s3b(sunrealtype *udata)
00227 inline sunrealtype s4f(sunrealtype *udata)
                                                                                    return s4f(udata, 6);
00228 inline sunrealtype s4c(sunrealtype *udata)
                                                                                    return s4c(udata, 6);
                                                                                    return s4b (udata, 6);
00229 inline sunrealtype s4b(sunrealtype *udata)
00230 inline sunrealtype s5f(sunrealtype *udata) {
                                                                                    return s5f (udata, 6):
00231 inline sunrealtype s5b(sunrealtype *udata) {
                                                                                    return s5b (udata, 6);
00232 inline sunrealtype s6f(sunrealtype *udata) {
                                                                                    return s6f(udata, 6);
00233 inline sunrealtype s6c(sunrealtype *udata)
                                                                                    return s6c (udata, 6);
00234 inline sunrealtype s6b(sunrealtype *udata)
                                                                                    return s6b(udata, 6);
00235 inline sunrealtype s7f(sunrealtype *udata) {
                                                                                    return s7f(udata, 6);
00236 inline sunrealtype s7b(sunrealtype *udata) {
                                                                                   return s7b (udata, 6);
00237 inline sunrealtype s8f(sunrealtype *udata) {
                                                                                   return s8f(udata, 6);
00238 inline sunrealtype s8c(sunrealtype *udata) {
                                                                                   return s8c(udata, 6);
00239 inline sunrealtype s8b(sunrealtype *udata) {
                                                                                   return s8b(udata, 6);
00240 inline sunrealtype s9f(sunrealtype *udata) {
                                                                                    return s9f(udata, 6);
00241 inline sunrealtype s9b(sunrealtype *udata) {
                                                                                   return s9b(udata, 6);
00242 inline sunrealtype s10f(sunrealtype *udata) { return s10f(udata, 6);
00243 inline sunrealtype s10c(sunrealtype *udata) { return s10c(udata, 6);
00244 inline sunrealtype s10b(sunrealtype *udata) { return s10b(udata, 6);
00245 inline sunrealtype s11f(sunrealtype *udata)
                                                                                  { return s11f(udata, 6);
00246 inline sunrealtype s11b(sunrealtype *udata)
                                                                                  { return s11b(udata, 6);
00247 inline sunrealtype s12f(sunrealtype *udata) {
                                                                                     return s12f(udata, 6);
00248 inline sunrealtype s12c(sunrealtype *udata) { return s12c(udata, 6);
00249 inline sunrealtype s12b(sunrealtype *udata) { return s12b(udata, 6);
00250 inline sunrealtype s13f(sunrealtype *udata) { return s13f(udata, 6);
00251 inline sunrealtype s13b(sunrealtype *udata) { return s13b(udata, 6);
00252
```

6.6 src/ICSetters.cpp File Reference

Implementation of the plane wave and Gaussian wave packets in 1D, 2D, 3D.

```
#include "ICSetters.h"
#include <math.h>
Include dependency graph for ICSetters.cpp:
```



6.6.1 Detailed Description

Implementation of the plane wave and Gaussian wave packets in 1D, 2D, 3D.

Definition in file ICSetters.cpp.

6.7 ICSetters.cpp

```
Go to the documentation of this file.
```

```
00002 /// @file ICSetters.cpp
00003 /// @brief Implementation of the plane wave and Gaussian wave packets in 1D, 2D,
00004 /// 3D
00007 #include "ICSetters.h"
80000
00009 #include <math.h>
00010
00011 /** PlaneWavelD construction with */
 00012 PlaneWave1D::PlaneWave1D(vector<sunrealtype> k, vector<sunrealtype> p,
00013
                                                                                       vector<sunrealtype> phi) {
                     00014
00015
00016
                     // Amplitude bug: lower by factor 3 px = p[0] / 3; /** - amplitude (polarization) in x-direction \f$ p_x \f$ */ py = p[1] / 3; /** - amplitude (polarization) in y-direction \f$ p_y \f$ */
00017
00018
00019
                     py = p[1] / 3, /** - amplitude (polarization) in y direction (10 p_y \ 10 \ 7)
pz = p[2] / 3; /** - amplitude (polarization) in z-direction \f$ p_z \ f$ */
phix = phi[0]; /** - phase shift in x-direction \f$ \phi_x \ f$ */
phiy = phi[1]; /** - phase shift in y-direction \f$ \phi_y \ f$ */
phiz = phi[2]; /** - phase shift in z-direction \f$ \phi_z \ f$ */
00020
00021
00022
00023
00024 }
00025
00026 /** PlaneWave1D implementation in space */
00027 //#pragma omp declare simd uniform(x,y,z) linear(pTo6Space:6)
{\tt 00028 \ void \ PlaneWavelD::addToSpace} ({\tt const \ sunrealtype \ x, \ const \ sunrealtype \ z, \
00029
                                                                                                   sunrealtype *pTo6Space) const {
00030
                     const sunrealtype wavelength =
00031
                                sqrt(kx * kx + ky * ky + kz * kz); /* \f$ 1/\lambda \f$ */
```

6.7 ICSetters.cpp 185

```
const sunrealtype kScalarX = (kx * x + ky * y + kz * z) * 2 *
                                     numbers::pi; /* \f$ 2\pi \ \vec{k} \cdot \vec{x} \f$ */
00033
          // Plane wave definition
00034
00035
         const array<sunrealtype, 3> E{{
                                                                                     /* E-field vector */
                                         00036
00037
00039
         // Put E-field into space
         pTo6Space[0] += E[0];
pTo6Space[1] += E[1];
00040
00041
         pTo6Space[2] += E[2];
00042
00043
         // and B-field
         pTo6Space[3] += (ky * E[2] - kz * E[1]) / wavelength;
pTo6Space[4] += (kz * E[0] - kx * E[2]) / wavelength;
pTo6Space[5] += (kx * E[1] - ky * E[0]) / wavelength;
00044
00045
00046
00047 }
00048
00049 /** PlaneWave2D construction with */
00050 PlaneWave2D::PlaneWave2D(vector<sunrealtype> k, vector<sunrealtype> p,
                                      vector<sunrealtype> phi) {
         00052
00053
00054
         // Amplitude bug: lower by factor 9 px = p[0] / 9; /** - amplitude (polarization) in x-direction \f$ p_x \f$ */ py = p[1] / 9; /** - amplitude (polarization) in y-direction \f$ p_y \f$ */
00055
00056
         pz = p[2] / 9; /** - amplitude (polarization) in z-direction <math>f p_z f */
00058
         phix = phi[0]; /** - phase shift in x-direction \f$ \phi_x \f$ */
phiy = phi[1]; /** - phase shift in y-direction \f$ \phi_y \f$ */
phiz = phi[2]; /** - phase shift in z-direction \f$ \phi_z \f$ */
00059
00060
00061
00062 }
00063
00064 /** PlaneWave2D implementation in space */
00065 //#pragma omp declare simd uniform(x,y,z) linear(pTo6Space:6)
00066 void PlaneWave2D::addToSpace(const sunrealtype x, const sunrealtype y, const sunrealtype z,
00067
                                          sunrealtype *pTo6Space) const {
         const sunrealtype wavelength =
00068
         sqrt(kx * kx + ky * ky + kz * kz); /* \f$ 1/\lambda \f$ */
const sunrealtype kScalarX = (kx * x + ky * y + kz * z) * 2 *
00070
00071
                                     numbers::pi; /* \f$ 2\pi \ \end{tabular} \ \cdot \end{tabular} $$ \f$ */
00072
         // Plane wave definition
         const array<sunrealtype, 3> E{{
00073
                                                                                     /* E-field vector */
                                        00074
00075
00076
00077
         // Put E-field into space
         pTo6Space[0] += E[0];
pTo6Space[1] += E[1];
00078
00079
         pTo6Space[2] += E[2];
00080
00081
         // and B-field
         pTo6Space[3] += (ky * E[2] - kz * E[1]) / wavelength;
pTo6Space[4] += (kz * E[0] - kx * E[2]) / wavelength;
pTo6Space[5] += (kx * E[1] - ky * E[0]) / wavelength;
00083
00084
00085 }
00086
00087 /** PlaneWave3D construction with */
00088 PlaneWave3D::PlaneWave3D(vector<sunrealtype> k, vector<sunrealtype> p,
00089
                                      vector<sunrealtype> phi) {
00090
         kx = k[0];
                            /** - wavevectors \f$ k_x \f$ */
                            /** - \f$ k_y \f$ */
/** - \f$ k_z \f$ normalized to \f$ 1/\lambda \f$ */
00091
         ky = k[1];
         kz = k[2]:
00092
                            /** - Amplitude (polarization) in x-direction \f$ p_x \f$ */ /** - amplitude (polarization) in y-direction \f$ p_y \f$ */
         px = p[0];
00093
00094
         py = p[1];
         py - p(1);  /** - amplitude (polarization) in y-direction \fs p_z \ (is */
pz = p[2];  /** - amplitude (polarization) in z-direction \fs p_z \ fs */
phix = phi[0]; /** - phase shift in x-direction \fs \ phi_z \ fs */
phiy = phi[1]; /** - phase shift in y-direction \fs \ phi_z \ fs */
phiz = phi[2]; /** - phase shift in z-direction \fs \ phi_z \ fs */
00095
00096
00097
00098
00099 }
00100
00101 /** PlaneWave3D implementation in space */
00102 //#pragma omp declare simd uniform(x,y,z) linear(pTo6Space:6)
00103 void PlaneWave3D::addToSpace(sunrealtype x, sunrealtype y, sunrealtype z,
00104
                                           sunrealtype *pTo6Space) const {
00105
         const sunrealtype wavelength =
         00106
00107
                                     numbers::pi; /* \f$ 2\pi \ \vec{k} \cdot \vec{x} \f$ */
00108
         // Plane wave definition
00109
00110
         const array<sunrealtype, 3 \ge E\{{/* E-field vector \f} \vec{E}\f^{**/e}
                                        00111
00112
                                         pz * cos(kScalarX - phiz)}}; /* \f$ E_z \f$ */
          // Put E-field into space
00114
00115
         pTo6Space[0] += E[0];
         pTo6Space[1] += E[1];
pTo6Space[2] += E[2];
00116
00117
         // and B-field
00118
```

```
00120
00121
00122 }
00123
00124 /** Gauss1D construction with */
00125 Gauss1D::Gauss1D(vector<sunrealtype> k, vector<sunrealtype> p,
                          vector<sunrealtype> xo, sunrealtype phig_,
00126
00127
                          vector<sunrealtype> phi) {
                         /** - wavevectors \f$ k_x \f$ */
/** - \f$ k_y \f$ */
/** - \f$ k_z \f$ normalized to \f$ 1/\lambda \f$*/
/** - amplitude (polarization) in x-direction */
00128
        kx = k[0];
         ky = k[1];
00129
00130
         kz = k[2]:
00131
         ;[0]q = xq
         py = p[1];
                          /** - amplitude (polarization) in y-direction */
00132
                          /** - amplitude (polarization) in z-direction */
00133
         pz = p[2];
         phix = phi[0]; /** - phase shift in x-direction */
phiy = phi[1]; /** - phase shift in y-direction */
00134
00135
         phiz = phi[2]; /** - phase shift in z-direction */
00136
         phig = phig_; /** - width */
        pring = pring.;
x0x = xo[0];    /** - shift from origin in x-direction...,
x0y = xo[1];    /** - shift from origin in y-direction*/
x0z = xo[2];    /** - shift from origin in z-direction*/
00138
00139
00140
00141 }
00142
00143 /** Gauss1D implementation in space */
00144 //#pragma omp declare simd uniform(x,y,z) linear(pTo6Space:6)
00145 void Gauss1D::addToSpace(sunrealtype x, sunrealtype y, sunrealtype z,
00146
                                   sunrealtype *pTo6Space) const {
00147
         const sunrealtype wavelength =
         sqrt(kx * kx + ky * ky + kz * kz); /* \f$ 1/\lambda \f$ */ x = x - x0x; /* x-coordinate minus shift from origin */
00148
00149
00150
         y = y - x0y; /* y-coordinate minus shift from origin */
         z = z - x0z; /* z-coordinate minus shift from origin */
00151
00152
         const sunrealtype kScalarX = (kx \star x + ky \star y + kz \star z) \star 2 \star
00153
                                   numbers::pi; /* \f$ 2\pi \ \cdot \ext{vec} x \f$ */
00154
         const sunrealtype envelopeAmp =
         exp(-(x * x + y * y + z * z) / phig / phig); /* enveloping Gauss shape */ // Gaussian wave definition
00155
00156
00157
         const array<sunrealtype, 3> E{
00158
                                                                 /* E-field vector */
               00159
00160
00161
00162
         // Put E-field into space
        pTo6Space[0] += E[0];
00163
00164
         pTo6Space[1] += E[1];
00165
         pTo6Space[2] += E[2];
00166
         // and B-field
         pTo6Space[3] += (ky * E[2] - kz * E[1]) / wavelength;
pTo6Space[4] += (kz * E[0] - kx * E[2]) / wavelength;
00167
00168
        pTo6Space[5] += (kx * E[1] - ky * E[0]) / wavelength;
00169
00170 }
00171
00172 /** Gauss2D construction with */
00173 Gauss2D::Gauss2D(vector/sunrealtype> dis_, vector/sunrealtype> axis_,
00174 sunrealtype Amp_, sunrealtype phip_, sunrealtype w0_,
00175 sunrealtype zr_, sunrealtype Ph0_, sunrealtype PhA_) {
00176 dis = dis_; /** - center it approaches */
00177 axis_= axis_: /** - direction form whose it correct */
00177
        axis = axis_;
                                  /** - direction form where it comes */
                                  /** - amplitude */
00178
        Amp = Amp_;
                                  /** - polarization rotation from TE-mode */
00179
         phip = phip_;
         w0 = w0_{;}
                                  /** - taille */
00180
00181
         zr = zr_{;}
                                  /** - Rayleigh length */
         Ph0 = Ph0_;
                                   /** - beam center */
00182
        PhA = PhA_;
00183
                                   /** - beam length */
        A1 = Amp * cos(phip); // amplitude in z-direction

A2 = Amp * sin(phip); // amplitude on xy-plane

lambda = numbers::pi * w0 * w0 / zr; // formula for wavelength
00184
00185
00186
00187 }
00189 //#pragma omp declare simd uniform(x,y,z) linear(pTo6Space:6)
00190 void Gauss2D::addToSpace(sunrealtype x, sunrealtype y, sunrealtype z,
         00191
00192
00193
         //origin
         x -= dis[0];
00194
00195
         y -= dis[1];
00196
         // z-=dis[2];
00197
         z = NAN;
         // \f$ z_g = \sqrt{x} \cdot \sqrt{f} projection on propagation axis
00198
         const sunrealtype zg =
00199
00200
             x * axis[0] + y * axis[1]; //+z*axis[2]; // =z-z0 -> propagation
                                             //direction, minus origin
00201
00202
         // \f$ r = \sqrt{\vec{x}^2 -z_g^2} \f$ -> pythagoras of radius minus
         00203
00204
00205
```

6.7 ICSetters.cpp 187

```
// \f$ w(z) = w0 \cdot \{1 + (z_g/z_R)^2\} \cdot f$
         const surrealtype wz = w0 * sqrt(1 + (zg * zg / zr / zr)); // waist at position z // \f$ g(z) = atan(z_g/z_r) \f$
00207
00208
         const sunrealtype gz = atan(zg / zr); // Gouy phase // \f$ R(z) = z_g*(1+(z_r/z_g)^2) \f$
00209
00210
00211
         sunrealtype Rz = NAN; // beam curvature
         if (zg != 0)
00213
           Rz = zg * (1 + (zr * zr / zg / zg));
00214
          Rz = 1e308;
00215
         // wavenumber \f$ k = 2\pi/\lambda k
00216
         const sunrealtype k = 2 * numbers::pi / lambda;
00217
         00218
00219
         const sunrealtype PhF =
00220
             -k * r * r^{\prime} (2 * Rz) + gz - k * zg; // to be inserted into cosine
         // \f$ G = \sqrt{w_0/w_z}\e^{-(r/w(z))^2}\e^{{(zg-Ph0)^2/PhA^2}\cos(PhF) \f$
00221
00222
        // CVode is a diva, no chance to remove the square in the second exponential
         // -> h too small
00223
         const sunrealtype G2D = sqrt(w0 / wz) * exp(-r * r / wz / wz) *
                             exp(-(zg - Ph0) * (zg - Ph0) / PhA / PhA) * cos(PhF); // gauss shape
00225
00226
00227
         // \f$ c_\alpha =\vec{e}_x\cdot\vec{axis} \f$
         // projection components; do like this for CVode convergence \rightarrow otherwise
00228
00229
        \ensuremath{//} results in machine error values for non-existant field components if
00230
         // axis[0] and axis[1] are given
00231
         const sunrealtype ca =
00232
             axis[0]; // x-component of propagation axis which is given as parameter
00233
         const sunrealtype sa = sqrt(1 - ca * ca); // no z-component for 2D propagation
00234
         // E-field to space: polarization in xy-plane (A2) is projection of
         // z-polarization (A1) on x- and y-directions
00235
         pTo6Space[0] += sa * (G2D * A2);
00236
         pTo6Space[1] += -ca * (G2D * A2);
pTo6Space[2] += G2D * A1;
00237
00238
00239
         // B-field -> negative derivative wrt polarization shift of E-field
         pTo6Space[3] += -sa * (G2D * A1);
pTo6Space[4] += ca * (G2D * A1);
00240
00241
00242
        pTo6Space[5] += G2D * A2;
00243 }
00244
00245 /** Gauss3D construction with */
00246 Gauss3D::Gauss3D(vector<sunrealtype> dis_, vector<sunrealtype> axis_,
00247
                          sunrealtype Amp_,
                          // vector<sunrealtype> pol_,
00248
                          sunrealtype phip_, sunrealtype w0_, sunrealtype zr_, sunrealtype Ph0_, sunrealtype PhA_) {
00249
        sunrealtype Ph0_, sunrealtype PhA_) {
dis = dis_; /** - center it approaches */
axis = axis_; /** - direction from where it comes */
Amp = Amp_; /** - amplitude */
// nol-prol
00250
00251
00252
00253
        // pol=pol_;
00254
         phip = phip_; /** - polarization rotation form TE-mode */
00255
                     /** - taille */
         w0 = w0_{;}
         zr = zr_;
00257
                         /** - Rayleigh length */
                        /** - beam center */
/** - beam length */
         Ph0 = Ph0_;
00258
        PhA = PhA_;
00259
00260
        lambda = numbers::pi * w0 * w0 / zr;
00261
        A1 = Amp * cos(phip);
        A2 = Amp * sin(phip);
00262
00263 }
00264
00265 /** Gauss3D implementation in space */
00266 void Gauss3D::addToSpace(sunrealtype\ x,\ sunrealtype\ y,\ sunrealtype\ z,
00267
                                   sunrealtype *pTo6Space) const {
00268
        x -= dis[0];
        y -= dis[1];
00269
         z -= dis[2];
00270
        const sunrealtype zg = x * axis[0] + y * axis[1] + z * axis[2];

const sunrealtype r = sqrt((x * x + y * y + z * z) - zg * zg);

const sunrealtype wz = w0 * sqrt(1 + (zg * zg / zr / zr));
00271
00272
00273
         const sunrealtype gz = atan(zg / zr);
00274
00275
         sunrealtype Rz = NAN;
00276
         if (zg != 0)
00277
          Rz = zg * (1 + (zr * zr / zg / zg));
00278
         else
00279
          Rz = 1e308;
00280
         const sunrealtype k = 2 * numbers::pi / lambda;
         const sunrealtype PhF = -k * r * r / (2 * Rz) + gz - k * zg;
00281
         const sunrealtype G3D = (w0 / wz) * exp(-r * r / wz / wz)
00282
                             \exp(-(zg - Ph0) * (zg - Ph0) / PhA / PhA) * \cos(PhF);
00283
        const sunrealtype ca = axis[0];
const sunrealtype sa = sqrt(1 - ca * ca);
pTo6Space[0] += sa * (G3D * A2);
00284
00285
00286
         pTo6Space[1] += -ca * (G3D * A2);
pTo6Space[2] += G3D * A1;
00287
00288
00289
         pTo6Space[3] += -sa * (G3D * A1);
         pTo6Space[4] += ca * (G3D * A1);
00290
         pTo6Space[5] += G3D \star A2;
00291
00292 }
```

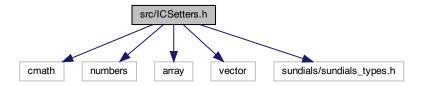
```
00294 /** Evaluate lattice point values to zero and add field values */
00295 //# pragma omp declare simd uniform(x,y,z) linear(pTo6Space:6)
00296 void ICSetter::eval(sunrealtype x, sunrealtype y, sunrealtype z,
00297
                         sunrealtype *pTo6Space) {
       pTo6Space[0] = 0;
00298
       pTo6Space[1] = 0;
00300
       pTo6Space[2] = 0;
00301
       pTo6Space[3] = 0;
00302
       pTo6Space[4] = 0;
       pTo6Space[5] = 0;
00303
00304
       add(x, y, z, pTo6Space);
00305 }
00306
00307 /** Add all initial field values to the lattice space */
00308 void ICSetter::add(sunrealtype x, sunrealtype y, sunrealtype z,
00309
                         sunrealtype *pTo6Space)
00310
       for (const auto &wave : planeWaves1D)
         wave.addToSpace(x, y, z, pTo6Space);
00312
       for (const auto &wave : planeWaves2D)
00313
         wave.addToSpace(x, y, z, pTo6Space);
00314
       for (const auto &wave : planeWaves3D)
00315
         wave.addToSpace(x, y, z, pTo6Space);
00316
       for (const auto &wave : gauss1Ds)
00317
         wave.addToSpace(x, y, z, pTo6Space);
       for (const auto &wave : gauss2Ds)
         wave.addToSpace(x, y, z, pTo6Space);
00319
00320
       for (const auto &wave : gauss3Ds)
00321
         wave.addToSpace(x, y, z, pTo6Space);
00322 }
00323
00324 /** Add plane waves in 1D to their container vector */
00325 void ICSetter::addPlaneWave1D(vector<sunrealtype> k, vector<sunrealtype> p,
00326
                                    vector < sunrealtype > phi)  {
00327
       planeWaves1D.emplace_back(PlaneWave1D(k, p, phi));
00328 }
00329
00330 /** Add plane waves in 2D to their container vector */
00331 void ICSetter::addPlaneWave2D(vector<sunrealtype> k, vector<sunrealtype> p,
00332
                                    vector<sunrealtype> phi) {
00333
       planeWaves2D.emplace_back(PlaneWave2D(k, p, phi));
00334 }
00335
00336 /** Add plane waves in 3D to their container vector */
00337 void ICSetter::addPlaneWave3D(vector<sunrealtype> k, vector<sunrealtype> p,
00338
                                    vector<sunrealtype> phi) {
00339
       planeWaves3D.emplace_back(PlaneWave3D(k, p, phi));
00340 }
00341
00342 /** Add Gaussian waves in 1D to their container vector */
00343 void ICSetter::addGauss1D(vector<sunrealtype> k, vector<sunrealtype> p,
00344
                                vector<sunrealtype> xo, sunrealtype phig_,
00345
                                vector<sunrealtype> phi) {
00346
       gauss1Ds.emplace_back(Gauss1D(k, p, xo, phig_, phi));
00347 }
00348
00349 /** Add Gaussian waves in 2D to their container vector */
00350 void ICSetter::addGauss2D(vector<sunrealtype> dis_, vector<sunrealtype> axis_,
00351
                                sunrealtype Amp_, sunrealtype phip_, sunrealtype w0_,
00352
                                sunrealtype zr_, sunrealtype PhO_, sunrealtype PhA_) {
00353
       gauss2Ds.emplace back(
00354
           Gauss2D (dis_, axis_, Amp_, phip_, w0_, zr_, Ph0_, PhA_));
00355 }
00357 /** Add Gaussian waves in 3D to their container vector */
00358 void ICSetter::addGauss3D(vector<sunrealtype> dis_, vector<sunrealtype> axis_,
00359
                                sunrealtype Amp_, sunrealtype phip_, sunrealtype w0_-,
                                sunrealtype zr_, sunrealtype PhO_, sunrealtype PhA_) {
00360
00361 gauss3Ds.emplace_back(
00362
           Gauss3D(dis_, axis_, Amp_, phip_, w0_, zr_, Ph0_, PhA_));
00363 }
```

6.8 src/ICSetters.h File Reference

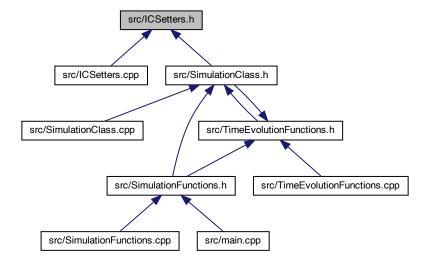
Declaration of the plane wave and Gaussian wave packets in 1D, 2D, 3D.

```
#include <cmath>
#include <numbers>
#include <array>
```

#include <vector>
#include <sundials/sundials_types.h>
Include dependency graph for ICSetters.h:



This graph shows which files directly or indirectly include this file:



Data Structures

class PlaneWave

super-class for plane waves

• class PlaneWave1D

class for plane waves in 1D

class PlaneWave2D

class for plane waves in 2D

class PlaneWave3D

class for plane waves in 3D

class Gauss1D

class for Gaussian waves in 1D

• class Gauss2D

class for Gaussian waves in 2D

· class Gauss3D

class for Gaussian waves in 3D

class ICSetter

ICSetter class to initialize wave types with default parameters.

6.8.1 Detailed Description

Declaration of the plane wave and Gaussian wave packets in 1D, 2D, 3D.

Definition in file ICSetters.h.

6.9 ICSetters.h

Go to the documentation of this file.

```
00001 //
           00002 /// @file ICSetters.h
00003 /// @brief Declaration of the plane wave and Gaussian wave packets in 1D, 2D, 3D
00005
00006 #pragma once
00007
00008 // math, constants, vector, and array
00009 #include <cmath>
00010 //#include <mathimf.h>
00011 #include <numbers>
00012 #include <arrav>
00013 #include <vector>
00014
00015 #include <sundials/sundials_types.h> /* definition of type sunrealtype */
00016
00017 using namespace std;
00018
00019 /** @brief super-class for plane waves
00020 *
00021 * They are given in the form \f$ \vec{E} = \vec{E}_0 \ \cos \left( \vec{k} 00022 * \cdot \vec{x} - \vec{\phi} \right) \f$ */
00023 class PlaneWave {
00024 protected:
       /// wavenumber f k_x f
00025
00026
       sunrealtype kx;
00027
       /// wavenumber \f$ k_y \f$
       sunrealtype ky;
00029
       /// wavenumber f k_z f
00030
        sunrealtype kz;
00031
        /// polarization & amplitude in x-direction, f p_x f
00032
       sunrealtype px;
00033
        /// polarization & amplitude in y-direction, \f$ p_y \f$
00034
       sunrealtype py;
        /// polarization & amplitude in z-direction, f p_z f
00035
00036
        sunrealtype pz;
00037
        /// phase shift in x-direction, f \phi_x \f$
00038
        sunrealtype phix;
00039
       /// phase shift in y-direction, \f$ \phi_y \f$
       sunrealtype phiy;
00041
       /// phase shift in z-direction, \f$ \phi_z \f$
00042
       sunrealtype phiz;
00043 };
00044
00045 /** @brief class for plane waves in 1D */
00046 class PlaneWave1D : public PlaneWave {
00047 public:
      /// construction with default parameters
00048
       \label{eq:planeWavelD} \begin{split} & \textbf{PlaneWavelD}(\text{vector} < \text{sunrealtype} > \ k = \{1, \ 0, \ 0\}, \\ & \text{vector} < \text{sunrealtype} > \ p = \{0, \ 0, \ 1\}, \\ & \text{vector} < \text{sunrealtype} > \ phi = \{0, \ 0, \ 0\}); \end{split}
00049
00050
00051
00052
       /// function for the actual implementation in the lattice
00053 void addToSpace(sunrealtype x, sunrealtype y, sunrealtype z,
00054
                        sunrealtype *pTo6Space) const;
00055 };
00056
00057 /** @brief class for plane waves in 2D */
00058 class PlaneWave2D : public PlaneWave {
00059 public:
```

6.9 ICSetters.h

```
/// construction with default parameters
       PlaneWave2D(vector<sunrealtype> k = {1, 0, 0}, vector<sunrealtype> p = {0, 0, 1},
00061
00062
                  vector<sunrealtype> phi = {0, 0, 0});
00063
       \ensuremath{///} function for the actual implementation in the lattice
00064
00065
       void addToSpace(sunrealtype x, sunrealtype y, sunrealtype z,
                      sunrealtype *pTo6Space) const;
00067 };
00068
00069 /** @brief class for plane waves in 3D */ 00070 class PlaneWave3D : public PlaneWave {
00071 public:
00072
       /// construction with default parameters
00073
       PlaneWave3D (vector<sunrealtype> k = \{1, 0, 0\},
00074
                  vector<sunrealtype> p = \{0, 0, 1\},
00075
                  vector<sunrealtype> phi = \{0, 0, 0\};
       /// function for the actual implementation in space
00076
00077
       void addToSpace(sunrealtype x, sunrealtype y, sunrealtype z,
                      sunrealtype *pTo6Space) const;
00078
00079 };
00080
00081 /** @brief class for Gaussian waves in 1D
00082
00086 class Gauss1D {
00087 private:
       /// wavenumber f k_x f
00088
00089
       sunrealtype kx;
00090
       /// wavenumber f k_y f
       sunrealtype ky;
00092
       /// wavenumber f k_z f
00093
       sunrealtype kz;
00094
       /// polarization & amplitude in x-direction, f p_x f
00095
       sunrealtype px;
00096
       /// polarization & amplitude in v-direction, \f$ p v \f$
       sunrealtype py;
00098
       /// polarization & amplitude in z-direction, f p_z f
00099
       sunrealtype pz;
00100
       /// phase shift in x-direction, f \phi_x \f$
00101
       sunrealtype phix;
00102
       /// phase shift in v-direction, \f$ \phi v \f$
00103
       sunrealtype phiy;
       /// phase shift in z-direction, f \phi_z \f$
00105
       sunrealtype phiz;
00106
       /// center of pulse in x-direction, f x_0 f
00107
       sunrealtype x0x;
00108
       /// center of pulse in y-direction, \f$ y_0 \f$
00109
       sunrealtype x0v:
00110
       /// center of pulse in z-direction, f z_0 f
00111
       sunrealtype x0z;
00112
       /// pulse width f \Phi_g \f$
00113
       sunrealtype phig;
00114
00115 public:
       /// construction with default parameters
       Gauss1D (vector<sunrealtype> k = \{1, 0, 0\}, vector<sunrealtype> p = \{0, 0, 1\},
00117
              vector/sunrealtype> xo = {0, 0, 0}, sunrealtype phig_ = 1.01,
vector/sunrealtype> phi = {0, 0, 0});
00118
00119
       /// function for the actual implementation in space
00120
00121
       void addToSpace(sunrealtype x, sunrealtype y, sunrealtype z,
00122
                      sunrealtype *pTo6Space) const;
00123
00124 public:
00125 };
00126
00127 /** @brief class for Gaussian waves in 2D
      * They are given in the form
00131
00132
00133
      * - radial distance to propagation axis f r = \sqrt{vec{x}^2 - z_g^2} f
00134
      \star - f k = 2\pi / \add f
00139 \star obtained via the chosen parameters \star/
00140 class Gauss2D {
00141 private:
       /// distance maximum to origin
00143
       vector<sunrealtype> dis;
00144
       /// normalized propagation axis
00145
       vector<sunrealtype> axis;
00146
      /// amplitude \f$ A\f$
```

```
sunrealtype Amp;
00148
               /// polarization rotation from TE-mode around propagation direction
00149
                // that determines f \vec{\epsilon}\f$ above
               sunrealtype phip;
/// taille \f$ \omega_0 \f$
00150
00151
               sunrealtype w0;
00152
00153
               /// Rayleigh length \f$ z_R = \pi \omega_0^2 / \lambda \f$
00154
               sunrealtype zr;
00155
               /// center of beam f \Phi_0 \f
00156
               sunrealtype Ph0;
00157
               /// length of beam \f$ \Phi_A \f$
               sunrealtype PhA;
00158
00159
               /// amplitude projection on TE-mode
00160
               sunrealtype A1;
00161
                /// amplitude projection on xy-plane
               sunrealtype A2;
/// wavelength \f$ \lambda \f$
00162
00163
00164
               sunrealtype lambda;
00165
00166 public:
                /// construction with default parameters
00167
              Gauss2D(vector<sunrealtype> dis_ = {0, 0, 0},
    vector<sunrealtype> axis_ = {1, 0, 0}, sunrealtype Amp_ = 1.01,
    sunrealtype phip_ = 0, sunrealtype w0_ = 1e-5, sunrealtype zr_ = 4e-5,
    sunrealtype Ph0_ = 2e-5, sunrealtype PhA_ = 0.45e-5);

/// function for the actual implementation in space
00168
00169
00170
00171
00172
00173
               void addToSpace(sunrealtype x, sunrealtype y, sunrealtype z,
00174
                                             sunrealtype *pTo6Space) const;
00175
00176 public:
00177 };
00178
00179 /** @brief class for Gaussian waves in 3D
00180
00181
            \star They are given in the form
00181 * Iney are given in the form 00182 * f\$ \vec\{E\} = A \, \vec\{\ensuremath{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\mbox{\m\s\m\s\\m\s\n\sin\\\\m\s\\\m\m\s\m\s\n\\\m\s\m\s\n\s\m\\
00186 * - radial distance to propagation axis \f$ r = \sqrt{\vec{x}^2 -z_g^2} \f$
00191 * obtained via the chosen parameters */
00192 class Gauss3D {
00193 private:
00194
              /// distance maximum to origin
               vector<sunrealtype> dis;
00195
00196
               \ensuremath{///} normalized propagation axis
               vector<sunrealtype> axis;
00198
               /// amplitude \f A\f$
00199
               sunrealtype Amp;
               /// polarization rotation from TE-mode around propagation direction // that determines f\ \c \
00200
00201
00202
               sunrealtype phip;
// polarization
00203
00204
               // vector<sunrealtype> pol;
00205
                /// taille \f$ \omega_0 \f$
00206
               sunrealtype w0;
00207
               /// Rayleigh length \f$ z_R = \pi \omega_0^2 / \lambda \f$
00208
               sunrealtype zr;
00209
               /// center of beam \f$ \Phi_0 \f$
               sunrealtype Ph0;
00210
00211
               /// length of beam \f$ \Phi_A \f$
00212
               sunrealtype PhA;
00213
               /// amplitude projection on TE-mode (z-axis)
00214
               sunrealtype A1:
00215
               /// amplitude projection on xv-plane
               sunrealtype A2;
00217
               /// wavelength \f$ \lambda \f$
00218
               sunrealtype lambda;
00219
00220 public:
               /// construction with default parameters
00221
               Gauss3D(vector<sunrealtype> dis_ = {0, 0, 0},
00222
00223
                              vector<sunrealtype> axis_ = {1, 0, 0}, sunrealtype Amp_ = 1.01,
00224
                               sunrealtype phip_ = 0,
                              // surrealtype pol_={0,0,1},
sunrealtype w0_ = 1e-5, sunrealtype zr_ = 4e-5,
sunrealtype Ph0_ = 2e-5, sunrealtype PhA_ = 0.45e-5);
00225
00226
00227
               /// function for the actual implementation in space
               void addToSpace(sunrealtype x, sunrealtype y, sunrealtype z,
00229
00230
                                              sunrealtype *pTo6Space) const;
00231
00232 public:
00233 };
```

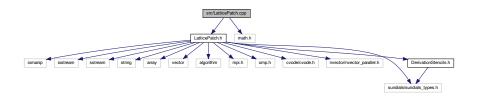
```
00235 /** @brief ICSetter class to initialize wave types with default parameters */
00236 class ICSetter {
00237 private:
00238
         /// container vector for plane waves in 1D
         vector<PlaneWave1D> planeWaves1D;
/// container vector for plane waves in 2D
         vector<PlaneWave2D> planeWaves2D;
00242
         /// container vector for plane waves in 3D
00243
         vector<PlaneWave3D> planeWaves3D;
00244
         /// container vector for Gaussian waves in 1D
00245
         vector<Gauss1D> gauss1Ds;
00246
         /// container vector for Gaussian waves in 2D
00247
         vector<Gauss2D> gauss2Ds;
00248
         /// container vector for Gaussian waves in 3D
00249
00250
         vector<Gauss3D> gauss3Ds;
00251 public:
00252
         /// function to set all coordinates to zero and then 'add' the field values
00253
         void eval(sunrealtype x, sunrealtype y, sunrealtype z,
00254
                      sunrealtype *pTo6Space);
00255
          /// function to fill the lattice space with initial field values
00256
         // of all field vector containers
00257
         void add(sunrealtype x, sunrealtype y, sunrealtype z, sunrealtype *pTo6Space); /// function to add plane waves in 1D to their container vector
00258
00259
         void addPlaneWave1D(vector<sunrealtype> k = {1, 0, 0},
00260
                                  vector<sunrealtype> p = \{0, 0,
00261
                                  vector<sunrealtype> phi = \{0, 0, 0\};
00262
         /// function to add plane waves in 2D to their container vector
         void addPlaneWave2D(vector<sunrealtype> k = \{1, 0, 0\}, vector<sunrealtype> p = \{0, 0, 1\},
00263
00264
         vector<sunrealtype> p - (0, 0, 1);
/// function to add plane waves in 3D to their container vector
00265
00266
         void addPlaneWave3D (vector<sunrealtype> k = \{1, 0, 0\}, vector<sunrealtype> p = \{0, 0, 1\},
00267
00268
         vector<sunrealtype> phi = {0, 0, 0});

/// function to add Gaussian waves in 1D to their container vector
void addGauss1D(vector<sunrealtype> k = {1, 0, 0},
00269
00270
00271
00272
                             vector<sunrealtype> p = \{0, 0, 1\},
                             vector<sunrealtype> xo = {0, 0, 0}, sunrealtype phig_ = 1.01,
vector<sunrealtype> phi = {0, 0, 0});
00273
00274
00275
         \ensuremath{///} function to add Gaussian waves in 2D to their container vector
         00276
00277
                             sunrealtype Amp_ = 1.01, sunrealtype phip_ = 0,
sunrealtype w0_ = 1e-5, sunrealtype zr_ = 4e-5,
00278
00279
00280
                             sunrealtype PhO_ = 2e-5, sunrealtype PhA_ = 0.45e-5);
         /// function to add Gaussian waves in 3D to their container vector
00281
         void addGauss3D (vector<sunrealtype> dis_ = {0, 0, 0}, vector<sunrealtype> axis_ = {1, 0, 0},
00282
00283
                             sunrealtype Amp = 1.01, sunrealtype phip = 0, sunrealtype w0 = 1e-5, sunrealtype zr = 4e-5,
00284
00285
00286
                             sunrealtype PhO_ = 2e-5, sunrealtype PhA_ = 0.45e-5);
00287 };
00288
```

6.10 src/LatticePatch.cpp File Reference

Costruction of the overall envelope lattice and the lattice patches.

```
#include "LatticePatch.h"
#include <math.h>
Include dependency graph for LatticePatch.cpp:
```



Functions

int generatePatchwork (const Lattice &envelopeLattice, LatticePatch &patchToMold, const int DLx, const int DLy, const int DLz)

Set up the patchwork.

void errorKill (const string &errorMessage)

Print a specific error message to stdout.

• int check retval (void *returnvalue, const char *funcname, int opt, int id)

6.10.1 Detailed Description

Costruction of the overall envelope lattice and the lattice patches.

Definition in file LatticePatch.cpp.

6.10.2 Function Documentation

6.10.2.1 check_retval()

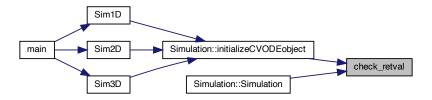
Check function return value. From CVode examples. opt == 0 means SUNDIALS function allocates memory so check if returned NULL pointer opt == 1 means SUNDIALS function returns an integer value so check if retval < 0 opt == 2 means function allocates memory so check if returned NULL pointer

Definition at line 982 of file LatticePatch.cpp.

```
00982
        int *retval = nullptr;
00983
00984
        /\star Check if SUNDIALS function returned NULL pointer - no memory allocated \star/
00985
00986
        if (opt == 0 && returnvalue == nullptr) {
00987
00988
                   "\nSUNDIALS_ERROR(%d): %s() failed - returned NULL pointer\n\n", id,
00989
                   funcname);
00990
          return (1);
00991
00992
00993
        /* Check if retval < 0 */
        else if (opt == 1) {
  retval = (int *)returnvalue;
00994
00995
          if (*retval < 0) {
   fprintf(stderr, "\nSUNDIALS_ERROR(%d): %s() failed with retval = %d\n\n",</pre>
00996
00997
00998
                      id, funcname, *retval);
00999
             return (1);
01000
01001
01002
        /\star Check if function returned NULL pointer - no memory allocated \star/
01003
01004
        else if (opt == 2 && returnvalue == nullptr) {
         fprintf(stderr,
01005
01006
                   "\nMEMORY_ERROR(%d): %s() failed - returned NULL pointer\n\n", id,
01007
01008
          return (1);
01009
01010
01011
        return (0);
01012 }
```

Referenced by Simulation::initializeCVODEobject(), and Simulation::Simulation().

Here is the caller graph for this function:



6.10.2.2 errorKill()

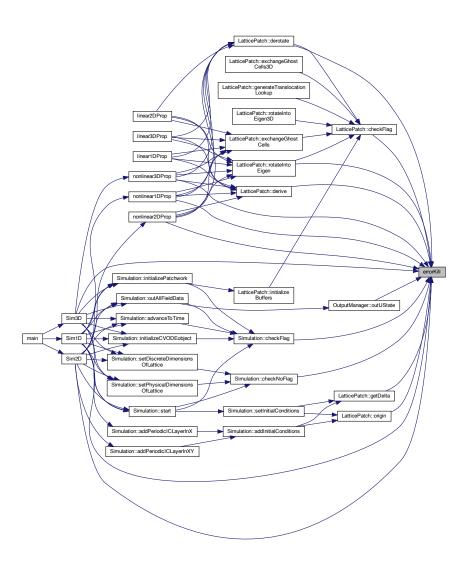
Print a specific error message to stdout.

```
Definition at line 969 of file LatticePatch.cpp.
```

```
00969
00970 cerr w endl w "Error: " w errorMessage w " Aborting..." w endl;
00971 MPI_Abort(MPI_COMM_WORLD, 1);
00972 return;
00973 }
```

Referenced by LatticePatch::checkFlag(), Simulation::checkFlag(), Simulation::checkNoFlag(), LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::getDelta(), nonlinear1DProp(), nonlinear2DProp(), nonlinear3DProp(), LatticePatch::origin(), OutputManager::outUState(), LatticePatch::rotateIntoEigen(), Sim1D(), Sim2D(), and Sim3D().

Here is the caller graph for this function:



6.10.2.3 generatePatchwork()

Set up the patchwork.

friend function for creating the patchwork slicing of the overall lattice

```
Definition at line 109 of file LatticePatch.cpp.
```

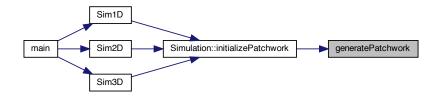
// Retrieve the ghost layer depth

{

```
const int gLW = envelopeLattice.get_ghostLayerWidth();
00113
         // Retrieve the data point dimension
00114
         const int dPD = envelopeLattice.get_dataPointDimension();
00115
         // MPI process/patch
00116
        const int my_prc = envelopeLattice.my_prc;
00117
         // Determine thicknes of the slice
        const sunindextype tot_NOXP = envelopeLattice.get_tot_nx(); // total points of lattice
00118
00119
         const sunindextype tot_NOYP = envelopeLattice.get_tot_ny();
00120
         const sunindextype tot_NOZP = envelopeLattice.get_tot_nz();
00121
         // position of the patch in the lattice of patches -> process associated to
        // position
00122
        const sunindextype LIx = my_prc % DLx;
00123
        const sunindextype LIy = (my_prc / DLx) % DLy;
const sunindextype LIz = (my_prc / DLx) / DLy;
00124
00125
00126
         // Determine the number of points in the patch and first absolute points in
00127
         // each dimension
        const sunindextype local_NOXP = tot_NOXP / DLx;
00128
        const sunindextype local_NOYP = tot_NOYP / DLy;
00129
        const sunindextype local_NOZP = tot_NOZP / DLz;
00130
         // absolute positions of the first point in each dimension
00131
        const sunindextype firstXPoint = local_NOXP * LIX;
const sunindextype firstYPoint = local_NOYP * LIY;
00132
00133
        const sunindextype firstZPoint = local_NOZP * LIZ;
00134
00135
        // total number of points in the patch
const sunindextype local_NODP = dPD * local_NOXP * local_NOYP * local_NOZP;
00136
00137
00138
         // Set patch up with above derived quantities
00139
         // Experiment: Resolution can be adapted for each process/patch
00140
        const int Scaler=4; // Better hand over as parameter via `initializePatchwork`
if(my_prc==0) {patchToMold.dx=envelopeLattice.get_dx();}
00141
00142
00143
         else if(my_prc==1) {patchToMold.dx=envelopeLattice.get_dx()*Scaler;}
00144
        else{errorKill("Only do this resolution barrier test with 2 processes.");}
00145
        patchToMold.dx = envelopeLattice.get_dx();
patchToMold.dy = envelopeLattice.get_dy();
00146
00147
        patchToMold.dz = envelopeLattice.get_dz();
00148
        patchToMold.x0 = firstXPoint * patchToMold.dx;
00150
        patchToMold.y0 = firstYPoint * patchToMold.dy;
00151
        patchToMold.z0 = firstZPoint * patchToMold.dz;
        patchToMold.LIx = LIx;
patchToMold.LIy = LIy;
00152
00153
        patchToMold.LIz = LIz;
00154
00155
        patchToMold.nx = local_NOXP;
        patchToMold.ny = local_NOYP;
00156
00157
        patchToMold.nz = local_NOZP;
00158
        patchToMold.lx = patchToMold.nx * patchToMold.dx;
        patchToMold.ly = patchToMold.ny * patchToMold.dy;
patchToMold.lz = patchToMold.nz * patchToMold.dz;
00159
00160
00161
         /* // Check name of lattice communicator
00162
         char lattice_comm_name[MPI_MAX_OBJECT_NAME];
         int lattice_namelen;
00163
        {\tt MPI\_Comm\_get\_name\,(envelopeLattice.comm,\ lattice\_comm\_name,\ \&lattice\_namelen)\,;}
00164
00165
         cout«"envelopeLattice.comm gives "« lattice_comm_name « endl;
00166
        /\star Create and allocate memory for parallel vectors with defined local and
00167
         * global lenghts *
00168
00169
         * (-> CVode problem sizes Nlocal and N)
00170
          \star for field data and temporal derivatives and set extra pointers to them \star/
        patchToMold.u =
00171
             00172
00173
00174
        patchToMold.uData = NV_DATA_P (patchToMold.u);
00175
        patchToMold.du =
00176
             N_VNew_Parallel(envelopeLattice.comm, local_NODP,
        envelopeLattice.get_tot_noDP(), envelopeLattice.sunctx);
patchToMold.duData = NV_DATA_P(patchToMold.du);
00177
00178
        // Allocate space for auxiliary uAux so that the lattice and all possible // directions of ghost Layers fit
00179
00180
00181
        const int s1 = patchToMold.nx, s2 = patchToMold.ny, s3 = patchToMold.nz;
        const int s_min = min(s1, min(s2, s3));
patchToMold.uAux.resize(s1 * s2 * s3 / s_min * (s_min + 2 * gLW) * dPD);
00182
00183
00184
         patchToMold.uAuxData = &patchToMold.uAux[0];
        patchToMold.envelopeLattice = &envelopeLattice;
// Set patch "name" to process number -> only for debugging
00185
00186
        // patchToMold.ID=my_prc;
00187
00188
         // set flag
00189
        patchToMold.statusFlags = FLatticePatchSetUp;
00190
         patchToMold.generateTranslocationLookup();
00191
         return 0:
00192 }
```

Referenced by Simulation::initializePatchwork().

Here is the caller graph for this function:



6.11 LatticePatch.cpp

```
Go to the documentation of this file.
```

```
00002 /// @file LatticePatch.cpp
00003 /// @brief Costruction of the overall envelope lattice and the lattice patches
00005
00006 #include "LatticePatch.h"
00007
00008 #include <math.h>
00009
00014 /// Initialize the cartesian communicator
00015 void Lattice::initializeCommunicator(const int nx, const int ny,
00016
             const int nz, const bool per) {
       const int dims[3] = {nz, ny, nx};
const int periods[3] = {static_cast<int>(per), static_cast<int>(per),
00017
00018
                         static_cast<int>(per) };
00020
        // Create the cartesian communicator for MPI_COMM_WORLD
00021
       MPI_Cart_create(MPI_COMM_WORLD, 3, dims, periods, 1, &comm);
00022
       // Set MPI variables of the lattice
00023
       \label{eq:mpi_comm_size} \texttt{MPI\_Comm\_size(comm, \&(n\_prc));}
       MPI_Comm_rank(comm, &(my_prc));
// Associate name to the communicator to identify it -> for debugging and
00024
00025
00026
       // nicer error messages
00027
        constexpr char lattice_comm_name[] = "Lattice";
00028
       MPI_Comm_set_name(comm, lattice_comm_name);
00029
00030
       \ensuremath{//} Test if process naming is the same for both communicators
00031
00033
       MPI_Comm_rank (MPI_COMM_WORLD, &MYPRC);
00034
       cout«"\r"«my_prc«"\t"«MYPRC«endl;
00035
00036 }
00037
00038 /// Construct the lattice and set the stencil order
00039 Lattice::Lattice(const int StO) : stencilOrder(StO),
00040
         ghostLayerWidth(StO/2+1) {
00041
       statusFlags = 0;
00042 }
00043
00044 /// Set the number of points in each dimension of the lattice
00045 void Lattice::setDiscreteDimensions(const sunindextype _nx,
00046
             const sunindextype _ny, const sunindextype _nz) {
00047
       \ensuremath{//} copy the given data for number of points
       tot_nx = _nx;
tot_ny = _ny;
tot_nz = _nz;
00048
00049
00050
00051
       // compute the resulting number of points and datapoints
00052
        tot_noP = tot_nx * tot_ny * tot_nz;
00053
       tot_noDP = dataPointDimension * tot_noP;
00054
       \ensuremath{//} compute the new Delta, the physical resolution
       dx = tot_lx / tot_nx;
dy = tot_ly / tot_ny;
00055
00056
       dz = tot_lz / tot_nz;
00057
00058 }
```

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```
00059
00060 /// Set the physical size of the lattice
00061 void Lattice::setPhysicalDimensions(const sunrealtype _lx,
00062
             const sunrealtype _ly, const sunrealtype _lz) {
       tot_lx = _lx;
tot_ly = _ly;
tot_lz = _lz;
00063
00064
00066
       // calculate physical distance between points
       dx = tot_lx / tot_nx;
dy = tot_ly / tot_ny;
dz = tot_lz / tot_nz;
00067
00068
00069
00070
       statusFlags |= FLatticeDimensionSet;
00071 }
00072
00076
00077 /// Construct the lattice patch
00078 LatticePatch::LatticePatch()
00079
       // set default origin coordinates to (0,0,0)
08000
        x0 = y0 = z0 = 0;
        // set default position in Lattice-Patchwork to (0,0,0)
00081
00082
        LIx = LIy = LIz = 0;
00083
        // set default physical lentgth for lattice patch to (0,0,0)
        1x = 1y = 1z = 0;
00084
        // set default discrete length for lattice patch to (0,1,1)
00085
00086
        /\star This is done in this manner as even in 1D simulations require a 1 point
00087
        * width */
00088
        nx = 0:
        ny = nz = 1;
00089
00090
00091
       // u is not initialized as it wouldn't make any sense before the dimensions
00092
        // are set idem for the enveloping lattice
00093
00094
       // set default statusFlags to non set
00095
       statusFlags = 0;
00097
00098 \ensuremath{///} Destruct the patch and thereby destroy the NVectors
00099 LatticePatch::~LatticePatch() {
00100
       // Deallocate memory for solution vector
00101
        if (statusFlags & FLatticePatchSetUp) {
00102
         // Destroy data vectors
          N_VDestroy_Parallel(u);
00103
00104
          N_VDestroy_Parallel(du);
00105
       }
00106 }
00107
00108 /// Set up the patchwork
00109 int generatePatchwork(const Lattice &envelopeLattice, LatticePatch &patchToMold,
00110
                            const int DLx, const int DLy, const int DLz) {
00111
        // Retrieve the ghost layer depth
00112
        const int gLW = envelopeLattice.get_ghostLayerWidth();
00113
        // Retrieve the data point dimension
        const int dPD = envelopeLattice.get_dataPointDimension();
00114
        // MPI process/patch
00116
        const int my_prc = envelopeLattice.my_prc;
        // Determine thicknes of the slice
00117
00118
        const sunindextype tot_NOXP = envelopeLattice.get_tot_nx(); // total points of lattice
        const sunindextype tot_NOYP = envelopeLattice.get_tot_ny();
00119
        const sunindextype tot_NOZP = envelopeLattice.get_tot_nz();
00120
00121
        // position of the patch in the lattice of patches -> process associated to
        // position
00122
00123
        const sunindextype LIx = my_prc % DLx;
        const sunindextype LIy = (my_prc / DLx) % DLy; const sunindextype LIz = (my_prc / DLx) / DLy;
00124
00125
        \ensuremath{//} Determine the number of points in the patch and first absolute points in
00126
00127
        // each dimension
00128
        const sunindextype local_NOXP = tot_NOXP / DLx;
        const sunindextype local_NOYP = tot_NOYP / DLy;
const sunindextype local_NOZP = tot_NOZP / DLz;
00129
00130
        \ensuremath{//} absolute positions of the first point in each dimension
00131
00132
        const sunindextype firstXPoint = local NOXP * LIx;
        const sunindextype firstYPoint = local_NOYP * LIy;
00133
00134
        const sunindextype firstZPoint = local_NOZP * LIZ;
        // total number of points in the patch
00135
00136
        const sunindextype local_NODP = dPD * local_NOXP * local_NOYP * local_NOZP;
00137
00138
        // Set patch up with above derived quantities
00139
        // Experiment: Resolution can be adapted for each process/patch
00140
        const int Scaler=4; // Better hand over as parameter via `initializePatchwork`
00141
00142
        if (my_prc==0) {patchToMold.dx=envelopeLattice.get_dx();}
00143
        \verb|else if (my_prc==1) {patchToMold.dx=envelopeLattice.get_dx() *Scaler;}|
        else{errorKill("Only do this resolution barrier test with 2 processes.");}
00144
00145
```

```
patchToMold.dx = envelopeLattice.get_dx();
        patchToMold.dy = envelopeLattice.get_dy();
00147
        patchToMold.dz = envelopeLattice.get_dz();
00148
        patchToMold.x0 = firstXPoint * patchToMold.dx;
patchToMold.y0 = firstYPoint * patchToMold.dy;
00149
00150
        patchToMold.z0 = firstZPoint * patchToMold.dz;
00151
        patchToMold.LIx = LIx;
00152
00153
        patchToMold.LIy = LIy;
00154
        patchToMold.LIz = LIz;
00155
        patchToMold.nx = local NOXP;
        patchToMold.ny = local_NOYP;
00156
00157
        patchToMold.nz = local NOZP;
00158
        patchToMold.lx = patchToMold.nx * patchToMold.dx;
00159
        patchToMold.ly = patchToMold.ny * patchToMold.dy;
00160
        patchToMold.lz = patchToMold.nz * patchToMold.dz;
00161
        /* // Check name of lattice communicator
00162
        char lattice_comm_name[MPI_MAX_OBJECT_NAME];
00163
        int lattice namelen;
00164
        MPI_Comm_get_name(envelopeLattice.comm, lattice_comm_name, &lattice_namelen);
00165
        cout«"envelopeLattice.comm gives "« lattice_comm_name « endl;
00166
00167
        /* Create and allocate memory for parallel vectors with defined local and
00168
         * global lenghts *
        * (-> CVode problem sizes Nlocal and N)
00169
00170
         \star for field data and temporal derivatives and set extra pointers to them \star/
00171
        patchToMold.u =
00172
            N_VNew_Parallel(envelopeLattice.comm, local_NODP,
00173
                              envelopeLattice.get_tot_noDP(), envelopeLattice.sunctx);
        patchToMold.uData = NV_DATA_P (patchToMold.u);
00174
        patchToMold.du =
00175
00176
            N VNew Parallel (envelopeLattice.comm, local NODP,
00177
                             envelopeLattice.get_tot_noDP(), envelopeLattice.sunctx);
00178
        patchToMold.duData = NV_DATA_P(patchToMold.du);
00179
        // Allocate space for auxiliary uAux so that the lattice and all possible
        // directions of ghost Layers fit const int s1 = patchToMold.nx, s2 = patchToMold.ny, s3 = patchToMold.nz;
00180
00181
        const int s_min = min(s1, min(s2, s3));
patchToMold.uAux.resize(s1 * s2 * s3 / s_min * (s_min + 2 * gLW) * dPD);
00182
00183
00184
        patchToMold.uAuxData = &patchToMold.uAux[0];
        patchToMold.envelopeLattice = &envelopeLattice;
// Set patch "name" to process number -> only for debugging
// patchToMold.ID=my_prc;
00185
00186
00187
        // set flag
00188
00189
        patchToMold.statusFlags = FLatticePatchSetUp;
00190
        patchToMold.generateTranslocationLookup();
00191
        return 0;
00192 }
00193
00194 /// Return the discrete size of the patch: number of lattice patch points in
00195 /// specified dimension
00196 int LatticePatch::discreteSize(int dir) const {
00197
       switch (dir) {
00198
        case 0:
00199
         return nx * ny * nz;
00200
       case 1:
00201
         return nx;
00202
        case 2:
00203
         return ny;
00204
        case 3:
          return nz;
00205
        // case 4: return uAux.size(); // for debugging
00206
00207
       default:
00208
         return -1;
00209
00210 }
00211
00212 /// Return the physical origin of the patch in a dimension
00213 sunrealtype LatticePatch::origin(const int dir) const {
00214
       switch (dir) {
00215
        case 1:
00216
          return x0;
00217
        case 2:
00218
         return y0;
00219
        case 3:
00220
          return z0;
00221
00222
        errorKill("LatticePatch::origin function called with wrong dir parameter");
00223
          return -1;
00224
       }
00225 }
00226
00227 /// Return the distance between points in the patch in a dimension
00228 sunrealtype LatticePatch::getDelta(const int dir) const {
00229
        switch (dir) {
00230
        case 1:
00231
         return dx;
00232
       case 2:
```

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```
00233
           return dy;
00234
         case 3:
00235
           return dz;
        default:
00236
          errorKill(
00237
00238
                "LatticePatch::getDelta function called with wrong dir parameter");
00239
           return -1;
00240
00241 }
00242
00243 /** To avoid cache misses:
00245 * and same for left and right ghost layers to space */
00246 void LatticePatch::generateTranslocationLookup() {
00247
        // Check that the lattice has been set up
00248
         checkFlag(FLatticeDimensionSet);
         // lenghts for auxilliary layers, including ghost layers
00249
         const int gLW = envelopeLattice->get_ghostLayerWidth();
00250
         const int mx = nx + 2 * gLW;
00251
         const int my = ny + 2 * gLW;
00252
00253
         const int mz = nz + 2 * gLW;
00254
         // sizes for lookup vectors
         // generate u->uAux
00255
00256
        uTox.resize(nx * ny * nz);
uToy.resize(nx * ny * nz);
00257
         uToz.resize(nx * ny * nz);
00258
00259
         // generate uAux->u with length including halo
00260
         xTou.resize(mx * ny * nz);
00261
         yTou.resize(nx * my * nz);
         zTou.resize(nx * ny * mz);
00262
00263
         // variables for cartesian position in the 3D discrete lattice
         int px = 0, py = 0, pz = 0; for (unsigned int i = 0; i < uToy.size(); i++) { // loop over all points in the patch
00264
00265
00266
           // calulate cartesian coordinates
           px = i % nx;
py = (i / nx) % ny;
pz = (i / nx) / ny;
// fill lookups extended by halos (useful for y and z direction)
00267
00268
00269
00270
00271
           uTox[i] = (px + gLW) + py * mx +
           pz * mx * ny; // unroll (de-flatten) cartesian dimension xTou[px + py * mx + pz * mx * ny] =
00272
00273
               i; // match cartesian point to u location
00274
           uToy[i] = (py + gLW) + pz * my + px * my * nz;
yTou[py + pz * my + px * my * nz] = i;
uToz[i] = (pz + gLW) + px * mz + py * mz * nx;
zTou[pz + px * mz + py * mz * nx] = i;
00275
00276
00277
00278
00279
         // same for ghost layer lookup tables
00280
         lgcTox.resize(gLW * ny * nz);
rgcTox.resize(gLW * ny * nz);
00281
00282
00283
         for (unsigned int i = 0; i < lgcTox.size(); i++) {</pre>
00284
          px = i % gLW;
          px = 1 ° gam,

py = (i / gLW) % ny;

pz = (i / gLW) / ny;

lgcTox[i] = px + py * mx + pz * mx * ny;

rgcTox[i] = px + nx + gLW + py * mx + pz * mx * ny;
00285
00286
00287
00288
00289
00290
         lgcToy.resize(gLW * nx * nz);
00291
         rgcToy.resize(gLW * nx * nz);
00292
         for (unsigned int i = 0; i < lgcToy.size(); i++) {</pre>
00293
          px = i % nx;
           py = (i / nx) % gLW;
00294
           pz = (i / nx) / gLW;
00295
00296
           lgcToy[i] = py + pz * my + px * my * nz;
00297
           rgcToy[i] = py + ny + gLW + pz * my + px * my * nz;
00298
00299
         lgcToz.resize(gLW * nx * ny);
         rgcToz.resize(gLW * nx * ny);
00300
00301
         for (unsigned int i = 0; i < lqcToz.size(); i++) {</pre>
00302
          px = i % nx;
           py = (i / nx) % ny;
pz = (i / nx) / ny;
00303
00304
           lgcToz[i] = pz + px * mz + py * mz * nx;
rgcToz[i] = pz + nz + gLW + px * mz + py * mz * nx;
00305
00306
00307
00308
        statusFlags |= TranslocationLookupSetUp;
00309 }
00310
00311 /** Rotate into eigenraum along R matrices of paper using below rotation
00312 * functions
00313 * -> uAuxData gets the rotated left-halo-, inner-patch-, right-halo-data */
00314 void LatticePatch::rotateIntoEigen(const int dir)
00315
        // Check that the lattice, ghost layers as well as the translocation lookups
00316
         // have been set up;
00317
         checkFlag(FLatticePatchSetUp);
         checkFlag(TranslocationLookupSetUp);
00318
00319
        checkFlag(GhostLayersInitialized); // this check is only after call to
```

```
// exchange ghost cells
         switch (dir) {
00321
         case 1:
00322
00323
         rotateToX(uAuxData, gCLData, lgcTox);
           rotateToX(uAuxData, uData, uTox);
rotateToX(uAuxData, gCRData, rgcTox);
00324
00325
00326
           break;
00327
         case 2:
00328
         rotateToY(uAuxData, gCLData, lgcToy);
00329
           rotateToY(uAuxData, uData, uToy);
00330
           rotateToY(uAuxData, gCRData, rgcToy);
00331
           break:
00332
        case 3:
         rotateToZ(uAuxData, gCLData, lgcToz);
00333
00334
           rotateToZ(uAuxData, uData, uToz);
00335
           rotateToZ(uAuxData, gCRData, rgcToz);
00336
           break:
00337
         default:
         errorKill("Tried to rotate into the wrong direction");
00338
00339
           break;
00340
00341 }
00342
00343 /// Same as 'rotateIntoEigen' but for neighborhood 3D halo buffers
00344 void LatticePatch::rotateIntoEigen3D() {
00345 checkFlag(FLatticePatchSetUp);
00346
         checkFlag(TranslocationLookupSetUp);
00347
         checkFlag(GhostLayersInitialized);
00348
        rotateToX(uAuxData, gCLData, lgcTox);
        rotateToX(uAuxData, uData, uTox);
00349
        rotateToX(uAuxData, gCRData, rgcTox);
rotateToY(uAuxData, gCBData, lgcToy);
00350
00351
00352
        rotateToY(uAuxData, uData, uToy);
00353
        rotateToY(uAuxData, gCTData, rgcToy);
00354
        rotateToZ(uAuxData, gCFData, lgcToz);
00355
        rotateToZ(uAuxData, uData, uToz);
00356
        rotateToZ(uAuxData, gCAData, rgcToz);
00357 }
00358
00359 /// Rotate halo and inner-patch data vectors with rotation matrix Rx into
00360 /// eigenspace of Z matrix and write to auxiliary vector
00361 inline void LatticePatch::rotateToX(sunrealtype *outArray,
00362
                                               const sunrealtype *inArray,
                                               const vector<int> &lookup) {
00363
00364
        int ii = 0, target = 0;
00365 #pragma ivdep
00366 #pragma omp simd // safelen(6) - also good
00367 #pragma distribute_point
         for (unsigned int i = 0; i < lookup.size(); i++) {</pre>
00368
00369
          // get correct u-vector and spatial indices along previously defined lookup
           // tables
00371
           target = envelopeLattice->get_dataPointDimension() * lookup[i];
00372
           ii = envelopeLattice->get_dataPointDimension() * i;
           outArray[target + 0] = -inArray[1 + ii] + inArray[5 + ii];
outArray[target + 1] = inArray[2 + ii] + inArray[4 + ii];
outArray[target + 2] = inArray[1 + ii] + inArray[5 + ii];
00373
00374
00375
00376
           outArray[target + 3] = -inArray[2 + ii] + inArray[4 + ii];
00377
           outArray[target + 4] = inArray[3 + ii];
           outArray[target + 5] = inArray[ii];
00378
00379
00380 }
00381
00382 /// Rotate halo and inner-patch data vectors with rotation matrix Ry into
00383 /// eigenspace of Z matrix and write to auxiliary vector
00384 inline void LatticePatch::rotateToY(sunrealtype *outArray,
00385
                                               const sunrealtype *inArray,
00386
                                               const vector<int> &lookup) {
00387
        int ii = 0, target = 0;
00388 #pragma ivdep
00389 #pragma omp simd // safelen(6)
00390 #pragma distribute_point
         for (unsigned int i = 0; i < lookup.size(); i++) {</pre>
00391
          target = envelopeLattice->get_dataPointDimension() * lookup[i];
ii = envelopeLattice->get_dataPointDimension() * i;
00392
00393
           outArray[target + 0] = inArray[ii] + inArray[5 + ii];
outArray[target + 1] = -inArray[2 + ii] + inArray[3 + ii];
00394
00395
00396
           outArray[target + 2] = -inArray[ii] + inArray[5 + ii];
           outArray[target + 3] = inArray[2 + ii] + inArray[3 + ii];
outArray[target + 4] = inArray[4 + ii];
outArray[target + 5] = inArray[1 + ii];
00397
00398
00399
00400
00401 }
00402
00403 /\!/\! Rotate halo and inner-patch data vectors with rotation matrix Rz into
00404 /// eigenspace of {\tt Z} matrix and write to auxiliary vector
00405 inline void LatticePatch::rotateToZ(sunrealtype *outArray
00406
                                               const sunrealtype *inArray.
```

```
00407
                                                     const vector<int> &lookup) {
         int ii = 0, target = 0;
00408
00409 #pragma ivdep
00410 \#pragma omp simd // safelen(6)
target = envelopeLattice->get_dataPointDimension() * lookup[i];
00414
            ii = envelopeLattice->get_dataPointDimension() * i;
            outArray[target + 0] = -inArray[ii] + inArray[4 + ii];
outArray[target + 1] = inArray[1 + ii] + inArray[3 + ii];
outArray[target + 2] = inArray[ii] + inArray[4 + ii];
outArray[target + 3] = -inArray[1 + ii] + inArray[3 + ii];
outArray[target + 4] = inArray[5 + ii];
00415
00416
00417
00418
00419
            outArray[target + 5] = inArray[2 + ii];
00420
00421
00422 }
00423
00424 /// Derotate uAux with transposed rotation matrices and write to derivative
00425 /// buffer -- normalization is done here by the factor 1/2
00426 void LatticePatch::derotate(int dir, sunrealtype *buffOut) {
         // Check that the lattice as well as the translocation lookups have been set
00427
          // up;
00428
00429
          checkFlag(FLatticePatchSetUp);
00430
          checkFlag(TranslocationLookupSetUp);
00431
          const int dPD = envelopeLattice->get_dataPointDimension();
          const int gLW = envelopeLattice->get_ghostLayerWidth();
00433
          const int uSize = discreteSize();
00434
          int ii = 0, target = 0;
00435
          switch (dir) {
00436
         case 1:
00437 #pragma ivdep
00438 #pragma omp simd // safelen(6) - also good
00439 #pragma distribute_point
00440
            for (int i = 0; i < uSize; i++) {</pre>
00441
               \ensuremath{//} get correct indices in u and rotation space
00442
               target = dPD * i;
               ii = dPD * (uTox[i] - gLW);
00443
               buffOut[target + 0] = uAux[5 + ii];
00445
               buffOut[target + 1] = (-uAux[ii] + uAux[2 + ii]) / 2.;
              buffout[target + 1] = (uAux[11] + uAux[2 + 11]) / 2.;
buffOut[target + 2] = (uAux[1 + ii] - uAux[3 + ii]) / 2.;
buffOut[target + 3] = uAux[4 + ii];
buffOut[target + 4] = (uAux[1 + ii] + uAux[3 + ii]) / 2.;
buffOut[target + 5] = (uAux[ii] + uAux[2 + ii]) / 2.;
00446
00447
00448
00449
00450
00451
            break;
00452
          case 2:
00453 #pragma omp simd // safelen(6)
00454 #pragma distribute_point
            for (int i = 0; i < uSize; i++) {
00455
              target = dPD * i;
00456
00457
               ii :
                    = dPD * (uToy[i] - gLW);
00458
               buffOut[target + 0] = (uAux[ii] - uAux[2 + ii]) / 2.;
00459
               buffOut[target + 1] = uAux[5 + ii];
              buffout[target + 2] = (-uAux[1 + ii] + uAux[3 + ii]) / 2.;
buffout[target + 3] = (uAux[1 + ii] + uAux[3 + ii]) / 2.;
buffout[target + 4] = uAux[4 + ii];
buffout[target + 5] = (uAux[ii] + uAux[2 + ii]) / 2.;
00460
00461
00462
00463
00464
00465
            break;
00466
          case 3:
00467 #pragma omp simd // safelen(6)
00468 #pragma distribute_point
            for (int i = 0; i < uSize; i++) {
               target = dPD * i;
00470
00471
               ii = dPD * (uToz[i] - gLW);
              buffOut[target + 0] = (-uAux[ii] + uAux[2 + ii]) / 2.;
buffOut[target + 1] = (uAux[1 + ii] - uAux[3 + ii]) / 2.;
buffOut[target + 2] = uAux[5 + ii];
00472
00473
00474
               buffOut[target + 3] = (uAux[1 + ii] + uAux[3 + ii]) / 2.;
00475
               buffOut[target + 4] = (uAux[ii] + uAux[2 + ii]) / 2.;
00476
00477
               buffOut[target + 5] = uAux[4 + ii];
00478
00479
            break;
00480
          default:
00481
           errorKill("Tried to derotate from the wrong direction");
00482
00483
00484 }
00485
00486 /// Create buffers to save derivative values, optimizing computational load
00487 void LatticePatch::initializeBuffers() {
          // Check that the lattice has been set up
          checkFlag(FLatticeDimensionSet);
00489
00490
          const int dPD = envelopeLattice->get_dataPointDimension();
         buffX.resize(nx * ny * nz * dPD);
buffY.resize(nx * ny * nz * dPD);
buffZ.resize(nx * ny * nz * dPD);
00491
00492
00493
```

```
// Set pointers used for propagation functions
        buffData[0] = &buffX[0];
buffData[1] = &buffY[0];
00495
00496
        buffData[2] = &buffZ[0];
00497
00498
        statusFlags |= BuffersInitialized;
00499 }
00500
00501 /// Perform the ghost cell exchange in a specified direction
00502 void LatticePatch::exchangeGhostCells(const int dir) {
00503
       // Check that the lattice has been set up
00504
        checkFlag(FLatticeDimensionSet);
00505
        checkFlag(FLatticePatchSetUp);
00506
        // Variables to per dimension calculate the halo indices, and distance to
00507
        // other side halo boundary
        int mx = 1, my = 1, mz = 1, distToRight = 1;
const int gLW = envelopeLattice->get_ghostLayerWidth();
00508
00509
00510
        // In the chosen direction m is set to ghost layer width while the others
        // remain to form the plane
00511
00512
        switch (dir) {
00513
        case 1:
00514
          mx = gLW;
          my = ny;

mz = nz;
00515
00516
          distToRight = (nx - gLW);
00517
00518
          break;
00519
        case 2:
00520
          mx = nx;
00521
          my = gLW;
00522
          mz = nz:
00523
          distToRight = nx * (ny - gLW);
00524
          break:
00525
        case 3:
00526
         mx = nx;
00527
          my = ny;
          mz = gLW;
00528
          distToRight = nx * ny * (nz - qLW);
00529
00530
          break;
00531
00532
        // total number of exchanged points
00533
        const int dPD = envelopeLattice->get_dataPointDimension();
00534
        const int exchangeSize = mx * my * mz * dPD;
        \ensuremath{//} provide size of the halos for ghost cells
00535
00536
        ghostCellLeft.resize(exchangeSize);
00537
        ghostCellRight.resize(ghostCellLeft.size());
00538
        ghostCellLeftToSend.resize(ghostCellLeft.size());
00539
        ghostCellRightToSend.resize(ghostCellLeft.size());
        gCLData = &ghostCellLeft[0];
gCRData = &ghostCellRight[0];
00540
00541
00542
        statusFlags |= GhostLayersInitialized;
00543
00544
        // Initialize running index li for the halo buffers, and index ui of uData for
00545
        // data transfer
00546
        int li = 0, ui = 0;
00547
00548 // #pragma omp parallel for reduction(+:ui) reduction(+:li) -> don't probably
00549 // bad idea to parallelize ghost cell exchange Loop over to be copied points in
00550 // z and y direction
00551 #pragma distribute_point
00552
        for (int iz = 0; iz < mz; iz++) {</pre>
00553
          for (int iy = 0; iy < my; iy++) {
            // uData vector start index of halo data to be transferred
00554
            // with each z-step add the whole xy-plane and with y-step the x-range ->
00555
            // iterate all x-ranges
00557
            ui = (iz * nx * ny + iy * nx) * dPD;
00558
            // copy left halo data from uData to buffer, transfer size is given by
00559
            // x-length (not x-range) perhaps faster but more fragile C lib copy
            // operation (contained in cstring header)
00560
00561
            memcpy(&ghostCellLeftToSend[li],
00562
                    &uData[ui],
00563
00564
                    sizeof(sunrealtype)*mx*dPD);
00565
            // increase ui by the distance to vis-a-vis boundary and copy right halo
00566
            data to buffer ui+=distToRight*dPD; memcpy(&ghostCellRightToSend[li],
00567
                    &uData[ui].
00568
                    sizeof(sunrealtype)*mx*dPD);
00569
            // perhaps more safe but slower copy operation (contained in algorithm // header) performance highly system dependent
00570
00571
            copy(&uData[ui], &uData[ui + mx * dPD], &ghostCellLeftToSend[li]);
00572
00573
            ui += distToRight * dPD;
00574
            copy(&uData[ui], &uData[ui + mx * dPD], &ghostCellRightToSend[li]);
00576
             // increase halo index by transferred items per y-iteration step
00577
            // (x-length)
00578
            li += mx * dPD;
00579
          }
00580
       1
```

```
00581
00582
        /\star Send and receive the data to and from neighboring latticePatches \star/
00583
        // Adjust direction to cartesian communicator
        int dim = 2; // default for dir==1
if (dir == 2) {
00584
00585
00586
          dim = 1:
        } else if (dir == 3) {
00588
          dim = 0;
00589
00590
        int rank_source = 0, rank_dest = 0;
        MPI_Cart_shift(envelopeLattice->comm, dim, -1, &rank_source,
00591
00592
                        &rank_dest); // s.t. rank_dest is left & v.v.
00593
00594
        // nonblocking Isend/Irecv
00595
00596
        MPI_Request requests[4];
        MPI_Irecv(&ghostCellRight[0], exchangeSize, MPI_SUNREALTYPE, rank_source, 1,
00597
        envelopeLattice->comm, &requests[0]);
00598
        MPI_Isend(&ghostCellLeftToSend[0], exchangeSize, MPI_SUNREALTYPE, rank_dest,
00599
00600
         1, envelopeLattice->comm, &requests[1]);
00601
        MPI_Irecv(&ghostCellLeft[0], exchangeSize, MPI_SUNREALTYPE, rank_dest, 2,
00602
        envelopeLattice->comm, &requests[2]);
        MPI_Isend(&ghostCellRightToSend[0], exchangeSize, MPI_SUNREALTYPE,
rank_source, 2, envelopeLattice->comm, &requests[3]);
00603
00604
00605
        MPI_Waitall(4, requests, MPI_STATUS_IGNORE);
00606
00607
00608
        // blocking Sendrecv:
00609
00610
        MPI_Sendrecv(&qhostCellLeftToSend[0], exchangeSize, MPI_SUNREALTYPE,
                       rank_dest, 1, &ghostCellRight[0], exchangeSize, MFI_SUNREALTYPE, rank_source, 1, envelopeLattice->comm, MFI_STATUS_IGNORE);
00611
00612
        MPI_Sendrecv(&ghostCellRightToSend[0], exchangeSize, MPI_SUNREALTYPE,
00613
00614
                      rank_source, 2, &ghostCellLeft[0], exchangeSize, MPI_SUNREALTYPE,
00615
                       rank_dest, 2, envelopeLattice->comm, MPI_STATUS_IGNORE);
00616
00617 }
00618
00619 /// Exchange ghost cells with a neighborhood collective operation
00620 void LatticePatch::exchangeGhostCells3D() {
00621
        // Check that the lattice has been set up
00622
        checkFlag(FLatticeDimensionSet);
00623
        // ghostlayerwidth
00624
        const int gLW = envelopeLattice->get_ghostLayerWidth();
        // datapoint dimension
00626
        const int dPD = envelopeLattice->get_dataPointDimension();
        // total number of exchanged points per halo const int n = nx; // only cubic patches allowed -> use general length n
00627
00628
        const int exchangeSize = n * n * gLW * dPD;

// Give ghostCells the total size of the ghost layers (the six halos)
00629
00630
        const int tot_exchangeSize = 6 * exchangeSize;
00631
00632
        ghostCells.resize(tot_exchangeSize);
00633
        ghostCellsToSend.resize(ghostCells.size());
        // ghost cell data in all directions: left,right,bottom,top,front,abaft; but // with MPI dim order "lefts" are the first receivers and "rights" are the
00634
00635
        // first senders -> see buffer creator below
00636
        gCFData = &ghostCells[0];
        gCAData = &ghostCells[exchangeSize];
00638
        gCBData = &ghostCells[2 * exchangeSize];
00639
00640
        gCTData = &ghostCells[3 * exchangeSize];
00641
        gCLData = &ghostCells[4 * exchangeSize];
        gCRData = &ghostCells[5 * exchangeSize];
00642
00643
        statusFlags |= GhostLayersInitialized;
00644
00645
        checkFlag(FLatticePatchSetUp);
00646
        // variables to set to ghost layer width and point distance to next
00647
        // communication point \rightarrow depends on direction
00648
        00649
00651
         // filling buffers along the MPI dim order
00652
        distToRight = n * n * (n - gLW);
        bufferCreator(li, n, n, gLW, distToRight);
li += 2 * exchangeSize; // li increases by two exchange sizes per dim
00653
00654
00655
        distToRight = n * (n - gLW);
bufferCreator(li, n, gLW, n, distToRight);
00656
00657
00658
        li += 2 * exchangeSize;
00659
00660
        distToRight = (n - qLW);
00661
        bufferCreator(li, gLW, n, n, distToRight);
00662
00663
        MPI_Neighbor_alltoall(&ghostCellsToSend[0], exchangeSize, MPI_SUNREALTYPE,
00664
                                 &ghostCells[0], exchangeSize, MPI_SUNREALTYPE,
00665
                                 envelopeLattice->comm);
00666 }
00667
```

```
00668 /// Fill the halo buffers for neighborhood collectives
00669 void LatticePatch::bufferCreator(int li, int mx, int my, int mz,
00670
               int distToRight) {
        const int dPD = envelopeLattice->get_dataPointDimension();
00671
        // Initialize running index ui for to be transferred uData
00672
00673
        int ui = 0:
00675 // #pragma omp parallel for reduction(+:ui) reduction(+:li) -> don't, probably
00676 // bad idea to parallelize ghost cell exchange Loop over all planes and pick to
00677 // be transferred points (uData indices)
00678 #pragma distribute_point
00679
        for (int iz = 0; iz < mz; iz++) {
  for (int iy = 0; iy < my; iy++) {</pre>
00680
             // start index of uData vector halo data to be transferred
00681
00682
             // Here, in contrast to above, start at right boundary to send to left
00683
             // s.t. updated left values are the first indices (bec of neighborhood
            // collective pattern) with each z-step add the whole xy-plane and with // y-step the x-range \rightarrow iterate all x-ranges
00684
00685
            ui = (iz * nx * ny + iy * nx + distToRight) * dPD;
00686
             // copy from uData from right boundary (at each dimension) into buffer,
00687
00688
             // halo transfer size is given by x length at each step
00689
             // memcpy(&ghostCellsToSend[li],
00690
                          &uData[ui], \
00691
            sizeof(sunrealtype)*mx*dPD);
copy(&uData[ui], &uData[ui + mx * dPD], &ghostCellsToSend[li]);
00692
             // increase li by transferred indices in this loop-step
00694
             li += mx * dPD;
00695
00696
        }
00697
00698 #pragma distribute_point
00699
        for (int iz = 0; iz < mz; iz++) {
00700
          for (int iy = 0; iy < my; iy++) {</pre>
00701
            \ensuremath{//} Now copy from left boundary into buffer
            ui = (iz * nx * ny + iy * nx) * dPD;
//memcpy(&ghostCellsToSend[li], \
00702
00703
00704
                          &uData[ui], \
                          sizeof(sunrealtype)*mx*dPD);
00705
00706
             copy(&uData[ui], &uData[ui + mx * dPD], &ghostCellsToSend[li]);
00707
            li += mx * dPD;
00708
          }
00709
       }
00710 }
00711
00712 /// Check if all flags are set
00713 void LatticePatch::checkFlag(unsigned int flag) const {
00714 if (!(statusFlags & flag)) {
00715
          string errorMessage;
00716
          switch (flag) {
00717
          case FLatticePatchSetUp:
            errorMessage = "The Lattice patch was not set up please make sure to "
"initilize a Lattice topology";
00718
00719
00720
          case TranslocationLookupSetUp:
    errorMessage = "The translocation lookup tables have not been generated, "
00721
00722
00723
                            "please be sure to run generateTranslocationLookup()";
00724
00725
          case GhostLaversInitialized:
           00726
00727
00728
           break:
          case BuffersInitialized:
00729
            errorMessage = "The space for the buffers has not been allocated, please "
00730
00731
                            "be sure to run initializeBuffers()";
00732
00733
          default:
00734
            errorMessage = "Uppss, you've made a non-standard error, sadly I can't "
00735
                            "help you there";
00736
            break:
00737
00738
          errorKill(errorMessage);
00739
00740
        return;
00741 }
00742
00743 /\!/\! Calculate derivatives in the patch (uAux) in the specified direction
00744 void LatticePatch::derive(const int dir) {
       // ghost layer width
const int gLW = envelopeLattice->get_ghostLayerWidth();
00745
00746
00747
        // dimensionality of data points -> 6
00748
        const int dPD = envelopeLattice->get_dataPointDimension();
00749
        // total width of patch in given direction including ghost layers at ends
00750
        const int dirWidth = discreteSize(dir) + 2 * gLW;
00751
        // width of patch only in given direction
00752
        const int dirWidthO = discreteSize(dir);
00753
        \ensuremath{//} size of plane perpendicular to given dimension
00754
        const int perpPlainSize = discreteSize() / discreteSize(dir);
```

```
// physical distance between points in that direction
          sunrealtype dxi = NAN;
00756
00757
          switch (dir) {
00758
          case 1:
           dxi = dx;
00759
00760
            break:
00761
          case 2:
00762
          dxi = dy;
00763
            break;
00764
          case 3:
           dxi = dz;
00765
00766
            break:
00767
          default:
00768
           dxi = 1;
00769
             errorKill("Tried to derive in the wrong direction");
00770
00771
00772
          // Derive according to chosen stencil accuracy order (which determines also
          // gLW)
00774
          const int order = envelopeLattice->get_stencilOrder();
00775
          switch (order) {
00776
          case 1:
            for (int i = 0; i < perpPlainSize; i++) {
    for (int j = (i * dirWidth + gLW) * dPD;
        j < (i * dirWidth + gLW + dirWidthO) * dPD; j += dPD) {
        uAux[j + 0 - gLW * dPD] = slb(&uAux[j + 0]) / dxi;
        uAux[j + 1 - gLW * dPD] = slb(&uAux[j + 1]) / dxi;
    }
}</pre>
00777
00778
00779
00780
00781
                  uAux[j + 2 - gLW * dPD] = slf(&uAux[j + 2]) / dxi;
uAux[j + 3 - gLW * dPD] = slf(&uAux[j + 3]) / dxi;
00782
00783
                  uAux[j + 4 - gLW * dPD] = slf(&uAux[j + 4]) / dxi;
00784
                  uAux[j + 5 - gLW * dPD] = s1f(&uAux[j + 5]) / dxi;
00785
00786
               }
00787
00788
            break;
00789
          case 2:
00790
            for (int i = 0; i < perpPlainSize; i++) {</pre>
               for (int j = (i * dirWidth + gLW) * dPD;
    j < (i * dirWidth + gLW + dirWidthO) * dPD; j += dPD) {</pre>
00791
00793
                  uAux[j + 0 - gLW * dPD] = s2b(&uAux[j + 0]) / dxi;
00794
                  uAux[j + 1 - gLW * dPD] = s2b(&uAux[j + 1]) / dxi;
00795
                  uAux[j + 2 - gLW * dPD] = s2f(&uAux[j + 2]) / dxi;
                  uAux[j + 3 - gLW * dPD] = s2f(&uAux[j + 3]) / dxi;
uAux[j + 4 - gLW * dPD] = s2c(&uAux[j + 4]) / dxi;
00796
00797
                  uAux[j + 5 - gLW * dPD] = s2c(&uAux[j + 5]) / dxi;
00798
00799
               }
00800
00801
            break:
00802
          case 3:
            for (int i = 0; i < perpPlainSize; i++) {</pre>
00803
               for (int j = (i * dirWidth + gLW) * dPD;

j < (i * dirWidth + gLW + dirWidthO) * dPD; j += dPD) {
00804
                  uAux[j + 0 - gLW * dPD] = s3b(&uAux[j + 0]) / dxi;

uAux[j + 1 - gLW * dPD] = s3b(&uAux[j + 1]) / dxi;
00806
00807
                  uAux[j + 2 - gLW * dPD] = s3f(&uAux[j + 2]) / dxi;
uAux[j + 3 - gLW * dPD] = s3f(&uAux[j + 3]) / dxi;
00808
00809
                  uAux[j + 4 - gLW * dPD] = s3f(&uAux[j + 4]) / dxi;
uAux[j + 5 - gLW * dPD] = s3f(&uAux[j + 5]) / dxi;
00810
00812
00813
            break;
00814
00815
          case 4:
            for (int i = 0; i < perpPlainSize; i++) {
    for (int j = (i * dirWidth + gLW) * dPD;
        j < (i * dirWidth + gLW + dirWidthO) * dPD; j += dPD) {</pre>
00816
00817
00818
                  uAux[j + 0 - gLW * dPD] = s4b(&uAux[j + 0]) / dxi;

uAux[j + 1 - gLW * dPD] = s4b(&uAux[j + 1]) / dxi;
00819
00820
                  uAux[j + 2 - gLW * dPD] = s4f(&uAux[j + 2]) / dxi;
00821
                  uAux[j + 3 - gLW * dPD] = s4f(&uAux[j + 3]) / dxi;
00822
                  uAux[j + 4 - gLW * dPD] = s4c(&uAux[j + 4]) / dxi;
00823
                  uAux[j + 5 - gLW * dPD] = s4c(&uAux[j + 5]) / dxi;
00825
00826
00827
            break;
00828
          case 5:
            for (int i = 0; i < perpPlainSize; i++) {</pre>
00829
                for (int j = (i * dirWidth + gLW) * dPD;
00831
                      j < (i * dirWidth + gLW + dirWidthO) * dPD; j += dPD) {</pre>
                  uAux[j + 0 - gLW * dPD] = s5b(&uAux[j + 0]) / dxi;

uAux[j + 1 - gLW * dPD] = s5b(&uAux[j + 1]) / dxi;
00832
00833
                  uAux[j + 2 - gLW * dPD] = s5f(&uAux[j + 2]) / dxi;
00834
                  uAux[j + 3 - gLW * dPD] = s5f(&uAux[j + 3]) / dxi;
00835
                  uAux[j + 4 - gLW * dPD] = s5f(&uAux[j + 4]) / dxi;
00836
                  uAux[j + 5 - gLW * dPD] = s5f(&uAux[j + 5]) / dxi;
00837
00838
00839
00840
            break;
00841
          case 6:
```

```
for (int i = 0; i < perpPlainSize; i++) {</pre>
                  for (int j = (i * dirWidth + gLW) * dPD;

j < (i * dirWidth + gLW + dirWidthO) * dPD; j += dPD) {
00844
                      uAux[j + 0 - gLW * dPD] = s6b(&uAux[j + 0]) / dxi;
uAux[j + 1 - gLW * dPD] = s6b(&uAux[j + 1]) / dxi;
00845
00846
                      uAux[j + 2 - gLW * dPD] = s6f(&uAux[j + 2]) / dxi;

uAux[j + 3 - gLW * dPD] = s6f(&uAux[j + 3]) / dxi;

uAux[j + 4 - gLW * dPD] = s6c(&uAux[j + 4]) / dxi;
00847
00849
                       uAux[j + 5 - gLW * dPD] = s6c(&uAux[j + 5]) / dxi;
00850
00851
00852
                }
00853
               break:
00854
            case 7:
               for (int i = 0; i < perpPlainSize; i++) {</pre>
00855
00856
                    for (int j = (i * dirWidth + gLW) * dPD;
                      j < (i * dirWidth + gLW + dirWidthO) * dPD; j += dPD) {
uAux[j + 0 - gLW * dPD] = s7b(&uAux[j + 0]) / dxi;
uAux[j + 1 - gLW * dPD] = s7b(&uAux[j + 1]) / dxi;
00857
00858
00859
                       uAux[j + 2 - gLW * dPD] = s7f(&uAux[j + 2]) / dxi;
                       uAux[j + 3 - gLW * dPD] = s7f(&uAux[j + 3]) / dxi;
00861
                      uAux[j + 4 - gLW * dPD] = s7f(&uAux[j + 4]) / dxi;

uAux[j + 5 - gLW * dPD] = s7f(&uAux[j + 5]) / dxi;
00862
00863
00864
00865
00866
               break;
             case 8:
00868
               for (int i = 0; i < perpPlainSize; i++) {</pre>
                   for (int j = (i * dirWidth + gLW) * dPD;

j < (i * dirWidth + gLW + dirWidth) * dPD; j += dPD) {

uAux[j + 0 - gLW * dPD] = s8b(&uAux[j + 0]) / dxi;

uAux[j + 1 - gLW * dPD] = s8b(&uAux[j + 1]) / dxi;
00869
00870
00871
00872
00873
                       uAux[j + 2 - gLW * dPD] = s8f(&uAux[j + 2]) / dxi;
                       uAux[j + 3 - gLW * dPD] = s8f(&uAux[j + 3]) / dxi;
uAux[j + 4 - gLW * dPD] = s8c(&uAux[j + 4]) / dxi;
uAux[j + 5 - gLW * dPD] = s8c(&uAux[j + 4]) / dxi;
00874
00875
00876
00877
00878
               break;
00880
             case 9:
               for (int i = 0; i < perpPlainSize; i++) {</pre>
00881
                   for (int j = (i * dirWidth + gLW) * dPD;
    j < (i * dirWidth + gLW + dirWidth) * dPD; j += dPD) {
    uAux[j + 0 - gLW * dPD] = s9b(&uAux[j + 0]) / dxi;
    uAux[j + 1 - gLW * dPD] = s9b(&uAux[j + 1]) / dxi;</pre>
00882
00883
00884
00885
                       uAux[j + 2 - gLW * dPD] = s9f(&uAux[j + 2]) / dxi;
00886
                       uAux[j + 3 - gLW * dPD] = s9f(&uAux[j + 3]) / dxi;
00887
                      uAux[j + 4 - gLW * dPD] = s9f(&uAux[j + 4]) / dxi;
uAux[j + 5 - gLW * dPD] = s9f(&uAux[j + 5]) / dxi;
00888
00889
00890
                   }
00891
00892
               break;
00893
             case 10:
00894
               for (int i = 0; i < perpPlainSize; i++) {</pre>
                   for (int j = (i * dirWidth + gLW) * dPD;

j < (i * dirWidth + gLW + dirWidthO) * dPD; j += dPD) {
00895
00896
                      uAux[j + 0 - gLW * dPD] = s10b(&uAux(j + 0]) / dxi;
uAux[j + 1 - gLW * dPD] = s10b(&uAux(j + 1)) / dxi;
00897
                       uAux[j + 2 - gLW * dPD] = s10f(&uAux[j + 2]) / dxi;
00899
                      uAux[j + 3 - gLW * dPD] = slof(&uAux[j + 3]) / dxi;
uAux[j + 4 - gLW * dPD] = sloc(&uAux[j + 4]) / dxi;
uAux[j + 5 - gLW * dPD] = sloc(&uAux[j + 5]) / dxi;
00900
00901
00902
00903
                   }
00904
00905
                break;
            case 11:
00906
00907
              for (int i = 0; i < perpPlainSize; i++) {</pre>
                   for (int j = (i * dirWidth + gLW) * dPD;

j < (i * dirWidth + gLW + dirWidthO) * dPD; j += dPD) {

uAux[j + 0 - gLW * dPD] = s1lb(&uAux[j + 0]) / dxi;

uAux[j + 1 - gLW * dPD] = s1lb(&uAux[j + 1]) / dxi;
00908
00909
00910
                      uAux[j + 2 - gLW * dPD] = sllf(&uAux[j + 2]) / dxi;

uAux[j + 3 - gLW * dPD] = sllf(&uAux[j + 2]) / dxi;

uAux[j + 4 - gLW * dPD] = sllf(&uAux[j + 3]) / dxi;

uAux[j + 5 - gLW * dPD] = sllf(&uAux[j + 4]) / dxi;
00912
00913
00914
00915
00916
00917
00918
                break;
00919
            case 12:
               00920
00921
00922
                      uAux[j + 0 - gLW * dPD] = s12b(&uAux[j + 0]) / dxi;
uAux[j + 1 - gLW * dPD] = s12b(&uAux[j + 1]) / dxi;
00924
                       uAux[j + 2 - gLW * dPD] = s12f(&uAux[j + 2]) / dxi;
00925
                      uAux[j + 3 - gLW * dPD] = sl2f(&uAux[j + 3]) / dxi;
uAux[j + 4 - gLW * dPD] = sl2c(&uAux[j + 4]) / dxi;
00926
00927
                       uAux[j + 5 - gLW * dPD] = s12c(&uAux[j + 5]) / dxi;
00928
```

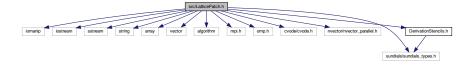
6.11 LatticePatch.cpp 209

```
00929
            }
00930
00931
          break;
00932
        case 13:
         //#pragma omp parallel for default(none) firstprivate(uAux)
00933
00934
          //shared(dxi,dirWidth,dirWidth0,gLW,dPD) collapse(2) schedule(static,6)
          //#pragma ivdep
00936
          //#pragma distribute_point -> No.
           //#pragma unroll_and_jam
00937
00938
          \ensuremath{//} Iterate through all points in the plane perpendicular to the given
          // direction
00939
          for (int i = 0; i < perpPlainSize; i++) {</pre>
00940
            // stencil functions range over 2*gLW+6 indices, attention to cache-line
00941
00942
             // false-sharing
00943
             //#pragma omp simd safelen(2*gLW+dPD)
            00944
00945
00946
00948
               * with a ghostlayer width adjusted to the order of the finite
00949
               * difference scheme */
00950
              uAux[j + 0 - gLW * dPD] = s13b(&uAux[j + 0]) / dxi;
              uAux[j + 1 - gLW * dPD] = sl3b(&uAux[j + 1]) / dxi;
uAux[j + 2 - gLW * dPD] = sl3f(&uAux[j + 2]) / dxi;
00951
00952
              uAux[j + 3 - gLW * dPD] = s13f(&uAux[j + 3]) / dxi;
uAux[j + 4 - gLW * dPD] = s13f(&uAux[j + 4]) / dxi;
00953
00954
00955
              uAux[j + 5 - gLW * dPD] = s13f(&uAux[j + 5]) / dxi;
00956
            }
00957
00958
          break:
00959
00960
        default:
00961
        errorKill("Please set an existing stencil order");
00962
00963
00964 }
00965
00966 /////// Helper functions ///////
00968 /// Print a specific error message to stdout
00969 void errorKill(const string & errorMessage) {
00970 cerr « endl « "Error: " « errorMessage « " Aborting..." « endl;
00971
        MPI Abort (MPI COMM WORLD, 1);
00972
        return;
00973 }
00974
00975 /** Check function return value. From CVode examples.
          opt == 0 means SUNDIALS function allocates memory so check if
00976
                    returned NULL pointer
00977
00978
           opt == 1 means SUNDIALS function returns an integer value so check if
                     retval < 0
00980
           opt == 2 means function allocates memory so check if returned
00981
                    NULL pointer */
00982 int check_retval(void *returnvalue, const char *funcname, int opt, int id) {
00983
        int *retval = nullptr;
00984
        /\star Check if SUNDIALS function returned NULL pointer - no memory allocated \star/
00986
        if (opt == 0 && returnvalue == nullptr) {
00987
        fprintf(stderr,
00988
                   "\nSUNDIALS_ERROR(%d): %s() failed - returned NULL pointer\n\n", id,
                  funcname);
00989
00990
          return (1);
00991
        }
00992
00993
        /* Check if retval < 0 */
00994
        else if (opt == 1) {
00995
         retval = (int *)returnvalue;
          if (*retval < 0) {
   fprintf(stderr, "\nSUNDIALS_ERROR(%d): %s() failed with retval = %d\n\n",</pre>
00996
00997
00998
                     id, funcname, *retval);
00999
             return (1);
01000
01001
        }
01002
        /\star Check if function returned NULL pointer - no memory allocated \star/
01003
        else if (opt == 2 && returnvalue == nullptr) {
01004
01005
         fprintf(stderr,
01006
                   "\nMEMORY_ERROR(%d): %s() failed - returned NULL pointer\n\n", id,
01007
                  funcname);
01008
          return (1);
01009
01011
        return (0);
01012 }
```

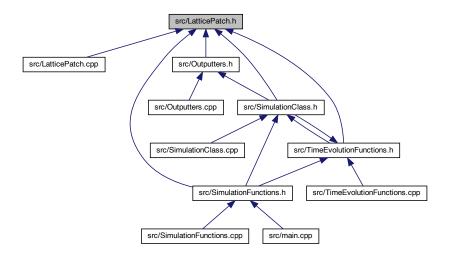
6.12 src/LatticePatch.h File Reference

Declaration of the lattice and lattice patches.

```
#include <iomanip>
#include <iostream>
#include <sstream>
#include <string>
#include <array>
#include <vector>
#include <algorithm>
#include <mpi.h>
#include <omp.h>
#include <cvode/cvode.h>
#include <nvector/nvector_parallel.h>
#include <sundials/sundials_types.h>
#include dependency graph for Lattice Patch.h:
```



This graph shows which files directly or indirectly include this file:



Data Structures

class Lattice

Lattice class for the construction of the enveloping discrete simulation space.

· class LatticePatch

LatticePatch class for the construction of the patches in the enveloping lattice.

Enumerations

```
• enum LatticeOptions { FLatticeDimensionSet = 0x01 }
```

```
• enum LatticePatchOptions { FLatticePatchSetUp = 0x01 , TranslocationLookupSetUp = 0x02 , GhostLayersInitialized = 0x04 , BuffersInitialized = 0x08 }
```

lattice patch construction checking flags

Functions

void errorKill (const string &errorMessage)

Print a specific error message to stdout.

• int check_retval (void *returnvalue, const char *funcname, int opt, int id)

6.12.1 Detailed Description

Declaration of the lattice and lattice patches.

Definition in file LatticePatch.h.

6.12.2 Enumeration Type Documentation

6.12.2.1 LatticeOptions

```
enum LatticeOptions
```

Enumerator

FLatticeDimensionSet

Definition at line 35 of file LatticePatch.h.

6.12.2.2 LatticePatchOptions

```
enum LatticePatchOptions
```

lattice patch construction checking flags

Enumerator

FLatticePatchSetUp	
TranslocationLookupSetUp	
GhostLayersInitialized	
BuffersInitialized	

Definition at line 125 of file LatticePatch.h.

```
00125
00126     FLatticePatchSetUp = 0x01,
00127     TranslocationLookupSetUp = 0x02,
00128     GhostLayersInitialized = 0x04,
00129     BuffersInitialized = 0x08,
00130     /*OPT_D = 0x08,
00131     OPT_E = 0x10,
00132     OPT_F = 0x20,*/
00133    };
```

6.12.3 Function Documentation

6.12.3.1 check_retval()

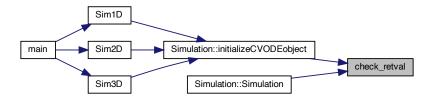
Check function return value. From CVode examples. opt == 0 means SUNDIALS function allocates memory so check if returned NULL pointer opt == 1 means SUNDIALS function returns an integer value so check if retval < 0 opt == 2 means function allocates memory so check if returned NULL pointer

Definition at line 982 of file LatticePatch.cpp.

```
00982
        int *retval = nullptr;
00983
00984
        /\star Check if SUNDIALS function returned NULL pointer - no memory allocated \star/
00985
00986
        if (opt == 0 && returnvalue == nullptr) {
00987
00988
                   "\nSUNDIALS_ERROR(%d): %s() failed - returned NULL pointer\n\n", id,
00989
                   funcname);
00990
          return (1);
00991
00992
00993
        /* Check if retval < 0 */
        else if (opt == 1) {
  retval = (int *)returnvalue;
00994
00995
          if (*retval < 0) {
   fprintf(stderr, "\nSUNDIALS_ERROR(%d): %s() failed with retval = %d\n\n",</pre>
00996
00997
                      id, funcname, *retval);
00998
00999
            return (1);
01000
01001
01002
        /\star Check if function returned NULL pointer - no memory allocated \star/
01003
01004
        else if (opt == 2 && returnvalue == nullptr) {
         fprintf(stderr,
01005
01006
                   "\nMEMORY_ERROR(%d): %s() failed - returned NULL pointer\n\n", id,
01007
01008
          return (1);
01009
01010
01011
        return (0);
01012 }
```

Referenced by Simulation::initializeCVODEobject(), and Simulation::Simulation().

Here is the caller graph for this function:



6.12.3.2 errorKill()

```
void errorKill ( {\tt const\ string\ \&\ errorMessage\ )}
```

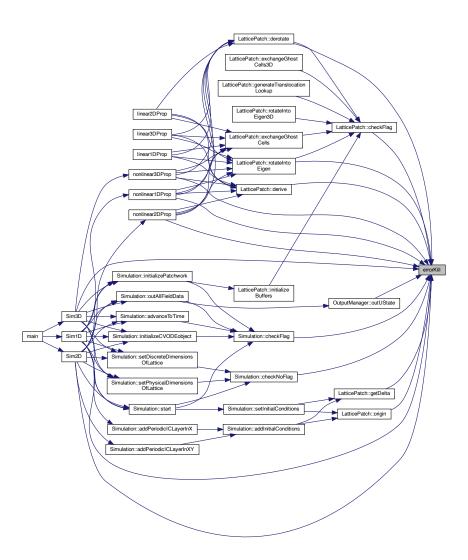
Print a specific error message to stdout.

```
Definition at line 969 of file LatticePatch.cpp.
```

```
00969 {
00970 cerr w endl w "Error: " w errorMessage w " Aborting..." w endl;
00971 MPI_Abort(MPI_COMM_WORLD, 1);
00972 return;
00973 }
```

Referenced by LatticePatch::checkFlag(), Simulation::checkFlag(), Simulation::checkNoFlag(), LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::getDelta(), nonlinear1DProp(), nonlinear2DProp(), nonlinear3DProp(), LatticePatch::origin(), OutputManager::outUState(), LatticePatch::rotateIntoEigen(), Sim1D(), Sim2D(), and Sim3D().

Here is the caller graph for this function:



6.13 LatticePatch.h

Go to the documentation of this file.

```
00005
00006 #pragma once
00007
00008 // IO
00009 #include <iomanip>
00010 #include <iostream>
00011 #include <sstream>
00012
00013 // string, container, algorithm
00014 #include <string>
00015 //#include <string_view>
00016 #include <array>
00017 #include <vector>
00018 #include <algorithm>
00019
00020 // MPI & OpenMP
00021 #include <mpi.h>
00022 #include <omp.h>
```

6.13 LatticePatch.h 215

```
00023
00024 // Sundials
00025 #include <cvode/cvode.h>
                                                                                                           /* prototypes for CVODE fcts. */
00026 \#include <nvector/nvector_parallel.h> /* definition of N_Vector and macros */
00027 \#include <sundials/sundials_types.h> /* definition of type sunrealtype */
00028
00030 #include "DerivationStencils.h"
00031
00032 using namespace std;
00033
00034 // lattice construction checking flags
00035 enum LatticeOptions {
00036
                      FLatticeDimensionSet = 0x01, // 1
00037
                        /*OPT_B = 0x02, // 2
                      OPT_C = 0x04, // 4
OPT_D = 0x08, // 8
OPT_E = 0x10, // 16
00038
00039
00040
                       OPT_F = 0x20, */ // 32
00041
00042 };
00043
00044 /** @brief Lattice class for the construction of the enveloping discrete
00045 * simulation space */
00046 class Lattice {
00047 private:
                 /// physical size of the lattice in x-direction
00049
                  sunrealtype tot_lx;
00050
                   /// physical size of the lattice in y-direction
00051
                  sunrealtype tot_ly;
                  /// physical size of the lattice in z-direction sunrealtype tot_lz;
00052
00053
00054
                   /// number of points in x-direction
00055
                  sunindextype tot_nx;
00056
                  /// number of points in y-direction
                  sunindextype tot_ny;
/// number of points in z-direction
00057
00058
00059
                  sunindextype tot_nz;
                  /// total number of lattice points
00060
00061
                  sunindextype tot_noP;
00062
                   /// dimension of each data point -> set once and for all
00063
                   static constexpr int dataPointDimension = 6;
00064
                  \ensuremath{///} number of lattice points times data dimension of each point
00065
                  sunindextype tot_noDP;
00066
                   /// physical distance between lattice points in x-direction
00067
                  sunrealtype dx;
00068
                   /// physical distance between lattice points in y-direction
00069
                   sunrealtype dy;
00070
                  /// physical distance between lattice points in z-direction % \left( 1\right) =\left( 1\right) \left( 1\right) 
00071
                  sunrealtype dz;
00072
                  /// stencil order
                  const int stencilOrder;
00074
                  ^{\prime} /// required width of ghost layers (depends on the stencil order)
00075
                   const int ghostLayerWidth;
00076
                  /// char for checking if lattice flags are set
00077
                  unsigned char statusFlags;
00078
00079 public:
00080
                  /// number of MPI processes
00081
                  int n_prc;
00082
                  /// number of MPI process
00083
                  int my_prc;
00084
                   /// personal communicator of the lattice
00085
                  MPI_Comm comm;
00086
                  /// function to create and deploy the cartesian communicator
00087
                  void initializeCommunicator(const int nx, const int ny,
00088
                                    const int nz, const bool per);
                  /// default construction
00089
00090
                  Lattice (const int StO):
                   /// SUNContext object
00091
                  SUNContext sunctx;
00093
                   /// SUNProfiler object
00094
                  SUNProfiler profobj;
00095
                   /// component function for resizing the discrete dimensions of the lattice
00096
                  void setDiscreteDimensions(const sunindextype _nx,
                   const sunindextype _ny, const sunindextype _nz);
/// component function for resizing the physical size of the lattice
00097
00098
00099
                   void setPhysicalDimensions(const sunrealtype _lx,
00100
                                     const sunrealtype _ly, const sunrealtype _lz);
00101
                   1//@{
00102
                   /** getter function */
                   [[nodiscard]] const sunrealtype &get_tot_lx() const { return tot_lx; }
00103
00104
                    [[nodiscard]] const sunrealtype &get_tot_ly() const { return tot_ly;
00105
                    [[nodiscard]] const sunrealtype &get_tot_lz() const { return tot_lz;
00106
                    [[nodiscard]] const sunindextype &get_tot_nx() const { return tot_nx;
00107
                   [[nodiscard]] const sunindextype &get_tot_ny() const { return tot_ny;
00108
                    [[nodiscard]] const sunindextype &get_tot_nz() const { return tot_nz;
00109
                   [[nodiscard]] const sunindextype &get_tot_noP() const { return tot_noP; }
```

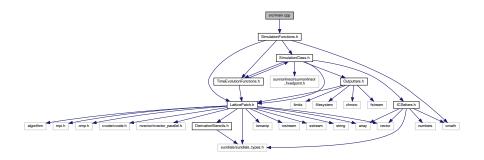
```
[[nodiscard]] const sunindextype &get_tot_noDP() const { return tot_noDP; }
        [[nodiscard]] const sunrealtype &get_dx() const { return dx; }
00111
00112
        [[nodiscard]] const sunrealtype &get_dy() const { return dy; }
00113
        [[nodiscard]] const sunrealtype &get_dz() const { return dz; }
00114
        [[nodiscard]] constexpr int get_dataPointDimension() const {
00115
         return dataPointDimension;
00116
00117
        [[nodiscard]] const int &get_stencilOrder() const { return stencilOrder; }
00118
       [[nodiscard]] const int &get_ghostLayerWidth() const {
00119
         return ghostLayerWidth;
00120
00121
       ///@}
00122 };
00123
00124 /// lattice patch construction checking flags
00125 enum LatticePatchOptions {
00126
       FLatticePatchSetUp = 0x01,
       TranslocationLookupSetUp = 0x02,
GhostLayersInitialized = 0x04,
00127
00129
       BuffersInitialized = 0x08
00130
        /*OPT_D = 0x08,
00131
       OPT\_E = 0x10,
       OPT_F = 0x20, */
00132
00133 };
00134
00135 /** @brief LatticePatch class for the construction of the patches in the
00136 * enveloping lattice */
00137 class LatticePatch {
00138 private:
00139
       /// origin of the patch in physical space; x-coordinate
00140
       sunrealtype x0:
00141
        /// origin of the patch in physical space; y-coordinate
00142
       sunrealtype y0;
00143
       /// origin of the patch in physical space; z-coordinate
00144
       sunrealtype z0;
00145
       /// inner position of lattice-patch in the lattice patchwork; x-points
00146
       sunindextype LIx;
00147
       /// inner position of lattice-patch in the lattice patchwork; y-points
00148
       sunindextype LIy;
00149
        /// inner position of lattice-patch in the lattice patchwork; z-points
00150
       sunindextype LIz;
00151
       /// physical size of the lattice-patch in the x-dimension
00152
       sunrealtype lx:
00153
       /// physical size of the lattice-patch in the y-dimension
00154
       sunrealtype ly;
00155
        /// physical size of the lattice-patch in the z-dimension
00156
       sunrealtype lz;
00157
       /// number of points in the lattice patch in the x-dimension
       sunindextype nx;
00158
00159
       /// number of points in the lattice patch in the \gamma-dimension
00160
       sunindextype ny;
00161
        /// number of points in the lattice patch in the z-dimension
00162
       sunindextype nz;
00163
       /// physical distance between lattice points in x-direction
00164
       sunrealtype dx;
00165
       /// physical distance between lattice points in y-direction
       sunrealtype dy;
00167
        /// physical distance between lattice points in z-direction
00168
        sunrealtype dz;
00169
       /// pointer to the enveloping lattice
00170
       const Lattice *envelopeLattice;
00171
       ///@{
00172
        /** translocation lookup table */
        vector<int> uTox, uToy, uToz, xTou, yTou, zTou;
00173
00174
00175
        /// aid (auxilliarly) vector including ghost cells to compute the derivatives
00176
       vector<sunrealtype> uAux;
00177
       ///@{
00178
        /** buffer to save spatial derivative values */
00179
        vector<sunrealtype> buffX, buffY, buffZ;
00180
00181
        1//01
       00182
00183
00184
00185
        ///@}
00186
       ///@{
00187
        /** ghost cell translocation lookup table */
00188
       vector<int> lgcTox, rgcTox, lgcToy, rgcToy, lgcToz, rgcToz;
00189
       ///@}
00190
       /** char for checking flags */
00191
       unsigned char statusFlags;
00192
00193
        /** rotate and translocate an input array according to a lookup into an output
00194
        * array */
00195
       inline void rotateToX(sunrealtype *outArray, const sunrealtype *inArray,
00196
                              const vector<int> &lookup);
```

```
inline void rotateToY(sunrealtype *outArray, const sunrealtype *inArray,
                               const vector<int> &lookup);
00198
00199
        inline void rotateToZ(sunrealtype *outArray, const sunrealtype *inArray,
00200
                              const vector<int> &lookup);
00201
00202 public:
       /// ID of the LatticePatch, corresponds to process number
        // (required solely for debugging)
00204
00205
00206
        /// N_Vector for saving field components u=(E,B) in lattice points
        N_Vector u;
00207
        /// N Vector for saving temporal derivatives of the field data
00208
        N Vector du;
00210
        /// pointer to field data
00211
        sunrealtype *uData;
00212
        /// pointer to auxiliary data vector
00213
        sunrealtype *uAuxData;
00214
        /// pointer to time-derivative data
        sunrealtype *duData;
00216
00217
        /** pointer to halo data */
00218
        sunrealtype *gCLData, *gCRData, *gCBData, *gCTData, *gCFData, *gCAData;
00219
        ///@}
        /// pointer to spatial derivative data buffers
00220
        array/sunrealtype *, 3> buffData;
/// constructor setting up a default first lattice patch
00221
00222
00223
        LatticePatch();
00224
        /// destructor freeing parallel vectors
00225
        ~LatticePatch();
00226
        /// friend function for creating the patchwork slicing of the overall lattice
00227
        friend int generatePatchwork(const Lattice &envelopeLattice.
00228
                                      LatticePatch &patchToMold, const int DLx,
00229
                                      const int DLy, const int DLz);
        /// function to get the discrete size of the LatticePatch
00230
00231
        // (0 direction corresponds to total)
        int discreteSize(int dir=0) const;
00232
        /// function to get the origin of the patch
sunrealtype origin(const int dir) const;
00233
00235
        /// function to get distance between points
00236
        sunrealtype getDelta(const int dir) const;
00237
        /// function to fill out the lookup tables for translocation
        // and de-translocation of data point
00238
00239
        void generateTranslocationLookup();
00240
        /// function to rotate u into Z-matrix eigenraum
        // and make it the primary lattice direction of dir
00241
00242
        void rotateIntoEigen(const int dir);
00243
        /// function to rotate as in 'rotateIntoEigen' with special 3D halo buffers
00244
        void rotateIntoEigen3D();
00245
        /// function to derotate uAux into dudata lattice direction of x
00246
        void derotate(int dir, sunrealtype *buffOut);
00247
        /// initialize ghost cells for halo exchange
00248
        void initializeGhostLayer();
00249
        /// initialize buffers to save derivatives
00250
        void initializeBuffers();
00251
        /// function to exchange ghost cells in uAux for the derivative
00252
        void exchangeGhostCells(const int dir);
        /// function to exchange ghost cells using a neighborhood collective operation
00254
        // for 3D simulations; requires cubic patches
00255
        void exchangeGhostCells3D();
00256
        /// outsourced convenience function to fill halo buffers with uData for 3D \,
00257
        void bufferCreator(int li, int mx, int my, int mz, int distToRight);
00258
       /// function to derive the centered values in uAux and save them noncentered
00259
        void derive(const int dir);
00260
       /// function to check if a flag has been set and if not abort
00261
        void checkFlag(unsigned int flag) const;
00262 };
00263
00264 // helper function for error messages
00265 void errorKill(const string & errorMessage);
00267 // helper function to check for CVode success
00268 int check_retval(void *returnvalue, const char *funcname, int opt, int id);
00269
```

6.14 src/main.cpp File Reference

Main function to configure the user's simulation settings.

#include "SimulationFunctions.h"
Include dependency graph for main.cpp:



Functions

• int main (int argc, char *argv[])

6.14.1 Detailed Description

Main function to configure the user's simulation settings.

Definition in file main.cpp.

6.14.2 Function Documentation

6.14.2.1 main()

```
int main (
          int argc,
          char * argv[] )
```

Determine the output directory.

A "SimResults" folder will be created if non-existent with a subdirectory named in the identifier format "yy-mm-dd_hh-MM-ss" that contains the csv files

A 1D simulation with specified

- · relative and absolute tolerances of the CVode solver
- accuracy order of the stencils in the range 1-13
- · physical length of the lattice in meters
- · number of lattice points
- periodic or vanishing boundary values

- included processes of the weak-field expansion, see README.md
- · physical total simulation time
- · discrete time steps
- · output step multiples
- output in csv (c) or binary (b)

Add electromagnetic waves.

A plane wave with

- wavevector (normalized to $1/\lambda$)
- · amplitude/polarization
- · phase shift

Another plane wave with

- wavevector (normalized to $1/\lambda$)
- amplitude/polarization
- · phase shift

A Gaussian wave with

- wavevector (normalized to $1/\lambda$)
- · polarization/amplitude
- · shift from origin
- width
- · phase shift

Another Gaussian with

- wavevector (normalized to $1/\lambda$)
- · polarization/amplitude
- · shift from origin
- width
- · phase shift

A 2D simulation with specified

- · relative and absolute tolerances of the CVode solver
- accuracy order of the stencils in the range 1-13

- · physical length of the lattice in the given dimensions in meters
- number of lattice points per dimension
- · slicing of discrete dimensions into patches
- · periodic or vanishing boundary values
- included processes of the weak-field expansion, see README.md
- · physical total simulation time
- · discrete time steps
- · output step multiples
- output in csv (c) or binary (b)

Add electromagnetic waves.

A plane wave with

- wavevector (normalized to $1/\lambda$)
- · amplitude/polarization
- · phase shift

Another plane wave with

- · wavevector
- · amplitude/polarization
- · phase shift

A Gaussian wave with

- · center it approaches
- normalized direction from which the wave approaches the center
- · amplitude
- polarization rotation from TE-mode (z-axis)
- · taille
- · Rayleigh length

the wavelength is determined by the relation $\lambda = \pi * w_0^2/z_R$

- · beam center
- · beam length

Another Gaussian wave with

- · center it approaches
- · normalized direction from which the wave approaches the center
- · amplitude
- polarization rotation fom TE-mode (z-axis)
- · taille
- · Rayleigh length
- · beam center
- · beam length

A 3D simulation with specified

- · relative and absolute tolerances of the CVode solver
- accuracy order of the stencils in the range 1-13
- · physical dimensions in meters
- · number of lattice points in any dimension
- · slicing of discrete dimensions into patches
- · perodic or non-periodic boundaries
- processes of the weak-field expansion, see README.md
- · physical total simulation time
- · discrete time steps
- · output step multiples
- output in csv (c) or binary (b)

Add electromagnetic waves.

A plane wave with

- wavevector (normalized to $1/\lambda$)
- · amplitude/polarization
- · phase shift

Another plane wave with

- wavevector (normalized to $1/\lambda$)
- · amplitude/polarization
- · phase shift

A Gaussian wave with

- · center it approaches
- · normalized direction from which the wave approaches the center
- · amplitude
- · polarization rotation from TE-mode (z-axis)
- · taille
- · Rayleigh length

the wavelength is determined by the relation $\lambda = \pi * w_0^2/z_R$

- · beam center
- · beam length

Another Gaussian wave with

- · center it approaches
- · normalized direction from which the wave approaches the center
- · amplitude
- · polarization rotation from TE-mode (z-axis)
- · taille
- · Rayleigh length
- · beam center
- · beam length

Definition at line 8 of file main.cpp.

```
00009 {
00010
             // Initialize MPI environment
           MPI_Init (&argc, &argv);
MPI_Comm comm = MPI_COMM_WORLD;
// Prepare MPI for Master-only threading
00011
00012
00013
00014
            //int provided;
00015
           //MPI_Init_thread(&argc, &argv, MPI_THREAD_FUNNELED, &provided);
00016
00017
00018
            MPI_Comm_rank(comm,&rank);
00019
           double ti=MPI_Wtime(); // Overall start time
00020
00021
           /** Determine the output directory.
  * A "SimResults" folder will be created if non-existent
00022
            * with a subdirectory named in the identifier format

* "yy-mm-dd_hh-MM-ss" that contains the csv files
00023
00024
           //constexpr auto outputDirectory = "/gpfs/scratch/uh3o1/ru68dab/ru68dab/HE/outputs";
//constexpr auto outputDirectory = "/home/andi/Documents/";
constexpr auto outputDirectory = "/Users/andi/Documents/";
00025
00026
00027
00028
00029
            if(rank==0 && !filesystem::exists(outputDirectory)) {
00030
                cerr«"\nOutput directory nonexistent.\n";
00031
                MPI_Abort(comm, 1);
00032
00033
00034
00035
            //---- BEGIN OF CONFIGURATION -----//
00036
00037
            00038
            /** A 1D simulation with specified */
00039
00040
            //// Specify your settings here ////
            constexpr array <sunrealtype,2> CVodeTolerances={1.0e-16,1.0e-16}; /// - relative and absolute
00041
        tolerances of the CVode solver
```

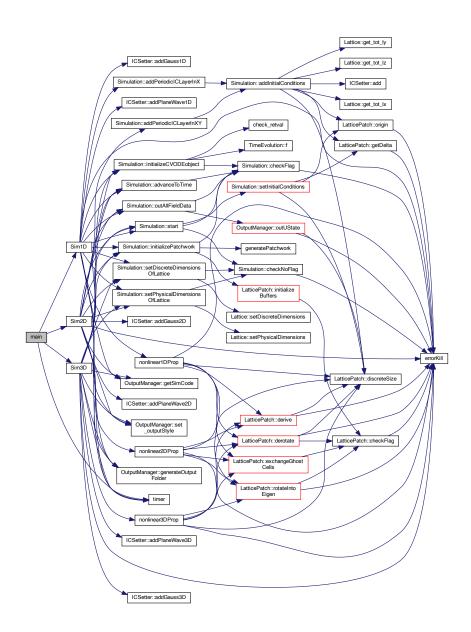
```
00042
          constexpr int StencilOrder=13;
                                                                              /// - accuracy order of the
       stencils in the range 1-13
00043
          constexpr sunrealtype physical_sidelength=300e-6;
                                                                              /// - physical length of the
       lattice in meters
00044
         constexpr sunindextype latticepoints=6e3;
                                                                              /// - number of lattice points
          constexpr bool periodic=true;
                                                                              /// - periodic or vanishing
00045
       boundary values
00046
          int processOrder=3;
                                                                              /// - included processes of the
       weak-field expansion, see README.md
00047
         constexpr sunrealtype simulationTime=100.0e-61;
                                                                              /// - physical total
       simulation time
00048
                                                                            /// - discrete time steps
/// - output step multiples
         constexpr int numberOfSteps=100;
00049
          constexpr int outputStep=1;
          constexpr char outputStyle='c';
                                                                             /// - output in csv (c) or binary
00050
00051
          /// Add electromagnetic waves.
00052
          planewave plane1;
plane1.k = {1e5,0,0};
                                           /// A plane wave with
00053
00054
                                           /// - wavevector (normalized to f 1/\lambda f)
          plane1.p = \{0,0,0.1\};
                                           /// - amplitude/polarization
00055
          plane1.phi = {0,0,0};
00056
                                           /// - phase shift
00057
          planewave plane2;
                                           /// Another plane wave with
          plane2.k = {-1e6,0,0};
plane2.p = {0,0,0.5};
                                            /// - wavevector (normalized to f 1/\lambda f)
00058
                                           /// - amplitude/polarization
00059
00060
          plane2.phi = \{0,0,0\};
                                           /// - phase shift
00061
          // Do not comment out this vector, even if no plane wave is used. But if, emplace used plane
00062
          vector<planewave> planewaves;
00063
          //planewaves.emplace_back(plane1);
00064
          //planewaves.emplace_back(plane2);
00065
00066
          gaussian1D gauss1;
                                            /// A Gaussian wave with
          gauss1.k = {1.0e6,0,0};
gauss1.p = {0,0,0.1};
00067
                                           /// - wavevector (normalized to \f$ 1/\lambda \f$)
00068
                                           /// - polarization/amplitude
          gauss1.x0 = \{100e-6,0,0\};
00069
                                          /// - shift from origin
          gauss1.phig = 5e-6;
gauss1.phi = {0,0,0};
                                           /// - width
00070
00071
                                           /// - phase shift
          gaussian1D gauss2;
                                           /// Another Gaussian with
00072
          gauss2.k = \{-0.2e6, 0, 0\};
00073
                                           /// - wavevector (normalized to f 1/\lambda f)
00074
          gauss2.p = \{0,0,0.5\};
                                          /// - polarization/amplitude
00075
          gauss2.x0 = \{200e-6,0,0\};
                                           /// - shift from origin
          gauss2.phig = 15e-6;
gauss2.phi = {0,0,0};
                                           /// - width
00076
                                           /// - phase shift
00077
00078
          // Do not comment out this vector, even if no Gaussian wave is used. But if, emplace used Gaussian
       waves.
00079
          vector<gaussian1D> Gaussians1D;
08000
          Gaussians1D.emplace_back(gauss1);
00081
          Gaussians1D.emplace_back(gauss2);
00082
00083
          //// Do not change this below ////
          int *interactions = &processOrder;
00084
00085
          Sim1D (CVodeTolerances, StencilOrder, physical_sidelength, latticepoints,
00086
                  periodic, interactions, simulationTime, numberOfSteps,
00087
                  outputDirectory,outputStep,outputStyle,
00088
                  planewaves, Gaussians1D);
00089
00090
          00091
00092
          00093
00094
          /** A 2D simulation with specified */
00095
00096
          //// Specify your settings here ////
          constexpr array<sunrealtype,2> CVodeTolerances={1.0e-12,1.0e-12}; /// - relative and absolute
00097
       tolerances of the CVode solver
00098
          constexpr int StencilOrder=13;
                                                                              /// - accuracy order of the
       stencils in the range 1-13
00099
          constexpr array<sunrealtype,2> physical_sidelengths={80e-6,80e-6}; /// - physical length of the
       lattice in the given dimensions in meters
00100
          constexpr array<sunindextype,2> latticepoints_per_dim={800,800}; /// - number of lattice points
00101
         constexpr array<int,2> patches_per_dim={2,2};
                                                                              /// - slicing of discrete
       dimensions into patches
00102
                                                                              /// - periodic or vanishing
         constexpr bool periodic=true;
       boundary values
00103
         int processOrder=3;
                                                                              /// - included processes of the
       weak-field expansion, see README.md
00104
          constexpr sunrealtype simulationTime=4e-61;
                                                                              /// - physical total simulation
       time
00105
         constexpr int numberOfSteps=10:
                                                                              /// - discrete time steps
                                                                              /// - output step multiples
          constexpr int outputStep=1;
00106
00107
          constexpr char outputStyle='c';
                                                                             /// - output in csv (c) or binary
00108
00109
          /// Add electromagnetic waves.
          planewave plane1;
plane1.k = {1e5,0,0};
                                             /// A plane wave with
00110
00111
                                             /// - wavevector (normalized to \f$ 1/\lambda \f$)
```

```
plane1.p = \{0,0,0.1\};
                                                /// - amplitude/polarization
                                                /// - phase shift
          plane1.phi = \{0,0,0\};
00113
00114
          planewave plane2;
                                                /// Another plane wave with
          plane2.k = {-1e6,0,0};
plane2.p = {0,0,0.5};
plane2.phi = {0,0,0};
00115
                                                /// - wavevector
                                                /// - amplitude/polarization
00116
                                                /// - phase shift
00117
00118
           // Do not comment out this vector, even if no plane wave is used. But if, emplace used plane
00119
          vector<planewave> planewaves;
00120
          //planewaves.emplace_back(plane1);
00121
          //planewaves.emplace_back(plane2);
00122
00123
          gaussian2D gauss1;
                                                /// A Gaussian wave with
          gauss1.x0 = \{40e-6, 40e-6\};
00124
                                                /// - center it approaches
00125
          gauss1.axis = {1,0};
                                                /// - normalized direction _from_ which the wave approaches the
       center
00126
                                                /// - amplitude
          gauss1.amp = 0.5;
                                               /// polarization rotation from TE-mode (z-axis) /// - taille
           gauss1.phip = 2*atan(0);
00127
          gauss1.w0 = 2.3e-6;
          gauss1.zr = 16.619e-6;
                                                /// - Rayleigh length
00129
00130
           /// the wavelength is determined by the relation \f$ \lambda = \pi*w_0^2/z_R \f$
          gauss1.ph0 = 2e-5;
gauss1.phA = 0.45e-5;
                                  /// - beam center
/// - beam length
00131
00132
          gaussian2D gauss2;
gauss2.x0 = {40e-6,40e-6};
                                               /// Another Gaussian wave with
00133
                                               /// - center it approaches
00134
          gauss2.axis = \{-0.7071, 0.7071\}; /// - normalized direction from which the wave approaches the
00135
00136
          gauss2.amp = 0.5;
                                                /// - amplitude
          gauss2.phip = 2*atan(0);
gauss2.w0 = 2.3e-6;
gauss2.zr = 16.619e-6;
                                                /// - polarization rotation fom TE-mode (z-axis)
00137
                                                /// - taille
00138
00139
                                                /// - Rayleigh length
          gauss2.ph0 = 2e-5;
gauss2.phA = 0.45e-5;
00140
                                                /// - beam center
                                                /// - beam length
00141
           // Do not comment out this vector, even if no Gaussian wave is used. But if, emplace used Gaussian
00142
       waves.
00143
          vector<gaussian2D> Gaussians2D;
00144
          Gaussians2D.emplace back(gauss1);
          Gaussians2D.emplace_back(gauss2);
00146
00147
           //// Do not change this below ////
00148
          static_assert(latticepoints_per_dim[0]%patches_per_dim[0]==0 &&
00149
                   latticepoints\_per\_dim[1] *patches\_per\_dim[1] == 0,
          "The number of lattice points in each dimension must be "
divisible by the number of patches in that direction.");
int * interactions = &processOrder;
00150
00151
00152
00153
          Sim2D (CVodeTolerances, StencilOrder, physical_sidelengths,
00154
                   latticepoints_per_dim,patches_per_dim,periodic,interactions,
00155
                   \verb|simulationTime|, \verb|numberOfSteps|, outputDirectory|, outputStep|,
00156
                   outputStyle, planewaves, Gaussians2D);
00157
00158
          00159
00160
00161
          /** A 3D simulation with specified */
00162
00163
00164
          //// Specify your settings here ////
           constexpr array<sunrealtype,2> CVodeTolerances={1.0e-12,1.0e-12};
00165
                                                                                        /// - relative and
       absolute tolerances of the CVode solver
00166
          constexpr int StencilOrder=4;
                                                                                         /// - accuracy order of
       the stencils in the range 1-13
          constexpr array<sunrealtype,3> physical_sidelengths={80e-6,80e-6,20e-6}; /// - physical dimensions
00167
       in meters
00168
          constexpr array<sunindextype, 3> latticepoints_per_dim={160,160,40};
                                                                                         /// - number of lattice
       points in any dimension
00169
          constexpr array<int,3> patches_per_dim= {2,2,1};
                                                                                         /// - slicing of discrete
       dimensions into patches
00170
          constexpr bool periodic=false;
                                                                                         /// - perodic or
       non-periodic boundaries
00171
           int processOrder=3;
                                                                                         /// - processes of the
       weak-field expansion, see README.md
00172
          constexpr sunrealtype simulationTime=2e-6;
                                                                                         /// - physical total
       simulation time
00173
          constexpr int numberOfSteps=5;
                                                                                         /// - discrete time steps
00174
          constexpr int outputStep=1;
                                                                                         /// - output step
       multiples
00175
          constexpr char outputStyle='b';
                                                                                /// - output in csv (c) or binary
        (b)
00176
00177
           /// Add electromagnetic waves.
00178
          planewave plane1;
                                                 /// A plane wave with
          plane1.k = {1e5,0,0};
plane1.p = {0,0,0.1};
00179
                                                 /// - wavevector (normalized to \f\$ 1/\lambda \f\$)
00180
                                                 /// - amplitude/polarization
                                                 /// - phase shift
00181
          plane1.phi = \{0,0,0\};
                                                 /// Another plane wave with
          planewave plane2;
plane2.k = {-1e6,0,0};
00182
00183
                                                 /// - wavevector (normalized to \f$ 1/\lambda \f$)
```

```
00184
          plane2.p = \{0,0,0.5\};
                                               /// - amplitude/polarization
          plane2.phi = \{0,0,0\};
                                                /// - phase shift
00185
00186
          // Do not comment out this vector, even if no plane wave is used. But if, emplace used plane
       waves.
00187
          vector<planewave> planewaves;
00188
          //planewaves.emplace back(plane1);
00189
          //planewaves.emplace_back(plane2);
00190
                                               /// A Gaussian wave with
00191
          gaussian3D gauss1;
          gauss1.x0 = {40e-6,40e-6,10e-6};
gauss1.axis = {1,0,0};
00192
                                               /// - center it approaches
                                               /// - normalized direction _from_ which the wave approaches
00193
       the center
                                               /// - amplitude
00194
         gauss1.amp = 0.05;
00195
          gauss1.phip = 2*atan(0);
                                               /// - polarization rotation from TE-mode (z-axis)
          gauss1.w0 = 3.5e-6;
gauss1.zr = 19.242e-6;
00196
                                               /// - taille
00197
                                               /// - Rayleigh length
          /// the wavelength is determined by the relation \f$ \lambda = \pi*w_0^2/z_R \f$
00198
00199
                                   /// - beam center
          gauss1.ph0 = 2e-5;
          gauss1.phA = 0.45e-5;
                                               /// - beam length
00200
          gaussian3D gauss2;
00201
                                               /// Another Gaussian wave with
          gauss2.x0 = {40e-6,40e-6,10e-6};  /// - center it approaches
gauss2.axis = {0,1,0};  /// - normalized direction
00202
                                               /// - normalized direction from which the wave approaches the
00203
       center
00204
                                               /// - amplitude
          gauss2.amp = 0.05;
00205
          qauss2.phip = 2*atan(0);
                                               /// - polarization rotation from TE-mode (z-axis)
          gauss2.w0 = 3.5e-6;
                                               /// - taille
                                               /// - Rayleigh length
00207
          gauss2.zr = 19.242e-6;
          gauss2.ph0 = 2e-5;
gauss2.phA = 0.45e-5;
00208
                                               /// - beam center
                                               /// - beam length
00209
          // Do not comment out this vector, even if no Gaussian wave is used. But if, emplace used Gaussian
00210
       waves.
00211
          vector<gaussian3D> Gaussians3D;
00212
          Gaussians3D.emplace_back(gauss1);
00213
          Gaussians3D.emplace_back(gauss2);
00214
          //// Do not change this below ////
00215
         static_assert(latticepoints_per_dim[0]*patches_per_dim[0]==0 && latticepoints_per_dim[1]*patches_per_dim[1]==0 &&
00216
00218
                  latticepoints_per_dim[2]%patches_per_dim[2]==0,
00219
                  "The number of lattice points in each dimension must be "
00220
                  "divisible by the number of patches in that direction.");
00221
          int *interactions = &processOrder;
00222
          Sim3D (CVodeTolerances, StencilOrder, physical_sidelengths,
00223
                  latticepoints_per_dim, patches_per_dim, periodic, interactions,
                  simulationTime, numberOfSteps, outputDirectory, outputStep,
00224
00225
                  outputStyle, planewaves, Gaussians3D);
00226
          00227
00228
00229
          00230
00231
          double tf=MPI_Wtime(); // Overall finish time
00232
          if(rank==0) {cout«endl; timer(ti,tf);} // Print the elapsed time
00233
00234
          // Finalize MPI environment
00235
          MPI Finalize();
00236
00237
          return 0:
00238 }
```

References planewave::k, gaussian1D::k, planewave::p, gaussian1D::p, planewave::phi, gaussian1D::phi, gaussian1D::phi, Sim1D(), Sim2D(), Sim3D(), timer(), and gaussian1D::x0.

Here is the call graph for this function:



6.15 main.cpp

Go to the documentation of this file.

```
00001 /// @file main.cpp
00002 /// @brief Main function to configure the user's simulation settings
00004
00005 #include "SimulationFunctions.h" /* complete simulation functions and all headers */
00006
00007
00008 int main(int argc, char *argv[])
00009 {
00010
             // Initialize MPI environment
            MPI_Init (&argc, &argv);
MPI_Comm comm = MPI_COMM_WORLD;
// Prepare MPI for Master-only threading
00011
00012
00013
            // Frequence Mer of Master-Only threading
//int provided;
//MPI_Init_thread(&argc, &argv, MPI_THREAD_FUNNELED, &provided);
00014
00015
00016
```

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```
int rank = 0;
          MPI_Comm_rank(comm,&rank);
00018
00019
          double ti=MPI_Wtime(); // Overall start time
00020
00021
          /** Determine the output directory.
  * A "SimResults" folder will be created if non-existent
00022
           * with a subdirectory named in the identifier format
* "yy-mm-dd_hh-MM-ss" that contains the csv files
00024
          //constexpr auto outputDirectory = "/gpfs/scratch/uh3o1/ru68dab/ru68dab/HE/outputs";
//constexpr auto outputDirectory = "/home/andi/Documents/";
constexpr auto outputDirectory = "/Users/andi/Documents/";
00025
00026
00027
00028
00029
          if(rank==0 && !filesystem::exists(outputDirectory)) {
00030
               cerr«"\nOutput directory nonexistent.\n";
00031
               MPI_Abort (comm, 1);
00032
00033
00034
00035
          //---- BEGIN OF CONFIGURATION -----//
00036
00037
           /** A 1D simulation with specified */
00038
00039
00040
          //// Specify your settings here ////
       constexpr array <sunrealtype,2> CVodeTolerances={1.0e-16,1.0e-16}; /// - relative and absolute tolerances of the CVode solver
00041
00042
          constexpr int StencilOrder=13;
                                                                                  /// - accuracy order of the
       stencils in the range 1-13
00043
          constexpr sunrealtype physical_sidelength=300e-6;
                                                                                  /// - physical length of the
       lattice in meters
00044
          constexpr sunindextype latticepoints=6e3;
                                                                                  /// - number of lattice points
00045
          constexpr bool periodic=true;
                                                                                  /// - periodic or vanishing
       boundary values
00046
          int processOrder=3;
                                                                                  /// - included processes of the
       weak-field expansion, see README.md
00047
          constexpr sunrealtype simulationTime=100.0e-61;
                                                                                  /// - physical total
       simulation time
00048
          constexpr int numberOfSteps=100;
                                                                                  /// - discrete time steps
00049
          constexpr int outputStep=1;
                                                                                /// - output step multiples
00050
          constexpr char outputStyle='c';
                                                                                /// - output in csv (c) or binary
00051
00052
          /// Add electromagnetic waves.
00053
                                             /// A plane wave with
          planewave plane1;
          plane1.k = \{1e5, 0, 0\};
                                             /// - wavevector (normalized to f 1/\lambda f)
00054
00055
          plane1.p = \{0,0,0.1\};
                                             /// - amplitude/polarization
00056
          plane1.phi = {0,0,0};
                                             /// - phase shift
00057
          planewave plane2;
                                              /// Another plane wave with
          plane2.k = {-le6,0,0};
plane2.p = {0,0,0.5};
00058
                                             /// - wavevector (normalized to \f$ 1/\lambda \f$)
                                             /// - amplitude/polarization
00059
          plane2.phi = \{0,0,0\};
                                              /// - phase shift
00060
           // Do not comment out this vector, even if no plane wave is used. But if, emplace used plane
00061
       waves.
00062
          vector<planewave> planewaves;
00063
          //planewaves.emplace_back(plane1);
00064
          //planewaves.emplace back(plane2);
00065
00066
          gaussian1D gauss1;
                                              /// A Gaussian wave with
          gauss1.k = {1.0e6,0,0};
gauss1.p = {0,0,0.1};
gauss1.x0 = {100e-6,0,0};
gauss1.phig = 5e-6;
gauss1.phi = {0,0,0};
00067
                                             /// - wavevector (normalized to \f$ 1/\lambda \f$)
                                             /// - polarization/amplitude
00068
                                             /// - shift from origin
00069
00070
                                             /// - width
00071
                                             /// - phase shift
00072
          gaussian1D gauss2;
                                             /// Another Gaussian with
00073
          gauss2.k = \{-0.2e6, 0, 0\};
                                             /// - wavevector (normalized to f 1/\lambda f)
          gauss2.p = \{0,0,0.5\};
gauss2.x0 = \{200e-6,0,0\};
                                              /// - polarization/amplitude
00074
                                              /// - shift from origin
00075
          gauss2.phig = 15e-6;
00076
                                             /// - width
          gauss2.phi = \{0,0,0\};
                                              /// - phase shift
00077
00078
           // Do not comment out this vector, even if no Gaussian wave is used. But if, emplace used Gaussian
00079
          vector<gaussian1D> Gaussians1D;
00080
          Gaussians1D.emplace_back(gauss1);
00081
          Gaussians1D.emplace_back(gauss2);
00082
00083
          //// Do not change this below ////
          int *interactions = &processOrder;
00084
00085
          Sim1D(CVodeTolerances, StencilOrder, physical_sidelength, latticepoints,
00086
                   periodic, interactions, simulationTime, numberOfSteps,
00087
                   outputDirectory,outputStep,outputStyle,
00088
                   planewaves, Gaussians1D);
00089
00090
          00091
00092
          00093
00094
          /** A 2D simulation with specified */
```

```
//// Specify your settings here ////
00096
00097
          constexpr array<sunrealtype,2> CVodeTolerances={1.0e-12,1.0e-12}; /// - relative and absolute
       tolerances of the CVode solver \,
00098
         constexpr int StencilOrder=13;
                                                                                /// - accuracy order of the
       stencils in the range 1-13
          constexpr array<sunrealtype,2> physical_sidelengths={80e-6,80e-6}; /// - physical length of the
00099
       lattice in the given dimensions in meters
00100
          constexpr array<sunindextype,2> latticepoints_per_dim={800,800}; /// - number of lattice points
       per dimension
00101
         constexpr array<int,2> patches_per_dim={2,2};
                                                                                 /// - slicing of discrete
       dimensions into patches
00102
         constexpr bool periodic=true;
                                                                                 /// - periodic or vanishing
       boundary values
00103
          int processOrder=3;
                                                                                 /// - included processes of the
       weak-field expansion, see README.md
00104
         constexpr sunrealtype simulationTime=4e-61;
                                                                                /// - physical total simulation
       time
00105
         constexpr int numberOfSteps=10;
                                                                                 /// - discrete time steps
00106
          constexpr int outputStep=1;
                                                                                /// - output step multiples
          constexpr char outputStyle='c';
                                                                               /// - output in csv (c) or binary
00107
00108
00109
          /// Add electromagnetic waves.
          planewave planel;
00110
                                               /// A plane wave with
          plane1.k = \{1e5, 0, 0\};
                                               /// - wavevector (normalized to f 1/\lambda f)
00111
          plane1.p = \{0,0,0.1\};
00112
                                               /// - amplitude/polarization
00113
          plane1.phi = \{0,0,0\};
                                               /// - phase shift
                                               /// Another plane wave with
00114
          planewave plane2;
          plane2.k = {-1e6,0,0};
plane2.p = {0,0,0.5};
00115
                                               /// - wavevector
00116
                                               /// - amplitude/polarization
00117
          plane2.phi = \{0,0,0\};
                                               /// - phase shift
           // Do not comment out this vector, even if no plane wave is used. But if, emplace used plane
00118
00119
          vector<planewave> planewaves;
00120
          //planewaves.emplace_back(plane1);
          //planewaves.emplace_back(plane2);
00121
00123
          gaussian2D gauss1;
                                               /// A Gaussian wave with
                                               /// - center it approaches
/// - normalized direction _from_ which the wave approaches the
00124
          gauss1.x0 = \{40e-6, 40e-6\};
          gauss1.axis = {1,0};
00125
       center
00126
          gauss1.amp = 0.5:
                                               /// - amplitude
00127
          gauss1.phip = 2*atan(0);
                                               /// - polarization rotation from TE-mode (z-axis)
          gauss1.w0 = 2.3e-6;
                                               /// - taille
00128
          gauss1.w0 = 2.3e-6;
gauss1.zr = 16.619e-6;
                                               /// - Rayleigh length
00129
00130
          /// the wavelength is determined by the relation f \lambda = \pi*w_0^2/z_R \f$
                                               /// - beam center /// - beam length
00131
          gauss1.ph0 = 2e-5;
          gauss1.phA = 0.45e-5;
00132
          gaussian2D gauss2;
00133
                                              /// Another Gaussian wave with
          gauss2.x0 = \{40e-6, 40e-6\};
00134
                                              /// - center it approaches
          gauss2.axis = \{-0.7071, 0.7071\}; /// - normalized direction from which the wave approaches the
00135
       center
00136
          qauss2.amp = 0.5;
                                               /// - amplitude
          gauss2.phip = 2*atan(0);
                                               /// - polarization rotation fom TE-mode (z-axis)
00137
          gauss2.w0 = 2.3e-6;
gauss2.zr = 16.619e-6;
                                               /// - taille
00138
                                               /// - Rayleigh length
          gauss2.ph0 = 2e-5;
                                               /// - beam center
00140
00141
          gauss2.phA = 0.45e-5;
                                               /// - beam length
00142
          // Do not comment out this vector, even if no Gaussian wave is used. But if, emplace used Gaussian
       waves.
00143
          vector<gaussian2D> Gaussians2D;
00144
          Gaussians2D.emplace_back(gauss1);
          Gaussians2D.emplace_back(gauss2);
00145
00146
00147
          //// Do not change this below ////
          static_assert(latticepoints_per_dim[0]%patches_per_dim[0]==0 &&
    latticepoints_per_dim[1]%patches_per_dim[1]==0,
    "The number of lattice points in each dimension must be "
00148
00149
00150
00151
                   "divisible by the number of patches in that direction.");
00152
          int * interactions = &processOrder;
00153
          Sim2D (CVodeTolerances, StencilOrder, physical_sidelengths,
00154
                   latticepoints_per_dim,patches_per_dim,periodic,interactions,
00155
                   simulationTime, numberOfSteps, outputDirectory, outputStep,
00156
                   outputStyle, planewaves, Gaussians2D);
00157
00158
          00159
00160
          00161
          /** A 3D simulation with specified */
00162
00163
00164
          //// Specify your settings here ////
00165
          constexpr array<sunrealtype,2> CVodeTolerances={1.0e-12,1.0e-12};
                                                                                      /// - relative and
       absolute tolerances of the CVode solver
00166
       constexpr int StencilOrder=4;
the stencils in the range 1-13
                                                                                       /// - accuracy order of
```

6.15 main.cpp 229

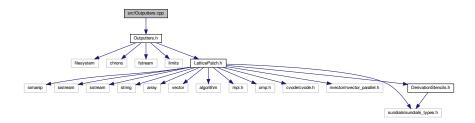
```
00167
          constexpr array<sunrealtype,3> physical_sidelengths={80e-6,80e-6,20e-6}; /// - physical dimensions
00168
          constexpr array<sunindextype, 3> latticepoints_per_dim={160,160,40};
                                                                                        /// - number of lattice
       points in any dimension
                                                                                        /// - slicing of discrete
00169
          constexpr array<int,3> patches_per_dim= {2,2,1};
       dimensions into patches

constexpr bool periodic=false;
00170
                                                                                        /// - perodic or
       non-periodic boundaries
          int processOrder=3;
00171
                                                                                        /// - processes of the
       weak-field expansion, see README.md
00172
          constexpr sunrealtype simulationTime=2e-6;
                                                                                        /// - physical total
       simulation time
00173
          constexpr int numberOfSteps=5;
                                                                                        /// - discrete time steps
                                                                                        /// - output step
00174
          constexpr int outputStep=1;
       multiples
00175
          constexpr char outputStyle='b';
                                                                                /// - output in csv (c) or binary
       (b)
00176
00177
          /// Add electromagnetic waves.
00178
          planewave planel;
                                                 /// A plane wave with
          plane1.k = {1e5,0,0};
plane1.p = {0,0,0.1};
plane1.phi = {0,0,0};
00179
                                                 /// - wavevector (normalized to f 1/\lambda \f$)
                                                 /// - amplitude/polarization
00180
                                                 /// - phase shift
00181
          planewave plane2;
plane2.k = {-1e6,0,0};
plane2.p = {0,0,0.5};
                                                /// Another plane wave with
00182
00183
                                                 /// - wavevector (normalized to \f$ 1/\lambda \f$)
                                                 /// - amplitude/polarization
00184
                                                 /// - phase shift
00185
          plane2.phi = \{0,0,0\};
00186
           // Do not comment out this vector, even if no plane wave is used. But if, emplace used plane
       waves.
00187
          vector<planewave> planewaves;
00188
          //planewaves.emplace back(plane1);
00189
          //planewaves.emplace back(plane2);
00190
00191
          gaussian3D gauss1;
                                                /// A Gaussian wave with
                                                /// - center it approaches
/// - normalized direction _from_ which the wave approaches
          gauss1.x0 = \{40e-6, 40e-6, 10e-6\};
gauss1.axis = \{1, 0, 0\};
00192
00193
       the center
00194
          gauss1.amp = 0.05;
                                                 /// - amplitude
00195
          gauss1.phip = 2*atan(0);
                                                /// - polarization rotation from TE-mode (z-axis)
          gauss1.w0 = 3.5e-6;
gauss1.zr = 19.242e-6;
00196
                                                 /// - taille
                                                 /// - Rayleigh length
00197
          /// the wavelength is determined by the relation \f$ \lambda = \pi*w_0^2/z_R \f$
00198
          gauss1.ph0 = 2e-5;
00199
                                                /// - beam center
          gauss1.phA = 0.45e-5;
                                                /// - beam length
00200
                                                /// Another Gaussian wave with
00201
          gaussian3D gauss2;
                                                /// - center it approaches
00202
          gauss2.x0 = \{40e-6, 40e-6, 10e-6\};
00203
          gauss2.axis = {0,1,0};
                                                /// - normalized direction from which the wave approaches the
       center
00204
          gauss2.amp = 0.05;
                                                 /// - amplitude
          gauss2.phip = 2*atan(0);
gauss2.w0 = 3.5e-6;
gauss2.zr = 19.242e-6;
00205
                                                /// - polarization rotation from TE-mode (z-axis)
                                                 /// - taille
00206
00207
                                                 /// - Rayleigh length
          gauss2.ph0 = 2e-5;
gauss2.phA = 0.45e-5;
00208
                                                 /// - beam center
00209
                                                 /// - beam length
          // Do not comment out this vector, even if no Gaussian wave is used. But if, emplace used Gaussian
00210
       waves.
00211
          vector<gaussian3D> Gaussians3D;
00212
          Gaussians3D.emplace_back(gauss1);
00213
          Gaussians3D.emplace_back(gauss2);
00214
00215
          //// Do not change this below ////
          static_assert(latticepoints_per_dim[0]%patches_per_dim[0]==0 &&
00216
00217
                   latticepoints_per_dim[1]%patches_per_dim[1] == 0 &&
00218
                   latticepoints_per_dim[2]%patches_per_dim[2]==0,
00219
                   "The number of lattice points in each dimension must be "
00220
                   "divisible by the number of patches in that direction.");
00221
          int *interactions = &processOrder;
00222
          Sim3D (CVodeTolerances, StencilOrder, physical_sidelengths,
00223
                   latticepoints_per_dim, patches_per_dim, periodic, interactions,
00224
                   simulationTime, numberOfSteps, outputDirectory, outputStep,
00225
                   outputStyle, planewaves, Gaussians3D);
00226
00227
          00228
00229
          00230
00231
          double tf=MPI_Wtime(); // Overall finish time
00232
          if(rank==0) {cout«endl; timer(ti,tf);} // Print the elapsed time
00233
00234
           // Finalize MPT environment
00235
          MPI Finalize();
00236
00237
          return 0;
00238 }
```

6.16 src/Outputters.cpp File Reference

Generation of output writing to disk.

```
#include "Outputters.h"
Include dependency graph for Outputters.cpp:
```



6.16.1 Detailed Description

Generation of output writing to disk.

\$

Definition in file Outputters.cpp.

6.17 Outputters.cpp

```
Go to the documentation of this file.
```

```
00005
00006 #include "Outputters.h"
00007
00008 /// Directly generate the simCode at construction
00009 OutputManager::OutputManager() {
00010    simCode = SimCodeGenerator();
00011
        outputStyle = 'c';
00012 }
00013
00014 /// Generate the identifier number reverse from year to minute in the format
00015 /// yy-mm-dd_hh-MM-ss
00016 string OutputManager::SimCodeGenerator() {
       const chrono::time_point<chrono::system_clock> now{
00018
           chrono::system_clock::now() };
00019
        const chrono::year_month_day ymd{chrono::floor<chrono::days>(now)};
       const auto tod = now - chrono::floor<chrono::days>(now);
const chrono::hh_mm_ss hms{tod};
00020
00021
00022
00023
        stringstream temp;
        temp « setfill('0') « setw(2)
00024
00025
              <\!\!<\!\!<\!\!\mathrm{setfill}('0')<\!\!<\!\!<\!\!\mathrm{setw}(2)<\!\!<\!\!\mathrm{static\_cast}<\!\!\mathrm{unsigned}>\!\!(\mathrm{ymd.month}())<\!\!<\!\!<\!\!"-"
00026
             00027
00028
00029
00030
             « hms.seconds().count();
00031
             //« "_" « hms.subseconds().count(); // subseconds render the filename
00032
             // too large
00033
        return temp.str();
00034 }
00036 /** Generate the folder to save the data to by one process:
```

6.17 Outputters.cpp 231

```
* In the given directory it creates a directory "SimResults" and a directory
       * with the simCode. The relevant part of the main file is written to a
00039 \, * "config.txt" file in that directory to log the settings. */
00040 void OutputManager::generateOutputFolder(const string &dir) {
00041
        // Do this only once for the first process
00042
         int mvPrc:
        MPI_Comm_rank (MPI_COMM_WORLD, &myPrc);
00044
         if (myPrc == 0) {
00045
          if (!fs::is_directory(dir))
          fs::create_directory(dir);
if (!fs::is_directory(dir + "/SimResults"))
fs::create_directory(dir + "/SimResults");
if (!fs::is_directory(dir + "/SimResults") +
00046
00047
00048
00049
                                                            + simCode))
             fs::create_directory(dir + "/SimResults/" + simCode);
00050
00051
        // path variable for the output generation
Path = dir + "/SimResults/" + simCode + "/";
00052
00053
00054
         // Logging configurations from main.cpp
        ifstream fin("main.cpp");
ofstream fout(Path + "config.txt");
00056
00057
00058
         string line;
        int begin=1000;
00059
00060
        for (int i = 1; !fin.eof(); i++) {
  getline(fin, line);
00061
           if (line.starts_with("
                                       //---- B")) {
00062
00063
               begin=i;
00064
          if (i < begin) {</pre>
00065
00066
            continue:
00067
00068
           fout « line « endl;
00069
           if (line.starts_with("
                                      //---- E")) {
00070
               break;
00071
00072
00073
        return;
00074 }
00075
00076 void OutputManager::set_outputStyle(const char _outputStyle){
00077
          outputStyle = _outputStyle;
00078 }
00079
00080 /** Write the field data either in csv format to one file per each process
00081 * (patch) or in binary form to a single file. Files are stores inthe simCode 00082 * directory. For csv files the state (simulation step) denotes the
00083 \,\,\star\,\,\mathrm{prefix} and the suffix after an underscore is given by the process/patch
00084 \, * number. Binary files are simply named after the step number. \star/
00085 void OutputManager::outUState(const int &state, const Lattice &lattice,
00086
              const LatticePatch &latticePatch) {
        switch(outputStyle){
             case 'c': { // one csv file per process
00088
        ofstream ofs;
00089
        ofs.open(Path + to_string(state) + "_" + to_string(lattice.my_prc) + ".csv");
00090
        of s. open (Path + to_string (state) + "_" + to_string (tattee.my_prc) + ".csv");

// Precision of sunrealtype in significant decimal digits; 15 for IEEE double
ofs « setprecision(numeric_limits<sunrealtype>::digits10);
00091
00092
00093
00094
         // Walk through each lattice point
        00095
00096
00097
00098
               « latticePatch.uData[i + 4] « "," « latticePatch.uData[i + 5]
00099
00100
00101
00102
        ofs.close();
00103
        break;
00104
00105
             case 'b': { // a single binary file
00107
         // Open the output file
00108
        MPI File fh;
00109
        const string filename = Path+to_string(state);
        MPI_File_open(lattice.comm,&filename[0],MPI_MODE_WRONLY|MPI_MODE_CREATE,
00110
00111
                  MPI INFO NULL, &fh);
00112
         // number of datapoints in the patch with process offset
00113
         const int count = latticePatch.discreteSize()*lattice.get_dataPointDimension();
00114
        MPI_Offset offset = lattice.my_prc*count*sizeof(MPI_SUNREALTYPE);
00115
         // Go to offset in file and write data to it; maximal precision in
         // "native" representation
00116
        MPI_File_set_view(fh,offset,MPI_SUNREALTYPE,MPI_SUNREALTYPE,"native",
00117
00118
                 MPI_INFO_NULL);
00119
        MPI_File_write_all(fh,latticePatch.uData,count,MPI_SUNREALTYPE,MPI_STATUS_IGNORE);
00120
        MPI_Request write_request;
00121
        MPI_File_iwrite_all(fh,latticePatch.uData,count,MPI_SUNREALTYPE,&write_request);
00122
00123
        MPI_Wait(&write_request, MPI_STATUS_IGNORE);
```

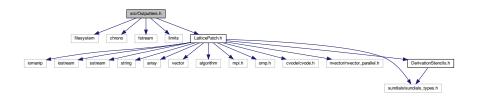
```
00124
00125
        MPI_File_write_at_all(fh,offset,latticePatch.uData,count,MPI_SUNREALTYPE,
00126
               MPI_STATUS_IGNORE);
00127
00128
                */
00129
        break;
00130
00131
            default: {
       errorKill("No valid output style defined.\
00132
                Choose between (c): one csv file per process, (b) one binary file");
00133
       break;
00134
00135
00136
        return;
00137
00138 }
00139
```

6.18 src/Outputters.h File Reference

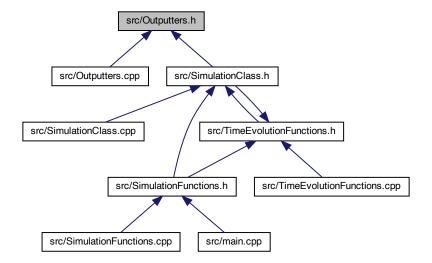
OutputManager class to outstream simulation data.

```
#include <filesystem>
#include <chrono>
#include <fstream>
#include <limits>
#include "LatticePatch.h"
```

Include dependency graph for Outputters.h:



This graph shows which files directly or indirectly include this file:



6.19 Outputters.h

Data Structures

· class OutputManager

Output Manager class to generate and coordinate output writing to disk.

6.18.1 Detailed Description

OutputManager class to outstream simulation data.

Definition in file Outputters.h.

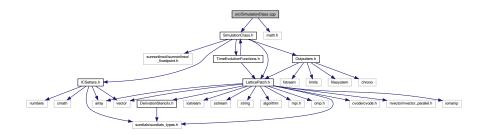
6.19 Outputters.h

```
Go to the documentation of this file.
         00002 /// @file Outputters.h
00003 /// @brief OutputManager class to outstream simulation data
00005
00006 #pragma once
00007
00008 // perform operations on the filesystem
00009 #include <filesystem>
00010
00011 // output controlling with limits and timestep
00012 #include <chrono>
00013 #include <fstream>
00014 #include <limits>
00015
00016 // project subfile header
00017 #include "LatticePatch.h'
00018
00019 using namespace std;
00020 namespace fs = std::filesystem;
00021 namespace chrono = std::chrono;
00022
00023 /** @brief Output Manager class to generate and coordinate output writing to
00024 * disk */
00025 class OutputManager {
00026 private:
      /// function to create the Code of the Simulations
00027
      static string SimCodeGenerator();
00028
      /// varible to safe the SimCode generated at execution
      string simCode;
00031
      /// variable for the path to the output folder
00032
       string Path;
00033
      /// output style; csv or binary
00034
       char outputStyle;
00035 public:
      /// default constructor
00037
       OutputManager();
00038
       /// function that creates folder to save simulation data
00039
       void generateOutputFolder(const string &dir);
      /// set the output style
void set_outputStyle(const char _outputStyle);
00040
00041
00042
       /// function to write data to disk in specified way
00043
       void outUState(const int &state, const Lattice &lattice, const LatticePatch);
00044
       \ensuremath{///} simCode getter function
00045
       [[nodiscard]] const string &getSimCode() const { return simCode; }
00046 };
00047
```

6.20 src/SimulationClass.cpp File Reference

Interface to the whole Simulation procedure: from wave settings over lattice construction, time evolution and outputs (also all relevant CVODE steps are performed here)

```
#include "SimulationClass.h"
#include <math.h>
Include dependency graph for SimulationClass.cpp:
```



6.20.1 Detailed Description

Interface to the whole Simulation procedure: from wave settings over lattice construction, time evolution and outputs (also all relevant CVODE steps are performed here)

Definition in file SimulationClass.cpp.

6.21 SimulationClass.cpp

Go to the documentation of this file.

```
00002 /// @file SimulationClass.cpp
00003 /// @brief Interface to the whole Simulation procedure:
00004 /// from wave settings over lattice construction, time evolution and outputs
00005 /// (also all relevant CVODE steps are performed here)
00007
00008 #include "SimulationClass.h"
00009
00010 #include <math.h>
00011
00012 /\!/\!/ Along with the simulation object, create the cartesian communicator and
00013 /// SUNContext object
00014 Simulation::Simulation(const int nx, const int ny, const int nz,
00015
               const int StencilOrder, const bool periodicity) :
00016
          lattice(StencilOrder) {
00017
        statusFlags = 0;
00018
        t = 0;
00019
        // Initialize the cartesian communicator
00020
        lattice.initializeCommunicator(nx, ny, nz, periodicity);
00021
00022
        // Create the SUNContext object associated with the thread of execution
00023
        int retval = 0;
00024
        retval = SUNContext_Create(&lattice.comm, &lattice.sunctx);
00025
        if (check_retval(&retval, "SUNContext_Create", 1, lattice.my_prc))
00026
          MPI_Abort(lattice.comm, 1);
        // if (flag != CV_SUCCESS) { printf("SUNContext_Create failed, flag=%d.\n", // flag);
00027
00028
00029
                MPI_Abort(lattice.comm, 1); }
00030 }
00031
00032 /\!/\!/ Free the CVode solver memory and Sundials context object with the finish of
00033 ///  the simulation
00034 Simulation::~Simulation() {
00035
       // Free solver memory
        if (statusFlags & CvodeObjectSetUp) {
    // PrintFinalStats(cvode_mem); // TODO write this function as in cvodes
00037
00038
           // cvAdvDiff_bnd.c SUNDIALS_MARK_FUNCTION_END(lattice.profobj);
00039
          CVodeFree(&cvode_mem);
00040
          SUNContext_Free (&lattice.sunctx);
00041
        }
00042 }
00043
```

```
00044 /\!/\!/ Set the discrete dimensions, the number of points per dimension
00045 void Simulation::setDiscreteDimensionsOfLattice(const sunindextype nx,
00046
               const sunindextype ny, const sunindextype nz) {
        checkNoFlag(LatticePatchworkSetUp);
00047
00048
        lattice.setDiscreteDimensions(nx, ny, nz);
00049
        statusFlags |= LatticeDiscreteSetUp;
00050 }
00051
00052 /// Set the physical dimensions with lenghts in micro meters
00053 void Simulation::setPhysicalDimensionsOfLattice(const sunrealtype lx,
        const sunrealtype ly, const sunrealtype lz) {
checkNoFlag(LatticePatchworkSetUp);
00054
00055
00056
        lattice.setPhysicalDimensions(lx, ly, lz);
        statusFlags |= LatticePhysicalSetUp;
00057
00058 }
00059
00060 /// Check that the lattice dimensions are set up and generate the patchwork
00061 void Simulation::initializePatchwork(const int nx, const int ny,
00062
               const int nz) {
00063
        checkFlag(LatticeDiscreteSetUp);
00064
        checkFlag(LatticePhysicalSetUp);
00065
00066
        // Generate the patchwork
00067
        generatePatchwork(lattice, latticePatch, nx, ny, nz);
00068
        latticePatch.initializeBuffers();
00069
00070
        statusFlags |= LatticePatchworkSetUp;
00071 }
00072
00073 /// Configure CVODE
00074 void Simulation::initializeCVODEobject(const sunrealtype reltol,
               const sunrealtype abstol) {
00076
        checkFlag(SimulationStarted);
00077
00078
        // CVode settings return value
00079
        int retval = 0;
08000
        // Set the profiler
00082
        retval = SUNContext_GetProfiler(lattice.sunctx, &lattice.profobj);
        if (check_retval(&retval, "SUNContext_GetProfiler", 1, lattice.my_prc))
    MPI_Abort(lattice.comm, 1);
// if (flag != CV_SUCCESS) { printf("SUNContext_GetProfiler failed,
    // flag=%d.\n", flag);
00083
00084
00085
00086
00087
                MPI_Abort(lattice.comm, 1); }
00088
00089
        // SUNDIALS_MARK_FUNCTION_BEGIN(profobj);
00090
00091
        // Create CVODE object \operatorname{\mathsf{--}} returns a pointer to the cvode memory structure
00092
        // with Adams method (Adams-Moulton formula) solver chosen for non-stiff ODE
        cvode_mem = CVodeCreate(CV_ADAMS, lattice.sunctx);
00093
00094
00095
         // Specify user data and attach it to the main cvode memory block
00096
        retval = CVodeSetUserData(
            cvode_mem,
00097
00098
             &latticePatch); // patch contains the user data as used in CVRhsFn
          f (check_retval(&retval, "CVodeSetUserData", 1, lattice.my_prc))
MPI_Abort(lattice.comm, 1);
00099
00100
         // if (flag != CV_SUCCESS) { printf("CVodeSetUserData failed, flag=%d.\n",
00101
00102
         // flag);
00103
                MPI_Abort(lattice.comm, 1); }
00104
00105
         // Initialize CVODE solver -> can only be called after start of simulation to
00106
        // have data ready Provide required problem and solution specifications,
         // allocate internal memory, and initialize cvode
00107
00108
        retval = CVodeInit(cvode_mem, TimeEvolution::f, 0,
                             00109
00110
        if (check_retval(&retval, "CVodeInit", 1, lattice.my_prc))
00111
          MPI_Abort(lattice.comm, 1);
00112
         // if (flag != CV_SUCCESS) { printf("CVodeInit failed, flag=%d.\n", flag);
00113
00114
                MPI_Abort(lattice.comm, 1); }
00115
00116
        // Create fixed point nonlinear solver object (suitable for non-stiff ODE) and
00117
         // attach it to CVode
        SUNNonlinearSolver NLS =
00118
00119
             SUNNonlinSol_FixedPoint(latticePatch.u, 0, lattice.sunctx);
00120
        retval = CVodeSetNonlinearSolver(cvode_mem, NLS);
00121
        if (check_retval(&retval, "CVodeSetNonlinearSolver", 1, lattice.my_prc))
        MPI_Abort(lattice.comm, 1);
// if (flag != CV_SUCCESS) {printf("CVodeSetNonlinearSolver failed,
// flag=%d.\n", flag);
00122
00123
00124
00125
                MPI_Abort(lattice.comm, 1); }
00126
00127
         // Specify the maximum number of steps to be taken by the solver in its
00128
        \ensuremath{//} attempt to reach the next output time
        retval = CVodeSetMaxNumSteps(cvode_mem, 10000);
if (check_retval(&retval, "CVodeSetMaxNumSteps", 1, lattice.my_prc))
00129
00130
```

```
MPI_Abort(lattice.comm, 1);
         // if (flag != CV_SUCCESS) { printf("CVodeSetMaxNumSteps failed, flag=%d.\n",
00132
00133
         // flag);
         11
00134
                 MPI Abort (lattice.comm, 1); }
00135
00136
         // Specify integration tolerances -- a scalar relative tolerance and scalar
00137
         // absolute tolerance
00138
         retval = CVodeSStolerances(cvode_mem, reltol, abstol);
         if (check_retval(&retval, "CVodeSStolerances", 1, lattice.my_prc))
    MPI_Abort(lattice.comm, 1);
// if (flag != CV_SUCCESS) { printf("CVodeSStolerances failed, flag=%d.\n",
00139
00140
00141
         // flag);
00142
00143
                 MPI_Abort(lattice.comm, 1); }
00144
00145
         statusFlags |= CvodeObjectSetUp;
00146 }
00147
00148 /// Check if the lattice patchwork is set up and set the initial conditions
00149 void Simulation::start() {
00150
        checkFlag(LatticeDiscreteSetUp);
         checkFlag(LatticePhysicalSetUp);
00151
00152
         checkFlag(LatticePatchworkSetUp);
00153
         checkNoFlag(SimulationStarted);
00154
         checkNoFlag(CvodeObjectSetUp):
00155
         setInitialConditions();
00156
        statusFlags |= SimulationStarted;
00157 }
00158
00159 /\!/\!/ Set initial conditions: Fill the lattice points with the initial field
00160 /// values
00161 void Simulation::setInitialConditions()
        const sunrealtype dx = latticePatch.getDelta(1);
const sunrealtype dy = latticePatch.getDelta(2);
00162
00163
00164
         const sunrealtype dz = latticePatch.getDelta(3);
         const int nx = latticePatch.discreteSize(1);
const int ny = latticePatch.discreteSize(2);
00165
00166
         const sunrealtype x0 = latticePatch.origin(1);
00167
         const sunrealtype y0 = latticePatch.origin(2);
00168
         const sunrealtype z0 = latticePatch.origin(3);
00169
00170
         int px = 0, py = 0, pz = 0;
00171
         // space coordinates
         for (int i = 0; i < latticePatch.discreteSize() * 6; i += 6) {
   px = (i / 6) % nx;</pre>
00172
00173
          py = ((i / 6) / nx) % ny;

pz = ((i / 6) / nx) / ny;
00174
00175
00176
           // Call the 'eval' function to fill the lattice points with the field data
00177
           icsettings.eval(static_cast<sunrealtype>(px) * dx + x0,
                    static_cast<sunrealtype>(py) * dy + y0,
static_cast<sunrealtype>(pz) * dz + z0, &latticePatch.uData[i]);
00178
00179
00180
00181
         return;
00182 }
00183
00184 /// Use parameters to add periodic IC layers
00185 void Simulation::addInitialConditions(const int xm, const int ym,
00186
               const int zm /* zm=0 always */ ) {
         const sunrealtype dx = latticePatch.getDelta(1);
00187
00188
         const sunrealtype dy = latticePatch.getDelta(2);
00189
         const sunrealtype dz = latticePatch.getDelta(3);
         const int nx = latticePatch.discreteSize(1);
const int ny = latticePatch.discreteSize(2);
00190
00191
00192
         // Correct for demanded displacement, rest as for setInitialConditions
00193
         const sunrealtype x0 = latticePatch.origin(1) + xm*lattice.get_tot_lx();
00194
         const sunrealtype y0 = latticePatch.origin(2) + ym*lattice.get_tot_ly();
         const sunrealtype z0 = latticePatch.origin(3) + zm*lattice.get_tot_lz();
00195
00196
         int px = 0, py = 0, pz = 0;
         for (int i = 0; i < latticePatch.discreteSize() * 6; i += 6) {
   px = (i / 6) % nx;</pre>
00197
00198
           py = ((i / 6) / nx) % ny;

pz = ((i / 6) / nx) / ny;
00199
00200
00201
           icsettings.add(static_cast<sunrealtype>(px) * dx + x0,
                    static_cast<sunrealtype>(py) * dy + y0,
static_cast<sunrealtype>(pz) * dz + z0, &latticePatch.uData[i]);
00202
00203
00204
00205
        return;
00206 }
00207
00208 /// Add initial conditions in one dimension
00209 void Simulation::addPeriodicICLayerInX() {
00210 addInitialConditions(-1, 0, 0);
00211
        addInitialConditions(1, 0, 0);
00212
        return;
00213 }
00214
00215 /// Add initial conditions in two dimensions
00216 void Simulation::addPeriodicICLayerInXY() {
00217
        addInitialConditions(-1, -1, 0);
```

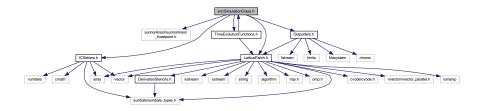
```
addInitialConditions(-1, 0, 0);
00219
       addInitialConditions(-1, 1, 0);
00220
        addInitialConditions(0, 1, 0);
       addInitialConditions(0, -1, 0);
00221
00222
       addInitialConditions(1, -1, 0);
       addInitialConditions(1, 0, 0);
00223
00224
       addInitialConditions(1, 1, 0);
00225
00226 }
00227
00228 /// Advance the solution in time -> integrate the ODE over an interval t
00229 void Simulation::advanceToTime(const sunrealtype &tEnd) {
00230
       checkFlag(SimulationStarted);
00231
        int flag = 0;
00232
       flag = CVode(cvode_mem, tEnd, latticePatch.u, &t,
                    CV_NORMAL); // CV_NORMAL: internal steps to reach tEnd, then // interpolate to return latticePatch.u, return time
00233
00234
00235
                                 // reached by the solver as t
00236
       if (flag != CV_SUCCESS)
        printf("CVode failed, flag=%d.\n", flag);
00237
00238 }
00239
00240 /// Write specified simulations steps to disk
00241 void Simulation::outAllFieldData(const int & state) {
00242
       checkFlag(SimulationStarted);
00243
       outputManager.outUState(state, lattice, latticePatch);
00244 }
00245
00246 /// Check the presence configuration flags
00247 void Simulation::checkFlag(unsigned int flag) const {
       if (!(statusFlags & flag)) {
00248
00249
         string errorMessage;
00250
         switch (flag) {
00251
         case LatticeDiscreteSetUp:
00252
           errorMessage = "The discrete size of the Simulation has not been set up";
00253
           break;
         case LatticePhysicalSetUp:
00254
           errorMessage = "The physical size of the Simulation has not been set up";
00256
           break;
00257
          case LatticePatchworkSetUp:
00258
           errorMessage = "The patchwork for the Simulation has not been set up";
00259
           break;
         case CvodeObjectSetUp:
00260
          errorMessage = "The CVODE object has not been initialized";
break;
00261
00262
00263
          case SimulationStarted:
00264
          errorMessage = "The Simulation has not been started";
00265
           break;
00266
         default:
          errorMessage = "Uppss, you've made a non-standard error, sadly I can't "
00267
00268
                          "help you there";
00269
00270
00271
         errorKill(errorMessage);
00272
00273
       return;
00274 }
00275
00276 /// Check the absence of configuration flags
00277 void Simulation::checkNoFlag(unsigned int flag) const {
00278
       if ((statusFlags & flag)) {
00279
         string errorMessage;
00280
         switch (flag) {
         case LatticeDiscreteSetUp:
00281
00282
           errorMessage =
00283
               "The discrete size of the Simulation has already been set up";
00284
           break;
00285
         case LatticePhysicalSetUp:
00286
           errorMessage
00287
                "The physical size of the Simulation has already been set up";
00288
           break;
00289
          case LatticePatchworkSetUp:
00290
           errorMessage = "The patchwork for the Simulation has already been set up";
00291
           break:
00292
         case CvodeObjectSetUp:
00293
           errorMessage = "The CVODE object has already been initialized";
00294
           break;
00295
         case SimulationStarted:
           00296
00297
00298
           break;
00299
         default:
00300
           errorMessage = "Uppss, you've made a non-standard error, sadly I can't "
00301
                          "help you there";
00302
           break;
00303
00304
         errorKill(errorMessage);
```

```
00305 }
00306 return;
00307 }
```

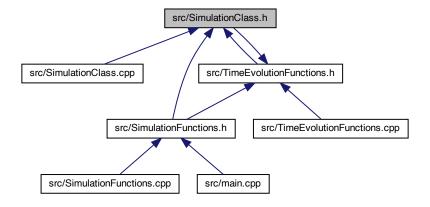
6.22 src/SimulationClass.h File Reference

Class for the Simulation object calling all functionality: from wave settings over lattice construction, time evolution and outputs initialization of the CVode object.

```
#include "sunnonlinsol/sunnonlinsol_fixedpoint.h"
#include "ICSetters.h"
#include "LatticePatch.h"
#include "Outputters.h"
#include "TimeEvolutionFunctions.h"
Include dependency graph for SimulationClass.h:
```



This graph shows which files directly or indirectly include this file:



Data Structures

· class Simulation

Simulation class to instantiate the whole walkthrough of a Simulation.

6.23 SimulationClass.h 239

Enumerations

```
    enum SimulationOptions {
        LatticeDiscreteSetUp = 0x01 , LatticePhysicalSetUp = 0x02 , LatticePatchworkSetUp = 0x04 ,
        CvodeObjectSetUp = 0x08 ,
        SimulationStarted = 0x10 }
        simulation checking flags
```

6.22.1 Detailed Description

Class for the Simulation object calling all functionality: from wave settings over lattice construction, time evolution and outputs initialization of the CVode object.

Definition in file SimulationClass.h.

6.22.2 Enumeration Type Documentation

6.22.2.1 SimulationOptions

```
enum SimulationOptions
```

simulation checking flags

Enumerator

LatticeDiscreteSetUp	
LatticePhysicalSetUp	
LatticePatchworkSetUp	
CvodeObjectSetUp	
SimulationStarted	

Definition at line 22 of file SimulationClass.h.

6.23 SimulationClass.h

```
Go to the documentation of this file.
```

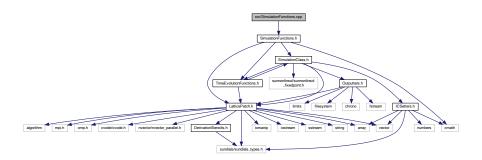
```
00002 /// @file SimulationClass.h
00003 /// @brief Class for the Simulation object calling all functionality:
00004 /// from wave settings over lattice construction, time evolution and outputs
00007
00008 #pragma once
00009
00010 /\star access to the fixed point SUNNonlinear
Solver \star/
00011 #include "sunnonlinsol/sunnonlinsol_fixedpoint.h"
00012
00013 // project subfile headers
00014 #include "ICSetters.h"
00015 #include "LatticePatch.h"
00016 #include "Outputters.h"
00017 #include "TimeEvolutionFunctions.h"
00018
00019 using namespace std;
00021 /// simulation checking flags
00022 enum SimulationOptions {
00023
       LatticeDiscreteSetUp = 0x01,
        LatticePhysicalSetUp = 0x02,
00024
        LatticePatchworkSetUp = 0x04, // not used anymore
00025
00026
        CvodeObjectSetUp = 0x08,
       SimulationStarted = 0x10
00027
00028
        /*OPT_B = 0x02,
00029
       OPT_C = 0x04,
00030
       OPT_D = 0x08,
       OPT_E = 0x10
00031
00032
       OPT F = 0x20.*/
00033 };
00034
00035 /** @brief Simulation class to instantiate the whole walkthrough of a Simulation
00036 */
00037 class Simulation {
00038 private:
       /// Lattice object
00040
        Lattice lattice:
00041
        /// LatticePatch object
00042
        LatticePatch latticePatch;
00043
       /// current time of the simulation
00044
       sunrealtype t;
00045
        /// char for checking simulation flags
       unsigned char statusFlags;
00046
00047
00048 public:
       /// IC Setter object
00049
00050
        ICSetter icsettings:
00051
        /// Output Manager object
        OutputManager outputManager;
00053
        /// Pointer to CVode memory object -- public to avoid cross library errors
00054
        void *cvode_mem;
00055
        /// constructor function for the creation of the cartesian communicator
00056
        Simulation(const int nx, const int ny, const int nz, const int StencilOrder,
00057
                const bool periodicity);
00058
        /// destructor function freeing CVode memory and Sundials context
00059
        ~Simulation();
00060
        /// Reference to the cartesian communicator of the lattice -> for debugging
00061
        MPI_Comm *get_cart_comm() { return &lattice.comm; };
00062
        /// function to set discrete dimensions of the lattice
00063
        void setDiscreteDimensionsOfLattice(const sunindextype _tot_nx,
        const sunindextype _tot_ny, const sunindextype _tot_nz);
/// function to set physical dimensions of the lattice
00064
00065
00066
        void setPhysicalDimensionsOfLattice(const sunrealtype lx, const sunrealtype ly,
00067
                                              const sunrealtype lz);
        /// function to initialize the Patchwork
00068
        void initializePatchwork(const int nx, const int ny, const int nz);
/// function to initialize the CVODE object with all requirements
00069
00070
00071
        void initializeCVODEobject(const sunrealtype reltol,
00072
                                    const sunrealtype abstol);
00073
        \ensuremath{///} function to start the simulation for time iteration
00074
        void start();
00075
        /// functions to set the initial field configuration onto the lattice
00076
        void setInitialConditions();
00077
        /// functions to add initial periodic field configurations
00078
        void addInitialConditions(const int xm, const int ym, const int zm = 0);
00079
        \ensuremath{/\!/} function to add a periodic IC Layer in one dimension
08000
        void addPeriodicICLayerInX();
00081
        /// function to add periodic IC Layers in two dimensions
        void addPeriodicICLayerInXY();
00082
00083
        /// function to advance solution in time with CVODE
00084
        void advanceToTime(const sunrealtype &tEnd);
00085
        /// function to generate Output of the whole field at a given time
00086
        void outAllFieldData(const int & state);
00087
        /// function to check that a flag has been set and if not print an error
00088
        // message and cause an abort on all ranks
```

```
00089    void checkFlag(unsigned int flag) const;
00090    /// function to check that if flag has not been set and if print an error
00091    // message and cause an abort on all ranks
00092    void checkNoFlag(unsigned int flag) const;
00093 };
00094
```

6.24 src/SimulationFunctions.cpp File Reference

Implementation of the complete simulation functions for 1D, 2D, and 3D, as called in the main function.

#include "SimulationFunctions.h"
Include dependency graph for SimulationFunctions.cpp:



Functions

- void timer (double &t1, double &t2)
- void Sim1D (const array< sunrealtype, 2 > CVodeTol, const int StencilOrder, const sunrealtype phys_
 dim, const sunindextype disc_dim, const bool periodic, int *interactions, const sunrealtype endTime, const
 int numberOfSteps, const string outputDirectory, const int outputStep, const char outputStyle, const vector<
 planewave > &planes, const vector< gaussian1D > &gaussians)

complete 1D Simulation function

void Sim2D (const array< sunrealtype, 2 > CVodeTol, int const StencilOrder, const array< sunrealtype, 2 > phys_dims, const array< sunindextype, 2 > disc_dims, const array< int, 2 > patches, const bool periodic, int *interactions, const sunrealtype endTime, const int numberOfSteps, const string outputDirectory, const int outputStep, const char outputStyle, const vector< planewave > &planes, const vector< gaussian2D > &gaussians)

complete 2D Simulation function

void Sim3D (const array< sunrealtype, 2 > CVodeTol, const int StencilOrder, const array< sunrealtype, 3 > phys_dims, const array< sunindextype, 3 > disc_dims, const array< int, 3 > patches, const bool periodic, int *interactions, const sunrealtype endTime, const int numberOfSteps, const string outputDirectory, const int outputStep, const char outputStyle, const vector< planewave > &planes, const vector< gaussian3D > &gaussians)

complete 3D Simulation function

6.24.1 Detailed Description

Implementation of the complete simulation functions for 1D, 2D, and 3D, as called in the main function.

Definition in file SimulationFunctions.cpp.

6.24.2 Function Documentation

6.24.2.1 Sim1D()

complete 1D Simulation function

Conduct the complete 1D simulation process

Definition at line 23 of file SimulationFunctions.cpp.

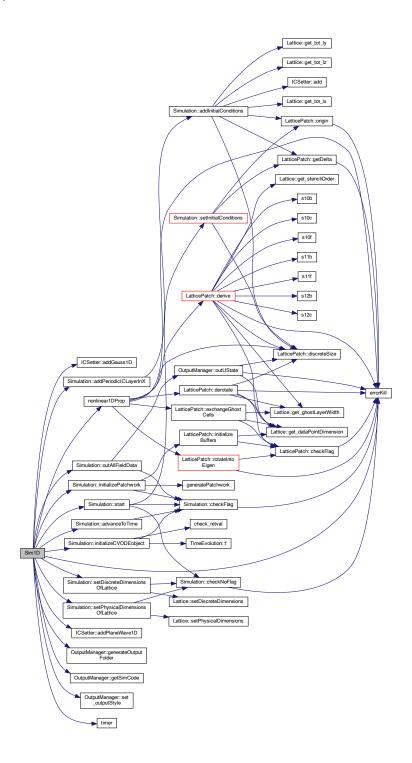
```
00031
         // MPI data
00032
        int myPrc = 0, nprc = 0;
00033
        MPI_Comm_size(MPI_COMM_WORLD, &nprc);
MPI_Comm_rank(MPI_COMM_WORLD, &myPrc);
00034
00035
00037
         // Check feasibility of the patchwork decomposition
00038
         if (myPrc == 0) {
             if (disc_dim % nprc != 0) {
  errorKill("The number of lattice points must be "
    "divisible by the number of processes.");
00039
00040
00041
00042
00043
00044
00045
        \ensuremath{//} Initialize the simulation, set up the cartesian communicator
00046
        array<int, 3> patches = {nprc, 1, 1};
        Simulation sim(patches[0], patches[1], patches[2], StencilOrder, periodic);
00047
00048
00049
        // Configure the patchwork
00050
        sim.setPhysicalDimensionsOfLattice(phys_dim,1,1);
00051
        sim.setDiscreteDimensionsOfLattice(disc_dim,1,1);
00052
        \verb|sim.initializePatchwork(patches[0], patches[1], patches[2]);\\
00053
00054
        // Add em-waves
00055
        for (const auto &gauss : gaussians)
00056
          sim.icsettings.addGauss1D(gauss.k, gauss.p, gauss.x0, gauss.phig,
00057
                                        gauss.phi);
00058
        for (const auto &plane : planes)
00059
          sim.icsettings.addPlaneWave1D(plane.k, plane.p, plane.phi);
00060
00061
        // Check that the patchwork is ready and set the initial conditions
        sim.start();
00062
00063
        sim.addPeriodicICLayerInX();
00064
00065
         // Initialize CVode with abs and rel tolerances
00066
        sim.initializeCVODEobject(CVodeTol[0], CVodeTol[1]);
00067
         \ensuremath{//} Configure the time evolution function
00068
00069
         TimeEvolution::c = interactions;
00070
00071
        TimeEvolution::TimeEvolver = nonlinear1DProp;
00072
        // Configure the output
00073
        sim.outputManager.generateOutputFolder(outputDirectory);
00074
        if (!myPrc) {
```

```
00075
          cout « "Simulation code: " « sim.outputManager.getSimCode() « endl;
00076
00077
        sim.outputManager.set_outputStyle(outputStyle);
00078
00079
        double ts = MPI Wtime();
08000
00081
        //sim.outAllFieldData(0); // output of initial state
00082
        // Conduct the propagation in space and time
00083
        for (int step = 1; step <= numberOfSteps; step++) {</pre>
          sim.advanceToTime(endTime / numberOfSteps * step);
if (step % outputStep == 0) {
00084
00085
00086
            sim.outAllFieldData(step);
00087
00088
          double tn = MPI_Wtime();
          if (!myPrc) {
  cout « "\rStep " « step « "\t\t" « flush;
00089
00090
00091
             timer(ts, tn);
00092
00093
00094
00095
00096 }
```

References ICSetter::addGauss1D(), Simulation::addPeriodicICLayerInX(), ICSetter::addPlaneWave1D(), Simulation::advanceToTime(), TimeEvolution::c, errorKill(), OutputManager::generateOutputFolder(), OutputManager::getSimCode(), Simulation::icsettings, Simulation::initializeCVODEobject(), Simulation::initializePatchwork(), nonlinear1DProp(), Simulation::outAllFieldData(), Simulation::outputManager, OutputManager::set_outputStyle(), Simulation::setDiscreteDimensionsOfLatice(), Simulation::start(), TimeEvolution::TimeEvolver, and timer().

Referenced by main().

Here is the call graph for this function:



Here is the caller graph for this function:



6.24.2.2 Sim2D()

complete 2D Simulation function

Conduct the complete 2D simulation process

Definition at line 99 of file SimulationFunctions.cpp.

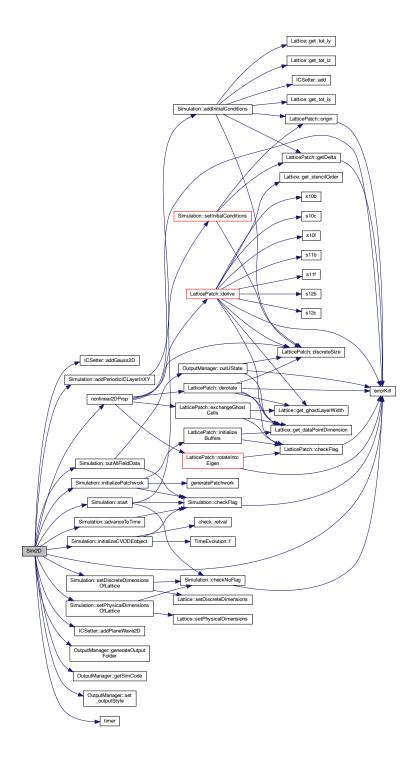
```
00104
00105
00106
        // MPI data
00107
        int myPrc = 0, nprc = 0; // Get process rank and number of processes
00108
       MPI_Comm_rank (MPI_COMM_WORLD,
00109
                      &myPrc); // Return process rank, number \in [1,nprc]
       MPI_Comm_size(MPI_COMM_WORLD,
00110
00111
                      &nprc); // Return number of processes (communicator size)
00112
00113
       // Check feasibility of the patchwork decomposition
00114
        if (myPrc == 0) {
         if (nprc != patches[0] * patches[1]) {
00115
00116
            errorKill(
00117
                "The number of MPI processes must match the number of patches.");
00118
00119
00120
00121
        // Initialize the simulation, set up the cartesian communicator
00122
       Simulation sim(patches[0], patches[1], 1, StencilOrder, periodic);
00123
00124
        /\star // Check that lattice communicator is unique; same as used in patchwork
00125
       generation char cart_comm_name[MPI_MAX_OBJECT_NAME]; int cart_namelen;
00126
       MPI_Comm_get_name(*sim.get_cart_comm(), cart_comm_name, &cart_namelen);
       printf("sim.get_cart_comm gives %s \n", cart_comm_name);
00127
00128
00129
00130
       // Configure the patchwork
00131
       sim.setPhysicalDimensionsOfLattice(phys_dims[0],
```

```
phys_dims[1],
00133
                                            1); // spacing of the lattice
00134
        sim.setDiscreteDimensionsOfLattice(
           disc_dims[0], disc_dims[1], 1); // Spacing equivalence to points
00135
00136
        sim.initializePatchwork(patches[0], patches[1], 1);
00137
00138
        // Add em-waves
00139
        for (const auto &gauss : gaussians)
00140
         sim.icsettings.addGauss2D(gauss.x0, gauss.axis, gauss.amp, gauss.phip,
00141
                                     gauss.w0, gauss.zr, gauss.ph0, gauss.phA);
00142
        for (const auto &plane : planes)
          sim.icsettings.addPlaneWave2D(plane.k, plane.p, plane.phi);
00143
00144
00145
        // Check that the patchwork is ready and set the initial conditions
00146
        sim.start(); // Check if the lattice is set up, set initial field
                     // configuration
00147
        \verb|sim.addPeriodicICLayerInXY()|; // insure periodicity in propagation directions| \\
00148
00149
00150
        // Initialize CVode with rel and abs tolerances
00151
        sim.initializeCVODEobject(CVodeTol[0], CVodeTol[1]);
00152
00153
        \ensuremath{//} Configure the time evolution function
00154
        TimeEvolution::c = interactions;
00155
        TimeEvolution::TimeEvolver = nonlinear2DProp;
00156
00157
        // Configure the output
00158
        sim.outputManager.generateOutputFolder(outputDirectory);
00159
        if (!myPrc) {
00160
          cout « "Simulation code: " « sim.outputManager.getSimCode() « endl;
00161
00162
        sim.outputManager.set_outputStyle(outputStyle);
00163
00164
        double ts = MPI_Wtime();
00165
00166
        //sim.outAllFieldData(0); // output of initial state
00167
        // Conduct the propagation in space and time
        for (int step = 1; step <= numberOfSteps; step++)</pre>
00168
         sim.advanceToTime(endTime / numberOfSteps * step);
00169
00170
          if (step % outputStep == 0) {
00171
            sim.outAllFieldData(step);
00172
          double tn = MPI_Wtime();
00173
00174
          if (!myPrc) {
            cout « "\rStep " « step « "\t\t" « flush;
00175
00176
            timer(ts, tn);
00177
00178
       }
00179
00180
       return:
00181 }
```

References ICSetter::addGauss2D(), Simulation::addPeriodicICLayerInXY(), ICSetter::addPlaneWave2D(), Simulation::advanceToTime(), TimeEvolution::c, errorKill(), OutputManager::generateOutputFolder(), OutputManager::getSimCode(), Simulation::icsettings, Simulation::initializeCVODEobject(), Simulation::initializePatchwork(), nonlinear2DProp(), Simulation::outAllFieldData(), Simulation::outputManager, OutputManager::set_outputStyle(), Simulation::setDiscreteDimensionsOfLatice(), Simulation::start(), TimeEvolution::TimeEvolver, and timer().

Referenced by main().

Here is the call graph for this function:



Here is the caller graph for this function:



6.24.2.3 Sim3D()

complete 3D Simulation function

Conduct the complete 3D simulation process

Definition at line 184 of file SimulationFunctions.cpp.

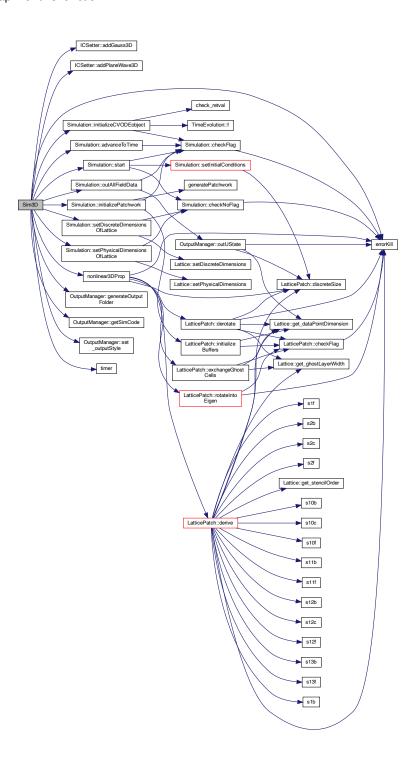
```
00190
00191
00192
        // MPI data
00193
        int myPrc = 0, nprc = 0; // Get process rank and numer of process
00194
        MPI_Comm_rank (MPI_COMM_WORLD,
00195
       &myPrc); // rank of the process inside the world communicator MPI_Comm_size(MPI_COMM_WORLD,
00196
00197
                      &nprc); // Size of the communicator is the number of processes
00198
00199
        // Check feasibility of the patchwork decomposition
00200
        if (myPrc == 0) {
          if (nprc != patches[0] * patches[1] * patches[2]) {
00201
00202
            errorKill(
00203
                "The number of MPI processes must match the number of patches.");
00204
          00205
00206
00207
                "\nWarning: Patches should be cubic in terms of the lattice "
"points for the computational efficiency of larger simulations.\n";
00208
00209
00210
00211
00212
00213
        // Initialize the simulation, set up the cartesian communicator
00214
        Simulation sim(patches[0], patches[1], patches[2],
00215
                       StencilOrder, periodic); // Simulation object with slicing
00216
00217
       // Create the SUNContext object associated with the thread of execution
```

```
00218
        sim.setPhysicalDimensionsOfLattice(phys_dims[0], phys_dims[1],
00219
                                            phys_dims[2]); // spacing of the box
00220
        sim.setDiscreteDimensionsOfLattice(
00221
            disc_dims[0], disc_dims[1],
00222
            disc_dims[2]); // Spacing equivalence to points
       sim.initializePatchwork(patches[0], patches[1], patches[2]);
00223
00225
00226
        for (const auto &plane : planes)
00227
         sim.icsettings.addPlaneWave3D(plane.k, plane.p, plane.phi);
        for (const auto &gauss : gaussians)
00228
00229
         sim.icsettings.addGauss3D(gauss.x0, gauss.axis, gauss.amp, gauss.phip,
00230
                                     gauss.w0, gauss.zr, gauss.ph0, gauss.phA);
00231
00232
        // Check that the patchwork is ready and set the initial conditions
00233
        sim.start();
00234
00235
        // Initialize CVode with abs and rel tolerances
        sim.initializeCVODEobject(CVodeTol[0], CVodeTol[1]);
00236
00237
00238
        // Configure the time evolution function
00239
        TimeEvolution::c = interactions;
       TimeEvolution::TimeEvolver = nonlinear3DProp;
00240
00241
00242
        // Configure the output
00243
        sim.outputManager.generateOutputFolder(outputDirectory);
00244
00245
         cout « "Simulation code: " « sim.outputManager.getSimCode() « endl;
00246
00247
        sim.outputManager.set_outputStyle(outputStyle);
00248
00249
        double ts = MPI_Wtime();
00250
00251
        //sim.outAllFieldData(0); // output of initial state
        // Conduct the propagation in space and time
for (int step = 1; step <= numberOfSteps; step++) {</pre>
00252
00253
          sim.advanceToTime(endTime / numberOfSteps * step);
00254
          if (step % outputStep == 0) {
00256
            sim.outAllFieldData(step);
00257
00258
          double tn = MPI_Wtime();
         if (!myPrc) {
  cout « "\rStep " « step « "\t\t" « flush;
00259
00260
00261
            timer(ts, tn);
00262
          }
00263
00264
       return;
00265 }
```

References ICSetter::addGauss3D(), ICSetter::addPlaneWave3D(), Simulation::advanceToTime(), TimeEvolution::c, errorKill(), OutputManager::generateOutputFolder(), OutputManager::getSimCode(), Simulation::icsettings, Simulation::initializeCVODEobject(), Simulation::initializePatchwork(), nonlinear3DProp(), Simulation::outAllFieldData(), Simulation::outputManager, OutputManager::set_outputStyle(), Simulation::setDiscreteDimensionsOfLattice(), Simulation::setPhysicalDimensionsOfLattice(), Simulation::start(), TimeEvolution::TimeEvolver, and timer().

Referenced by main().

Here is the call graph for this function:



Here is the caller graph for this function:



6.24.2.4 timer()

```
void timer ( \label{eq:condition} \text{double & $t1$,} \\ \text{double & $t2$ )}
```

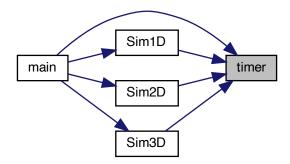
Calculate and print the total simulation time

```
Definition at line 12 of file SimulationFunctions.cpp.
```

```
00012 {
00013 printf("Elapsed time: %fs\n", (t2 - t1));
00014 }
```

Referenced by main(), Sim1D(), Sim2D(), and Sim3D().

Here is the caller graph for this function:



6.25 SimulationFunctions.cpp

```
Go to the documentation of this file.
00006
00007 #include "SimulationFunctions.h"
80000
00009 using namespace std;
00011 /** Calculate and print the total simulation time */
00012 void timer(double &t1, double &t2) {
00013 printf("Elapsed time: %fs\n", (t2 - t1)); 00014 }
00015
00016 // Instantiate and preliminarily initialize the time evolver
00017 // non-const statics to be defined in actual simulation process
00018 int *TimeEvolution::c = nullptr;
00019 void (*TimeEvolution::TimeEvolver) (LatticePatch *, N_Vector, N_Vector,
00020
                                         int *) = nonlinear1DProp;
00021
00022 /** Conduct the complete 1D simulation process */
00023 void Sim1D(const array<sunrealtype,2> CVodeTol, const int StencilOrder,
             const sunrealtype phys_dim, const sunindextype disc_dim,
00024
00025
              const bool periodic, int *interactions,
00026
              const sunrealtype endTime, const int numberOfSteps,
00027
             const string outputDirectory, const int outputStep,
00028
             const char outputStyle,
             const vector<planewave> &planes,
00030
             const vector<gaussian1D> &gaussians) {
00031
00032
       // MPI data
       int myPrc = 0, nprc = 0;
00033
       MPI_Comm_size(MPI_COMM_WORLD, &nprc);
00034
00035
       MPI_Comm_rank (MPI_COMM_WORLD, &myPrc);
00036
00037
        // Check feasibility of the patchwork decomposition
       if (myPrc == 0) {
00038
            if (disc_dim % nprc != 0) {
00039
             errorKill ("The number of lattice points must be "
"divisible by the number of processes.");
00040
00041
00042
00043
00044
       \ensuremath{//} Initialize the simulation, set up the cartesian communicator
00045
       array(int, 3> patches = {nprc, 1, 1};
Simulation sim(patches[0], patches[1], patches[2], StencilOrder, periodic);
00046
00047
00048
00049
        // Configure the patchwork
00050
        sim.setPhysicalDimensionsOfLattice(phys_dim,1,1);
00051
       sim.setDiscreteDimensionsOfLattice(disc_dim,1,1);
00052
       sim.initializePatchwork(patches[0], patches[1], patches[2]);
00053
00054
        // Add em-waves
00055
       for (const auto &gauss : gaussians)
00056
         sim.icsettings.addGauss1D(gauss.k, gauss.p, gauss.x0, gauss.phig,
00057
                                    gauss.phi);
00058
       for (const auto &plane : planes)
00059
         sim.icsettings.addPlaneWave1D(plane.k, plane.p, plane.phi);
00060
00061
       // Check that the patchwork is ready and set the initial conditions
00062
        sim.start();
00063
       sim.addPeriodicICLayerInX();
00064
00065
        // Initialize CVode with abs and rel tolerances
00066
       sim.initializeCVODEobject(CVodeTol[0], CVodeTol[1]);
00067
00068
        \ensuremath{//} Configure the time evolution function
00069
        TimeEvolution::c = interactions;
00070
       TimeEvolution::TimeEvolver = nonlinear1DProp;
00071
00072
        // Configure the output
        sim.outputManager.generateOutputFolder(outputDirectory);
00074
00075
          cout « "Simulation code: " « sim.outputManager.getSimCode() « endl;
00076
00077
       sim.outputManager.set_outputStyle(outputStyle);
00078
       double ts = MPI_Wtime();
08000
00081
        //sim.outAllFieldData(0); // output of initial state
00082
       \ensuremath{//} Conduct the propagation in space and time
```

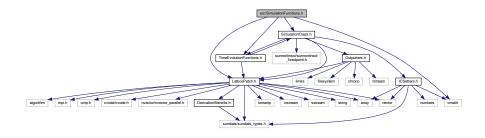
```
for (int step = 1; step <= numberOfSteps; step++) {</pre>
         sim.advanceToTime(endTime / numberOfSteps * step);
00084
00085
          if (step % outputStep == 0) {
00086
           sim.outAllFieldData(step);
00087
00088
          double tn = MPI Wtime();
          if (!myPrc) {
00090
            cout « "\rStep " « step « "\t\t" « flush;
00091
            timer(ts, tn);
00092
       }
00093
00094
00095
        return;
00096 }
00097
00098 /** Conduct the complete 2D simulation process */
00099 void Sim2D(const array<sunrealtype,2> CVodeTol, int const StencilOrder,
00100
              const array<sunrealtype,2> phys_dims, const array<sunindextype,2> disc_dims, const array<int,2> patches, const bool periodic, int *interactions,
              const sunrealtype endTime, const int numberOfSteps,
00102
00103
              const string outputDirectory, const int outputStep, const char outputStyle,
00104
              const vector<planewave> &planes, const vector<gaussian2D> &gaussians) {
00105
       // MPI data
00106
        int myPrc = 0, nprc = 0; // Get process rank and number of processes
00107
       MPI_Comm_rank (MPI_COMM_WORLD,
00108
00109
                       &myPrc); // Return process rank, number \in [1,nprc]
00110
       MPI_Comm_size(MPI_COMM_WORLD,
00111
                      &nprc); // Return number of processes (communicator size)
00112
00113
        // Check feasibility of the patchwork decomposition
00114
        if (myPrc == 0) {
00115
         if (nprc != patches[0] * patches[1]) {
            errorKill(
00116
00117
                "The number of MPI processes must match the number of patches.");
00118
00119
        }
00120
00121
        // Initialize the simulation, set up the cartesian communicator
00122
        Simulation sim(patches[0], patches[1], 1, StencilOrder, periodic);
00123
00124
        /* // Check that lattice communicator is unique; same as used in patchwork
00125
        generation char cart_comm_name[MPI_MAX_OBJECT_NAME]; int cart_namelen;
        MPI_Comm_get_name(*sim.get_cart_comm(), cart_comm_name, &cart_namelen);
printf("sim.get_cart_comm gives %s \n", cart_comm_name);
00126
00127
00128
00129
00130
        // Configure the patchwork
        sim.setPhysicalDimensionsOfLattice(phys_dims[0],
00131
00132
                                            phys_dims[1],
00133
                                             1); // spacing of the lattice
00134
        \verb|sim.setDiscreteDimensionsOfLattice|| \\
00135
           disc_dims[0], disc_dims[1], 1); // Spacing equivalence to points
00136
        sim.initializePatchwork(patches[0], patches[1], 1);
00137
00138
        // Add em-waves
00139
        for (const auto &gauss : gaussians)
00140
          sim.icsettings.addGauss2D(gauss.x0, gauss.axis, gauss.amp, gauss.phip,
00141
                                     gauss.w0, gauss.zr, gauss.ph0, gauss.phA);
00142
        for (const auto &plane : planes)
00143
         sim.icsettings.addPlaneWave2D(plane.k, plane.p, plane.phi);
00144
00145
        // Check that the patchwork is ready and set the initial conditions
        00146
00147
00148
        sim.addPeriodicICLayerInXY(); // insure periodicity in propagation directions
00149
00150
        // Initialize CVode with rel and abs tolerances
00151
        sim.initializeCVODEobject(CVodeTol[0], CVodeTol[1]);
00152
00153
        // Configure the time evolution function
00154
        TimeEvolution::c = interactions;
00155
        TimeEvolution::TimeEvolver = nonlinear2DProp;
00156
00157
        // Configure the output
00158
        sim.outputManager.generateOutputFolder(outputDirectory);
00159
00160
          cout « "Simulation code: " « sim.outputManager.getSimCode() « endl;
00161
00162
        sim.outputManager.set outputStyle(outputStyle);
00163
00164
        double ts = MPI_Wtime();
00165
00166
        //sim.outAllFieldData(0); // output of initial state
        // Conduct the propagation in space and time
for (int step = 1; step <= numberOfSteps; step++) {</pre>
00167
00168
          sim.advanceToTime(endTime / numberOfSteps * step);
00169
```

```
if (step % outputStep == 0) {
          sim.outAllFieldData(step);
00171
00172
00173
         double tn = MPI Wtime();
         if (!myPrc) {
00174
           cout « "\rStep " « step « "\t\t" « flush;
00175
00176
           timer(ts, tn);
00177
00178
       }
00179
00180
       return:
00181 }
00182
00183 /** Conduct the complete 3D simulation process */
00184 void Sim3D(const array<sunrealtype, 2> CVodeTol, const int StencilOrder,
00185
             const array<sunrealtype,3> phys_dims,
00186
             const array<sunindextype,3> disc_dims, const array<int,3> patches,
             const bool periodic, int *interactions, const surrealtype endTime, const int numberOfSteps, const string outputDirectory,
00187
00188
00189
             const int outputStep, const char outputStyle,
00190
             const vector<planewave> &planes, const vector<gaussian3D> &gaussians) {
00191
00192
       // MPT data
       int myPrc = 0, nprc = 0; // Get process rank and numer of process
00193
00194
       MPI_Comm_rank (MPI_COMM_WORLD,
00195
                     &myPrc); // rank of the process inside the world communicator
00196
       MPI_Comm_size(MPI_COMM_WORLD,
00197
                     &nprc); // Size of the communicator is the number of processes
00198
00199
       \ensuremath{//} Check feasibility of the patchwork decomposition
00200
       if (myPrc == 0) {
00201
         if (nprc != patches[0] * patches[1] * patches[2]) {
00202
           errorKill(
00203
                "The number of MPI processes must match the number of patches.");
00204
         00205
00206
            clog
00208
               « "\nWarning: Patches should be cubic in terms of the lattice "
00209
                   "points for the computational efficiency of larger simulations.\n";
00210
00211
       1
00212
00213
        // Initialize the simulation, set up the cartesian communicator
       Simulation sim(patches[0], patches[1], patches[2],
00214
00215
                       StencilOrder, periodic); // Simulation object with slicing
00216
00217
       \ensuremath{//} Create the SUNContext object associated with the thread of execution
       00218
00219
00220
       sim.setDiscreteDimensionsOfLattice(
00221
            disc_dims[0], disc_dims[1],
00222
            disc_dims[2]); // Spacing equivalence to points
00223
       sim.initializePatchwork(patches[0], patches[1], patches[2]);
00224
00225
        // Add em-waves
00226
       for (const auto &plane : planes)
00227
         sim.icsettings.addPlaneWave3D(plane.k, plane.p, plane.phi);
00228
       for (const auto &gauss : gaussians)
00229
         sim.icsettings.addGauss3D(gauss.x0, gauss.axis, gauss.amp, gauss.phip,
00230
                                   gauss.w0, gauss.zr, gauss.ph0, gauss.phA);
00231
00232
        // Check that the patchwork is ready and set the initial conditions
00233
       sim.start();
00234
00235
        // Initialize CVode with abs and rel tolerances
00236
       sim.initializeCVODEobject(CVodeTol[0], CVodeTol[1]);
00237
00238
        // Configure the time evolution function
00239
        TimeEvolution::c = interactions;
00240
       TimeEvolution::TimeEvolver = nonlinear3DProp;
00241
00242
        // Configure the output
       sim.outputManager.generateOutputFolder(outputDirectory);
00243
00244
       if (!myPrc) {
00245
         cout « "Simulation code: " « sim.outputManager.getSimCode() « endl;
00246
00247
       sim.outputManager.set_outputStyle(outputStyle);
00248
00249
       double ts = MPT Wtime():
00250
00251
       //sim.outAllFieldData(0); // output of initial state
00252
        // Conduct the propagation in space and time
00253
        for (int step = 1; step <= numberOfSteps; step++) {</pre>
         sim.advanceToTime(endTime / numberOfSteps * step);
00254
00255
         if (step % outputStep == 0) {
           sim.outAllFieldData(step);
00256
```

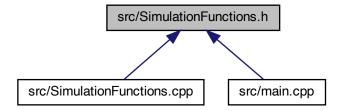
6.26 src/SimulationFunctions.h File Reference

Full simulation functions for 1D, 2D, and 3D used in main.cpp.

```
#include <cmath>
#include "LatticePatch.h"
#include "SimulationClass.h"
#include "TimeEvolutionFunctions.h"
Include dependency graph for SimulationFunctions.h:
```



This graph shows which files directly or indirectly include this file:



Data Structures

· struct planewave

plane wave structure

struct gaussian1D

1D Gaussian wave structure

• struct gaussian2D

2D Gaussian wave structure

struct gaussian3D

3D Gaussian wave structure

Functions

void Sim1D (const array< sunrealtype, 2 >, const int, const sunrealtype, const sunindextype, const bool, int *, const sunrealtype, const int, const string, const int, const char, const vector< planewave > &, const vector< gaussian1D > &)

```
complete 1D Simulation function
```

• void Sim2D (const array< sunrealtype, 2 >, const int, const array< sunrealtype, 2 >, const array< sunindextype, 2 >, const array< int, 2 >, const bool, int *, const sunrealtype, const int, const string, const int, const char, const vector< planewave > &, const vector< gaussian2D > &)

```
complete 2D Simulation function
```

• void Sim3D (const array< sunrealtype, 2 >, const int, const array< sunrealtype, 3 >, const array< sunindextype, 3 >, const array< int, 3 >, const bool, int *, const sunrealtype, const int, const string, const int, const char, const vector< planewave > &, const vector< gaussian3D > &)

```
complete 3D Simulation function
```

• void timer (double &, double &)

6.26.1 Detailed Description

Full simulation functions for 1D, 2D, and 3D used in main.cpp.

Definition in file SimulationFunctions.h.

6.26.2 Function Documentation

6.26.2.1 Sim1D()

complete 1D Simulation function

Conduct the complete 1D simulation process

Definition at line 23 of file SimulationFunctions.cpp.

```
00030

00031

00032  // MPI data

00033  int myPrc = 0, nprc = 0;

00034  MPI_Comm_size(MPI_COMM_WORLD, &nprc);

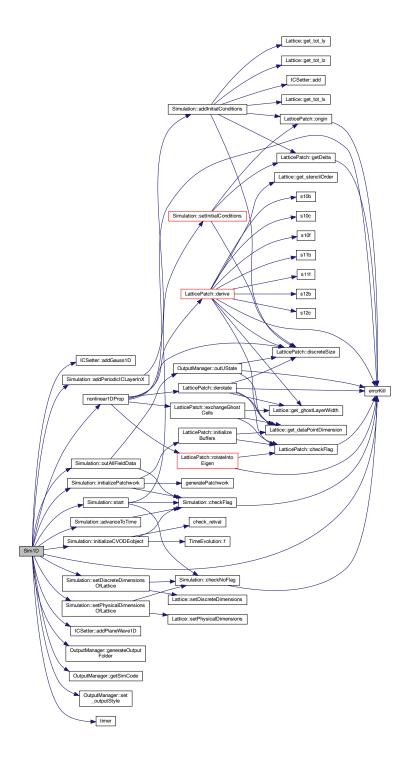
00035  MPI_Comm_rank(MPI_COMM_WORLD, &myPrc);
```

```
00036
00037
        // Check feasibility of the patchwork decomposition
00038
        if (myPrc == 0) {
            if (disc_dim % nprc != 0) {
   errorKill("The number of lattice points must be "
        "divisible by the number of processes.");
00039
00040
00041
00042
00043
00044
00045
        // Initialize the simulation, set up the cartesian communicator
00046
        array<int, 3> patches = {nprc, 1, 1};
00047
        Simulation sim(patches[0], patches[1], patches[2], StencilOrder, periodic);
00048
00049
        // Configure the patchwork
00050
        sim.setPhysicalDimensionsOfLattice(phys_dim,1,1);
00051
        sim.setDiscreteDimensionsOfLattice(disc_dim,1,1);
00052
        sim.initializePatchwork(patches[0], patches[1], patches[2]);
00053
00054
        // Add em-waves
00055
        for (const auto &gauss : gaussians)
00056
          sim.icsettings.addGauss1D(gauss.k, gauss.p, gauss.x0, gauss.phig,
00057
                                       gauss.phi);
        for (const auto &plane : planes)
00058
00059
          sim.icsettings.addPlaneWave1D(plane.k, plane.p, plane.phi);
00060
00061
        // Check that the patchwork is ready and set the initial conditions
00062
00063
        sim.addPeriodicICLayerInX();
00064
        // Initialize CVode with abs and rel tolerances
00065
00066
        sim.initializeCVODEobject(CVodeTol[0], CVodeTol[1]);
00067
00068
        \ensuremath{//} Configure the time evolution function
00069
        TimeEvolution::c = interactions;
00070
        TimeEvolution::TimeEvolver = nonlinear1DProp;
00071
00072
        // Configure the output
00073
        sim.outputManager.generateOutputFolder(outputDirectory);
00074
        if (!myPrc) {
00075
          cout « "Simulation code: " « sim.outputManager.getSimCode() « endl;
00076
00077
        sim.outputManager.set_outputStyle(outputStyle);
00078
00079
        double ts = MPI_Wtime();
08000
00081
        //sim.outAllFieldData(0); // output of initial state
00082
        \ensuremath{//} Conduct the propagation in space and time
00083
        for (int step = 1; step <= numberOfSteps; step++) {</pre>
          sim.advanceToTime(endTime / numberOfSteps * step);
00084
          if (step % outputStep == 0) {
00085
00086
            sim.outAllFieldData(step);
00087
00088
          double tn = MPI_Wtime();
          if (!myPrc) {
  cout « "\rStep " « step « "\t\t" « flush;
00089
00090
00091
             timer(ts, tn);
00092
00093
00094
        return;
00095
00096 }
```

References ICSetter::addGauss1D(), Simulation::addPeriodicICLayerInX(), ICSetter::addPlaneWave1D(), Simulation::advanceToTime(), TimeEvolution::c, errorKill(), OutputManager::generateOutputFolder(), OutputManager::getSimCode(), Simulation::icsettings, Simulation::initializeCVODEobject(), Simulation::initializePatchwork(), nonlinear1DProp(), Simulation::outAllFieldData(), Simulation::outputManager, OutputManager::set_outputStyle(), Simulation::setDiscreteDimensionsOfLattice(), Simulation::start(), TimeEvolution::TimeEvolver, and timer().

Referenced by main().

Here is the call graph for this function:



Here is the caller graph for this function:



6.26.2.2 Sim2D()

complete 2D Simulation function

Conduct the complete 2D simulation process

Definition at line 99 of file SimulationFunctions.cpp.

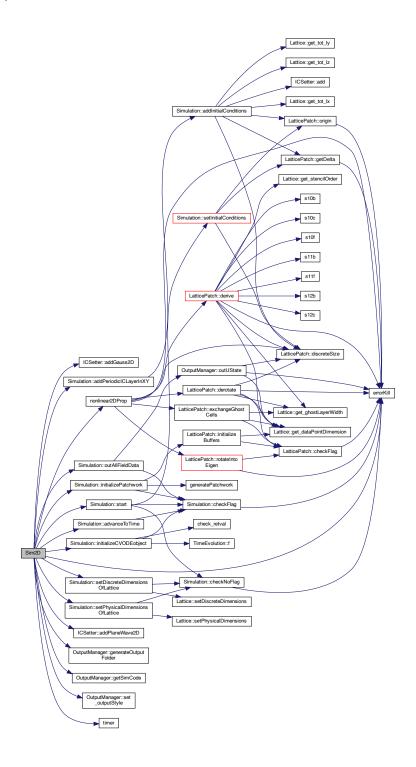
```
00104
00105
00106
        // MPI data
00107
        int myPrc = 0, nprc = 0; // Get process rank and number of processes
00108
       MPI_Comm_rank (MPI_COMM_WORLD,
00109
                      &myPrc); // Return process rank, number \in [1,nprc]
       MPI_Comm_size(MPI_COMM_WORLD,
00110
00111
                      &nprc); // Return number of processes (communicator size)
00112
00113
       // Check feasibility of the patchwork decomposition
00114
        if (myPrc == 0) {
         if (nprc != patches[0] * patches[1]) {
00115
00116
            errorKill(
00117
                "The number of MPI processes must match the number of patches.");
00118
00119
00120
00121
        // Initialize the simulation, set up the cartesian communicator
00122
       Simulation sim(patches[0], patches[1], 1, StencilOrder, periodic);
00123
00124
        /\star // Check that lattice communicator is unique; same as used in patchwork
00125
       generation char cart_comm_name[MPI_MAX_OBJECT_NAME]; int cart_namelen;
00126
       MPI_Comm_get_name(*sim.get_cart_comm(), cart_comm_name, &cart_namelen);
       printf("sim.get_cart_comm gives %s \n", cart_comm_name);
00127
00128
00129
00130
       // Configure the patchwork
00131
       sim.setPhysicalDimensionsOfLattice(phys_dims[0],
```

```
phys_dims[1],
00133
                                            1); // spacing of the lattice
00134
        sim.setDiscreteDimensionsOfLattice(
           disc_dims[0], disc_dims[1], 1); // Spacing equivalence to points
00135
00136
        sim.initializePatchwork(patches[0], patches[1], 1);
00137
00138
        // Add em-waves
00139
        for (const auto &gauss : gaussians)
00140
         sim.icsettings.addGauss2D(gauss.x0, gauss.axis, gauss.amp, gauss.phip,
00141
                                     gauss.w0, gauss.zr, gauss.ph0, gauss.phA);
00142
        for (const auto &plane : planes)
          sim.icsettings.addPlaneWave2D(plane.k, plane.p, plane.phi);
00143
00144
00145
        // Check that the patchwork is ready and set the initial conditions
00146
        sim.start(); // Check if the lattice is set up, set initial field
                     // configuration
00147
        \verb|sim.addPeriodicICLayerInXY()|; // insure periodicity in propagation directions| \\
00148
00149
00150
        // Initialize CVode with rel and abs tolerances
00151
        sim.initializeCVODEobject(CVodeTol[0], CVodeTol[1]);
00152
00153
        \ensuremath{//} Configure the time evolution function
00154
        TimeEvolution::c = interactions;
00155
        TimeEvolution::TimeEvolver = nonlinear2DProp;
00156
00157
        // Configure the output
00158
        sim.outputManager.generateOutputFolder(outputDirectory);
00159
        if (!myPrc) {
00160
          cout « "Simulation code: " « sim.outputManager.getSimCode() « endl;
00161
00162
        sim.outputManager.set_outputStyle(outputStyle);
00163
00164
        double ts = MPI_Wtime();
00165
00166
        //sim.outAllFieldData(0); // output of initial state
00167
        // Conduct the propagation in space and time
        for (int step = 1; step <= numberOfSteps; step++)</pre>
00168
         sim.advanceToTime(endTime / numberOfSteps * step);
00169
00170
          if (step % outputStep == 0) {
00171
            sim.outAllFieldData(step);
00172
          double tn = MPI_Wtime();
00173
00174
          if (!myPrc) {
            cout « "\rStep " « step « "\t\t" « flush;
00175
00176
            timer(ts, tn);
00177
00178
       }
00179
00180
       return:
00181 }
```

References ICSetter::addGauss2D(), Simulation::addPeriodicICLayerInXY(), ICSetter::addPlaneWave2D(), Simulation::advanceToTime(), TimeEvolution::c, errorKill(), OutputManager::generateOutputFolder(), OutputManager::getSimCode(), Simulation::icsettings, Simulation::initializeCVODEobject(), Simulation::initializePatchwork(), nonlinear2DProp(), Simulation::outAllFieldData(), Simulation::outputManager, OutputManager::set_outputStyle(), Simulation::setDiscreteDimensionsOfLatice(), Simulation::start(), TimeEvolution::TimeEvolver, and timer().

Referenced by main().

Here is the call graph for this function:



Here is the caller graph for this function:



6.26.2.3 Sim3D()

complete 3D Simulation function

Conduct the complete 3D simulation process

Definition at line 184 of file SimulationFunctions.cpp.

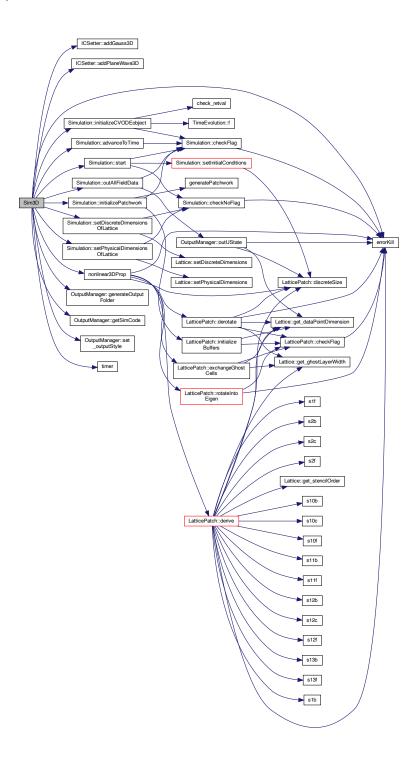
```
00190
00191
00192
        // MPI data
00193
        int myPrc = 0, nprc = 0; // Get process rank and numer of process
00194
        MPI_Comm_rank (MPI_COMM_WORLD,
00195
       &myPrc); // rank of the process inside the world communicator MPI_Comm_size(MPI_COMM_WORLD,
00196
00197
                      &nprc); // Size of the communicator is the number of processes
00198
00199
        // Check feasibility of the patchwork decomposition
00200
        if (myPrc == 0) {
          if (nprc != patches[0] * patches[1] * patches[2]) {
00201
00202
            errorKill(
00203
                "The number of MPI processes must match the number of patches.");
00204
          00205
00206
00207
                "\nWarning: Patches should be cubic in terms of the lattice "
"points for the computational efficiency of larger simulations.\n";
00208
00209
00210
00211
00212
00213
        // Initialize the simulation, set up the cartesian communicator
00214
        Simulation sim(patches[0], patches[1], patches[2],
00215
                       StencilOrder, periodic); // Simulation object with slicing
00216
00217
       // Create the SUNContext object associated with the thread of execution
```

```
sim.setPhysicalDimensionsOfLattice(phys_dims[0], phys_dims[1],
00219
                                             phys_dims[2]); // spacing of the box
00220
        sim.setDiscreteDimensionsOfLattice(
00221
            disc_dims[0], disc_dims[1],
00222
            disc_dims[2]); // Spacing equivalence to points
00223
       sim.initializePatchwork(patches[0], patches[1], patches[2]);
00225
00226
        for (const auto &plane : planes)
00227
         sim.icsettings.addPlaneWave3D(plane.k, plane.p, plane.phi);
        for (const auto &gauss : gaussians)
00228
00229
         sim.icsettings.addGauss3D(gauss.x0, gauss.axis, gauss.amp, gauss.phip,
00230
                                     gauss.w0, gauss.zr, gauss.ph0, gauss.phA);
00231
00232
        // Check that the patchwork is ready and set the initial conditions
00233
        sim.start();
00234
00235
        // Initialize CVode with abs and rel tolerances
        sim.initializeCVODEobject(CVodeTol[0], CVodeTol[1]);
00236
00237
00238
        // Configure the time evolution function
00239
        TimeEvolution::c = interactions;
       TimeEvolution::TimeEvolver = nonlinear3DProp;
00240
00241
00242
        // Configure the output
00243
        sim.outputManager.generateOutputFolder(outputDirectory);
00244
00245
         cout « "Simulation code: " « sim.outputManager.getSimCode() « endl;
00246
00247
        sim.outputManager.set_outputStyle(outputStyle);
00248
00249
        double ts = MPI_Wtime();
00250
00251
        //sim.outAllFieldData(0); // output of initial state
        // Conduct the propagation in space and time
for (int step = 1; step <= numberOfSteps; step++) {</pre>
00252
00253
          sim.advanceToTime(endTime / numberOfSteps * step);
00254
          if (step % outputStep == 0) {
00256
            sim.outAllFieldData(step);
00257
00258
          double tn = MPI_Wtime();
         if (!myPrc) {
  cout « "\rStep " « step « "\t\t" « flush;
00259
00260
00261
            timer(ts, tn);
00262
          }
00263
00264
       return;
00265 }
```

References ICSetter::addGauss3D(), ICSetter::addPlaneWave3D(), Simulation::advanceToTime(), TimeEvolution::c, errorKill(), OutputManager::generateOutputFolder(), OutputManager::getSimCode(), Simulation::icsettings, Simulation::initializeCVODEobject(), Simulation::initializePatchwork(), nonlinear3DProp(), Simulation::outAllFieldData(), Simulation::outputManager, OutputManager::set_outputStyle(), Simulation::setDiscreteDimensionsOfLattice(), Simulation::setPhysicalDimensionsOfLattice(), Simulation::start(), TimeEvolution::TimeEvolver, and timer().

Referenced by main().

Here is the call graph for this function:



Here is the caller graph for this function:



6.26.2.4 timer()

```
void timer ( \mbox{double \& $t1$,} \\ \mbox{double \& $t2$ )}
```

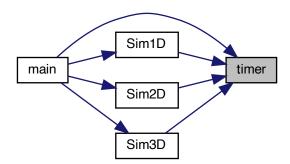
MPI timer function

Calculate and print the total simulation time

```
Definition at line 12 of file SimulationFunctions.cpp.
```

Referenced by main(), Sim1D(), Sim2D(), and Sim3D().

Here is the caller graph for this function:



6.27 SimulationFunctions.h

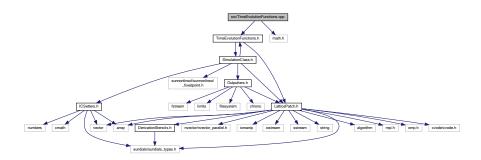
```
Go to the documentation of this file.
00003 /// @brief Full simulation functions for 1D, 2D, and 3D used in main.cpp
00005
00006 #pragma once
00007
00008 // math
00009 #include <cmath>
00010 //#include <mathimf.h>
00012 // project subfile headers
00013 #include "LatticePatch.h"
00014 #include "SimulationClass.h"
00015 #include "TimeEvolutionFunctions.h"
00016
00017 /***** EM-wave structures *****/
00018
00019 /// plane wave structure
00020 struct planewave {
00021 vector<sunrealtype> k;
00022 vector<sunrealtype> p;
                                    /**< wavevector (normalized to \f$ 1/\lambda \f$) */ /**< amplitde & polarization vector */
00023
        vector<sunrealtype> phi; /**< phase shift */
00024 };
00025
00026 /// 1D Gaussian wave structure
        vector<sunrealtype> k;    /**< wavevector (normalized to \f$ 1/\lambda \f$) */
vector<sunrealtype> p;    /**< amplitude & polarization vector */
vector<sunrealtype> x0;    /**< shift from origin */
sunrealtype phig;    /**</pre>
00027 struct gaussian1D {
00028 vector<sunrealtype> k;
00030
00031
00032
        vector<sunrealtype> phi; /**< phase shift */
00033 };
00034
00035 /// 2D Gaussian wave structure
00036 struct gaussian2D {
00037 vector<sunrealtype> x0; /**< center */
00038
        vector<sunrealtype> axis; /**< direction to center */
                               /**< amplitude */
00039
        sunrealtype amp;
00040
                                      /**< polarization rotation */
        sunrealtype phip;
                                     /**< taille */
/**< Rayleigh length */
/**< beam center */
/**< beam length */
        sunrealtype w0;
00041
00042
        sunrealtype zr;
00043 sunrealtype ph0;
00044 sunrealtype phA;
00045 };
00046
00047 /// 3D Gaussian wave structure
00048 struct gaussian3D {
00049 vector<sunrealtype> x0; /**< center */
00050
        vector<sunrealtype> axis; /**< direction to center */</pre>
                             /**< amplitude */
/**< polarization rotation */
/**< taille */
/**< Rayleigh length */
/**< beam center */
/**< beam length */
00051
        sunrealtype amp;
00052
        sunrealtype phip;
        sunrealtype w0;
00053
00054
        sunrealtype zr;
00055
        sunrealtype ph0;
00056
        sunrealtype phA;
00057 };
00058
00059 /***** simulation function declarations ******/
00061 /// complete 1D Simulation function
00062 void Sim1D(const array<sunrealtype, 2>, const int, const sunrealtype,
              const sunindextype, const bool, int *, const sunrealtype, const int,
const string, const int, const char, const vector<planewave> &,
const vector<gaussian1D> &);
00063
00064
00065
00066 /// complete 2D Simulation function
00067 void Sim2D(const array<sunrealtype,2>, const int, const array<sunrealtype,2>,
               const array<sunindextype,2>, const array<int,2>, const bool, int *,
00068
00069
                const sunrealtype, const int, const string, const int, const char,
00070
               const vector<planewave> &, const vector<gaussian2D> &);
00071 /// complete 3D Simulation function
00072 void Sim3D(const array<sunrealtype,2>, const int, const array<sunrealtype,3>,
         const array<sunindextype,3>, const array<int,3>, const bool, int *, const sunrealtype, const int, const string, const int, const char,
00074
00075
               const vector<planewave> &, const vector<gaussian3D> &);
00076
00077 /** MPI timer function */
00078 void timer(double &, double &);
```

6.28 src/TimeEvolutionFunctions.cpp File Reference

Implementation of functions to propagate data vectors in time according to Maxwell's equations, and various orders in the HE weak-field expansion.

```
#include "TimeEvolutionFunctions.h"
#include <math.h>
```

Include dependency graph for TimeEvolutionFunctions.cpp:



Functions

- void linear1DProp (LatticePatch *data, N_Vector u, N_Vector udot, int *c)
 only under-the-hood-callable Maxwell propagation in 1D
- void nonlinear1DProp (LatticePatch *data, N_Vector u, N_Vector udot, int *c) nonlinear 1D HE propagation
- void linear2DProp (LatticePatch *data, N_Vector u, N_Vector udot, int *c) only under-the-hood-callable Maxwell propagation in 2D
- void nonlinear2DProp (LatticePatch *data, N_Vector u, N_Vector udot, int *c) nonlinear 2D HE propagation
- void linear3DProp (LatticePatch *data, N_Vector u, N_Vector udot, int *c) only under-the-hood-callable Maxwell propagation in 3D
- void nonlinear3DProp (LatticePatch *data, N_Vector u, N_Vector udot, int *c) nonlinear 3D HE propagation

6.28.1 Detailed Description

Implementation of functions to propagate data vectors in time according to Maxwell's equations, and various orders in the HE weak-field expansion.

Definition in file TimeEvolutionFunctions.cpp.

6.28.2 Function Documentation

6.28.2.1 linear1DProp()

only under-the-hood-callable Maxwell propagation in 1D

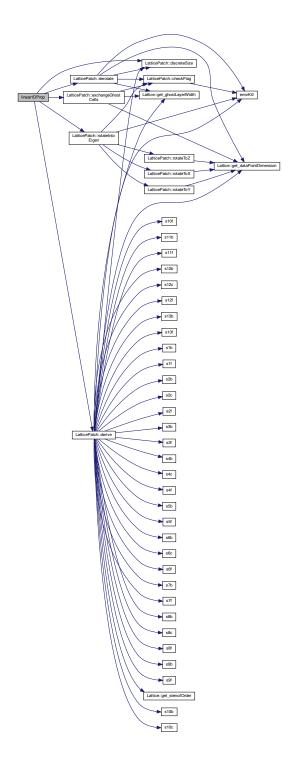
Maxwell propagation function for 1D – only for reference.

Definition at line 46 of file TimeEvolutionFunctions.cpp.

```
00047
00048
         \ensuremath{//} pointers to temporal and spatial derivative data
00049
         sunrealtype *duData = data->duData;
sunrealtype *dxData = data->buffData[1 - 1];
00050
00051
00052
         // sequence along any dimension:
00053
         data->exchangeGhostCells(1); // exchange halos
00054
         data->rotateIntoEigen(
00055
                            // -> rotate all data to prepare derivative operation
             1);
         data->derive(1); // -> perform derivative on it
00056
00057
         data->derotate(
00058
              1, dxData); // -> derotate derivative data to x-space for further use
00059
00060
         int totalNP = data->discreteSize();
00061 int pp = 0;
00062 #pragma distribute_point
00063
         for (int i = 0; i < totalNP; i++) {</pre>
           pp = i * 6;
00064
00065
00066
            simple vacuum Maxwell equations for spatial deriative only in x-direction
00067
            temporal derivative is approximated by spatial derivative according to the numerical scheme with Jacobi=0 -> no polarization or magnetization terms
00068
00069
00070
            duData[pp + 0] = 0;
00071
            duData[pp + 1] = -dxData[pp + 5];
           duData[pp + 2] = dxData[pp + 4];
duData[pp + 3] = 0;
duData[pp + 4] = dxData[pp + 2];
00072
00073
00074
00075
            duData[pp + 5] = -dxData[pp + 1];
00076
00077 }
```

References LatticePatch::buffData, LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::discreteSize(), LatticePatch::duData, LatticePatch::exchangeGhostCells(), and LatticePatch::rotateIntoEigen().

Here is the call graph for this function:



6.28.2.2 linear2DProp()

```
N_Vector u,
N_Vector udot,
int * c )
```

only under-the-hood-callable Maxwell propagation in 2D

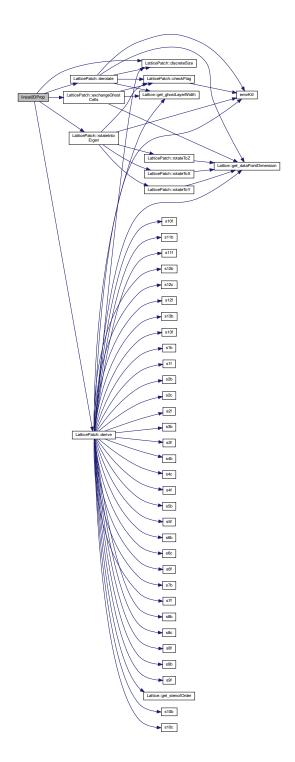
Maxwell propagation function for 2D – only for reference.

Definition at line 273 of file TimeEvolutionFunctions.cpp.

```
00274
00275
           sunrealtype *duData = data->duData;
           sunrealtype *dxData = data->buffData[1 - 1];
sunrealtype *dyData = data->buffData[2 - 1];
00276
00277
00278
00279
           data->exchangeGhostCells(1);
00280
           data->rotateIntoEigen(1);
00281
           data->derive(1);
00282
           data->derotate(1, dxData);
00283
           data->exchangeGhostCells(2);
           data->rotateIntoEigen(2);
00284
00285
           data->derive(2);
00286
           data->derotate(2, dyData);
00287
00288
           int totalNP = data->discreteSize();
00289 int pp = 0;
00290 #pragma distribute_point
           for (int i = 0; i < totalNP; i++) {</pre>
00292
              pp = i * 6;
              pp = 1 * 6;
duData[pp + 0] = dyData[pp + 5];
duData[pp + 1] = -dxData[pp + 5];
duData[pp + 2] = -dyData[pp + 3] + dxData[pp + 4];
duData[pp + 3] = -dyData[pp + 2];
duData[pp + 4] = dxData[pp + 2];
duData[pp + 5] = dyData[pp + 0] - dxData[pp + 1];
00293
00294
00295
00296
00297
00298
00299
00300 }
```

References LatticePatch::buffData, LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::discreteSize(), LatticePatch::duData, LatticePatch::exchangeGhostCells(), and LatticePatch::rotateIntoEigen().

Here is the call graph for this function:



6.28.2.3 linear3DProp()

```
N_Vector u,
N_Vector udot,
int * c )
```

only under-the-hood-callable Maxwell propagation in 3D

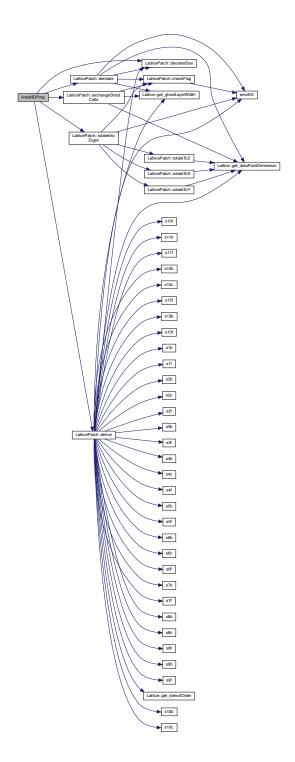
Maxwell propagation function for 3D – only for reference.

Definition at line 489 of file TimeEvolutionFunctions.cpp.

```
00490
00491
         sunrealtype *duData = data->duData;
00492
        sunrealtype *dxData = data->buffData[1 - 1];
sunrealtype *dyData = data->buffData[2 - 1];
00493
00494
        sunrealtype *dzData = data->buffData[3 - 1];
00495
00496
         /\star Under the hood call of point-to-point or collective communication \star/
00497
         // Point-to-Point:
00498
        data->exchangeGhostCells(1);
00499
        data->rotateIntoEigen(1);
00500
        data->derive(1);
00501
         data->derotate(1, dxData);
00502
        data->exchangeGhostCells(2);
00503
         data->rotateIntoEigen(2);
00504
        data->derive(2);
00505
        data->derotate(2, dyData);
00506
        data->exchangeGhostCells(3);
        data->rotateIntoEigen(3);
00508
         data->derive(3);
00509
        data->derotate(3, dzData);
00510
00511
         // Collective:
00512
00513
             data->exchangeGhostCells3D();
00514
             data->rotateIntoEigen3D();
00515
             data->derive(1);
00516
             data->derotate(1,dxData);
00517
             data->derive(2);
00518
             data->derotate(2,dvData);
00519
             data->derive(3);
00520
             data->derotate(3,dzData);
00521
00522
00523
        int totalNP = data->discreteSize();
00524
        int pp = 0;
00525 #pragma distribute_point
        for (int i = 0; i < totalNP; i++) {</pre>
          pp = i * 6;
00527
           duData[pp + 0] = dyData[pp + 5] - dzData[pp + 4];
duData[pp + 1] = dzData[pp + 3] - dxData[pp + 5];
duData[pp + 2] = dxData[pp + 4] - dyData[pp + 3];
00528
00529
00530
           duData[pp + 3] = -dyData[pp + 2] + dzData[pp + 1];
00531
00532
           duData[pp + 4] = -dzData[pp + 0] + dxData[pp + 2];
00533
           duData[pp + 5] = -dxData[pp + 1] + dyData[pp + 0];
00534
00535 }
```

References LatticePatch::buffData, LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::derotate(), LatticePatch::derotate(), LatticePatch::derotate(), LatticePatch::rotateIntoEigen().

Here is the call graph for this function:



6.28.2.4 nonlinear1DProp()

```
N_Vector u,
N_Vector udot,
int * c )
```

nonlinear 1D HE propagation

HE propagation function for 1D. Calculation of the Jacobi matrix

Definition at line 80 of file TimeEvolutionFunctions.cpp.

```
00081
00082
          // pointer to spatial derivative data sufficient, temporal derivative data
00083
         // provided with udot
         sunrealtype *dxData = data->buffData[1 - 1];
00084
00085
00086
         // same sequence as in the linear case
00087
         data->exchangeGhostCells(1);
00088
         data->rotateIntoEigen(1);
00089
         data->derive(1);
00090
         data->derotate(1, dxData);
00091
00092
00093
         F and G are nonzero in the nonlinear case,
00094
         polarization and magnetization contributions in Jacobi matrix style
00095
         with derivatives of polarization and magnetization % \left( {{\mathbf{p}}_{1}}\right) ={{\mathbf{p}}_{2}}
00096
         w.r.t. E- and B-field
00097
         sunrealtype f = NAN, g = NAN; // em field invariants F, G sunrealtype lf = NAN, lff = NAN, lfg = NAN, lg = NAN,
00098
00099
00100
                       lgg = NAN; // derivatives of Lagrangian w.r.t. field invariants
         array<sunrealtype, 36> JMM; // Jacobi matrix array<sunrealtype, 6> Quad; // array to hold E^2 and B^2 components array<sunrealtype, 6> h; // holding temporal derivatives of E and B components
00101
00102
00103
                                       // before operating (1+Z)^-1
00104
         sunrealtype pseudoDenom = NAN; // needed for inversion of 1+Z
00105
         00106
00107
         udata = NV_DATA_P(u);
dudata = NV_DATA_P(udot);
int totalNP = data->discreteSize(); // number of points in the patch
00108
00109
00110
00111
         // #pragma omp parallel for private(...) reduction(...) \rightarrow unsafe due to
00112
         // reductions and many variables, how to deal with / reduction?
00113
         //#pragma block_loop
00114
         //#pragma unroll_and_jam
00115
         //#pragma distribute_point
         for (int pp = 0; pp < totalNP * 6;</pre>
00116
               00117
00118
00119
                            11
                                     for(int pp=ppB;pp<min(totalNP*6,ppB+6*6);pp+=6){</pre>
           /// Calculation of the Jacobi matrix // 1. Calculate F and G
00120
00121
           f = 0.5 * ((Quad[0] = udata[pp] * udata[pp]) +
00122
                         (Quad[1] = udata[pp + 1] * udata[pp + 1]) + (Quad[2] = udata[pp + 2] * udata[pp + 2]) -
00123
00124
           (Quad[3] = udata[pp + 2] * udata[pp + 2]) -

(Quad[3] = udata[pp + 3] * udata[pp + 3]) -

(Quad[4] = udata[pp + 4] * udata[pp + 4]) -

(Quad[5] = udata[pp + 5] * udata[pp + 5]));

g = udata[pp] * udata[pp + 3] + udata[pp + 1] * udata[pp + 4] +

udata[pp + 2] * udata[pp + 5];
00125
00126
00127
00128
00129
00130
           // 2. Choose process/expansion order and assign derivative values of \ensuremath{\mathtt{L}}
00131
           // w.r.t. F, G
           switch (*c) {
case 0:
00132
00133
             lf = 0;
00134
00135
              lff = 0;
              lfg = 0;
00136
00137
              lg = 0;
00138
              lgg = 0;
00139
              break;
00140
           case 2:
00141
             1f = 0.000354046449700427580438254 * f * f +
                   0.000191775160254398272737387 * g * g;
00142
              lff = 0.0007080928994008551608765075 * f;
00143
00144
              lfg = 0.0003835503205087965454747749 * g;
00145
              lg = 0.0003835503205087965454747749 * f * g;
              lgg = 0.0003835503205087965454747749 * f;
00146
00147
              break;
00148
           case 1:
00149
              1f = 0.000206527095658582755255648 * f;
00150
              lff = 0.000206527095658582755255648;
00151
              lfg = 0;
              lg = 0.0003614224174025198216973841 * g;
00152
              lgg = 0.0003614224174025198216973841;
00153
```

```
break;
00155
                  lf = (0.000206527095658582755255648 + 0.000354046449700427580438254 * f) *
00156
00157
                                 f +
                           0.000191775160254398272737387 * g * g;
00158
                   lff = 0.000206527095658582755255648 + 0.0007080928994008551608765075 * f;
00159
                   lfg = 0.0003835503205087965454747749 * g;
00160
                   lg = (0.0003614224174025198216973841 +
00161
00162
                            0.0003835503205087965454747749 * f) *
00163
                   lgg = 0.0003614224174025198216973841 + 0.0003835503205087965454747749 * f:
00164
00165
                   break:
                default:
00166
                  errorKill(
00167
00168
                         "You need to specify a correct order in the weak-field expansion.");
00169
                // 3. Assign Jacobi components
00170
               00171
00173
                JMM[6] =
                      lff * udata[pp] * udata[1 + pp] + lfg * udata[1 + pp] * udata[3 + pp] +
lfg * udata[pp] * udata[4 + pp] + lgg * udata[3 + pp] * udata[4 + pp];
00174
00175
                JMM[7] = lf + lff * Quad[1] +
00176
00177
                             udata[4 + pp] * (2 * lfg * udata[1 + pp] + lgg * udata[4 + pp]);
00178
                JMM[12] =
                    lff * udata[pp] * udata[2 + pp] + lfg * udata[2 + pp] * udata[3 + pp] +
lfg * udata[pp] * udata[5 + pp] + lgg * udata[3 + pp] * udata[5 + pp];
00179
00180
00181
                JMM[13] = lff * udata[1 + pp] * udata[2 + pp] +
                               lfg * udata[2 + pp] * udata[4 + pp] +
00182
00183
                                lfg * udata[1 + pp] * udata[5 + pp] +
               lgg * udata[4 + pp] * udata[5 + pp];

JMM[14] = lf + lff * Quad[2] +
00184
00185
                Udata[5 + pp] * (2 * lfg * udata[2 + pp] + lgg * udata[5 + pp]);

JMM[18] = lg + lfg * (Quad[0] - Quad[3 + 0]) +
00186
00187
                00188
00189
00190
                00191
00192
00193
                JMM[21] = -1f + lgg * Quad[0] +
               00194
00195
00196
00197
                (-lff + lgg) * udata[1 + pp] * udata[4 + pp];

JMM[26] = -(udata[4 + pp] * (lff * udata[2 + pp] + lfg * udata[5 + pp])) +
00198
00199
00200
                                udata[1 + pp] * (lfg * udata[2 + pp] + lgg * udata[5 + pp]);
               00201
00202
00203
00204
                00205
00206
00207
               00208
00209
00210
00211
                                (-lff + lgg) * udata[2 + pp] * udata[5 + pp];
00212
                JMM[33] = lgg * udata[pp] * udata[2 + pp] +
                               lff * udata[3 + pp] * udata[5 + pp] -
lfg * (udata[2 + pp] * udata[3 + pp] + udata[pp] * udata[5 + pp]);
00213
00214
00215
                JMM[34] =
00216
                      lgg * udata[1 + pp] * udata[2 + pp] +
                      lff * udata[4 + pp] * udata[5 + pp]
00217
00218
                      lfg * (udata[2 + pp] * udata[4 + pp] + udata[1 + pp] * udata[5 + pp]);
00219
                JMM[35] = -lf + lgg * Quad[2] +
00220
                              udata[5 + pp] * (-2 * lfg * udata[2 + pp] + lff * udata[5 + pp]);
                //#pragma unroll_and_jam
00221
00222
                //#pragma distribute_point
00223
                for (int i = 0; i < 6; i++) {
                   for (int j = i + 1; j < 6; j++)
00224
00225
                      JMM[i * 6 + j] = JMM[j * 6 + i];
00226
                  }
00227
00228
                // 4. Final values for temporal derivatives of field values
                h[1] = dxData[pp] * JMM[30] + dxData[1 + pp] * JMM[31]
00230
                           dxData[2 + pp] * JMM[32] + dxData[3 + pp] * JMM[33] +
dxData[4 + pp] * JMM[34] + dxData[5 + pp] * (-1 + JMM[35]);
00231
00232
                h[2] = -(dxData[pp] * JMM[24]) - dxData[1 + pp] * JMM[25] - dxData[2 + pp] * JMM[26] - dxData[3 + pp] * JMM[27] - dxData[3 + p
00233
00234
                           dxData[4 + pp] * (1 - JMM[28]) - dxData[5 + pp] * JMM[29];
00235
00236
00237
               h[4] = dxData[2 + pp];
               h[5] = -dxData[1 + pp];
00238
               h(0) = h(3) * JMM(3) + h(4) * JMM(4) + h(5) * JMM(5);

h(1) = h(3) * JMM(9) + h(4) * JMM(10) + h(5) * JMM(11);
00239
00240
```

```
h[2] = h[3] * JMM[15] + h[4] * JMM[16] + h[5] * JMM[17];
                   // (1+Z)^-1 applies only to E components dudata[pp + 0] =
00242
00243
                          h(2) * (-(JMM[2] * (1 + JMM[7])) + JMM[1] * JMM[8]) +
h[1] * (JMM[2] * JMM[13] - JMM[1] * (1 + JMM[14])) +
h[0] * (1 - JMM[8] * JMM[13] + JMM[14] + JMM[7] * (1 + JMM[14]));
00244
00245
00246
                   dudata[pp + 1] =
                         h[2] * (JMM[2] * JMM[6] - (1 + JMM[0]) * JMM[8]) +
h[1] * (1 - JMM[2] * JMM[12] + JMM[14] + JMM[0] * (1 + JMM[14])) +
h[0] * (JMM[8] * JMM[12] - JMM[6] * (1 + JMM[14]));
00248
00249
00250
                 h[0] * (OHM[0] * OHM[12] - OHM[0] * (1 + OHM[14])),

dudata[pp + 2] =

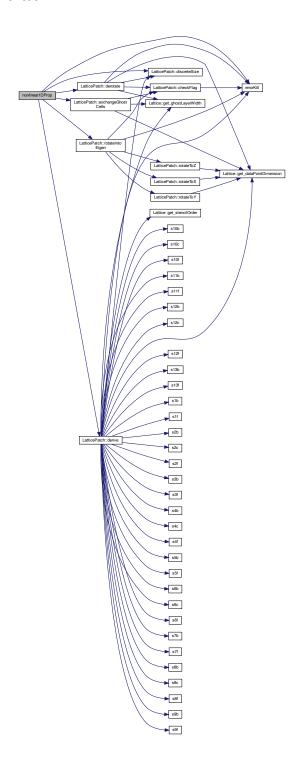
h[2] * (1 - JMM[1] * JMM[6] + JMM[7] + JMM[0] * (1 + JMM[7])) +

h[1] * (JMM[1] * JMM[12] - (1 + JMM[0]) * JMM[13]) +

h[0] * (-((1 + JMM[7]) * JMM[12]) + JMM[6] * JMM[13]);
00251
00252
00253
00254
00255
               pseudoDenom =
                   -((1 + JMM[7]) * (-1 + JMM[2] * JMM[12])) +
(JMM[2] * JMM[6] - JMM[8]) * JMM[13] + JMM[14] + JMM[7] * JMM[14] +
JMM[0] * (1 + JMM[7] - JMM[8] * JMM[13] + (1 + JMM[7]) * JMM[14]) -
JMM[1] * (-(JMM[8] * JMM[12]) + JMM[6] * (1 + JMM[14]));
00256
00257
00258
                  dudata[pp + 0] /= pseudoDenom;
dudata[pp + 1] /= pseudoDenom;
00260
00261
                  dudata[pp + 2] /= pseudoDenom;
dudata[pp + 3] = h[3];
dudata[pp + 4] = h[4];
00262
00263
00264
00265
                   dudata[pp + 5] = h[5];
00266
00267
               return;
00268 }
```

References LatticePatch::buffData, LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::discreteSize(), errorKill(), LatticePatch::exchangeGhostCells(), and LatticePatch::rotateIntoEigen().

Referenced by Sim1D().



Here is the caller graph for this function:



6.28.2.5 nonlinear2DProp()

```
void nonlinear2DProp (
    LatticePatch * data,
    N_Vector u,
    N_Vector udot,
    int * c )
```

nonlinear 2D HE propagation

HE propagation function for 2D.

Definition at line 303 of file TimeEvolutionFunctions.cpp.

```
00303
00304
         sunrealtype *dxData = data->buffData[1 - 1];
sunrealtype *dyData = data->buffData[2 - 1];
00305
00306
00307
00308
         data->exchangeGhostCells(1);
00309
         data->rotateIntoEigen(1);
00310
         data->derive(1);
00311
         data->derotate(1, dxData);
00312
         data->exchangeGhostCells(2);
00313
         data->rotateIntoEigen(2);
00314
         data->derive(2);
00315
         data->derotate(2, dyData);
00316
         sunrealtype f = NAN, g = NAN; sunrealtype lf = NAN, lff = NAN, lfg = NAN, lg = NAN, lgg = NAN; array<sunrealtype, 36> JMM;
00317
00318
00319
00320
         array<sunrealtype, 6> Quad;
00321
         array<sunrealtype, 6> h;
00322
         sunrealtype pseudoDenom = NAN;
00323
         sunrealtype *udata = nullptr, *dudata = nullptr;
udata = NV_DATA_P(u);
00324
         dudata = NV_DATA_P(udot);
int totalNP = data->discreteSize();
00325
00326
00327
          //#pragma distribute_point
00328
          //#pragma unroll_and_jam
         for (int pp = 0; pp < totalNP * 6; pp += 6) {
    // 1</pre>
00329
00330
           00331
00332
00333
00334
                          (Quad[4] = udata[pp + 4] * udata[pp + 4]) -
00335
            (Quad[5] = udata[pp + 4] * udata[pp + 4]) -
(Quad[5] = udata[pp + 5] * udata[pp + 5]));

g = udata[pp] * udata[pp + 3] + udata[pp + 1] * udata[pp + 4] +
udata[pp + 2] * udata[pp + 5];
00336
00337
00338
            // 2
00339
00340
            switch (*c) {
            case 0:
lf = 0;
00341
00342
              lff = 0;
00343
00344
              lfg = 0;
00345
              lg = 0;
```

```
lgg = 0;
00347
            break;
00348
          case 2:
00349
            1f = 0.000354046449700427580438254 * f * f +
                 0.000191775160254398272737387 * g * g;
00350
             lff = 0.0007080928994008551608765075 * f;
00351
             lfg = 0.0003835503205087965454747749 * g;
             lg = 0.0003835503205087965454747749 * f
00353
00354
             lgg = 0.0003835503205087965454747749 * f;
00355
            break;
00356
          case 1:
            lf = 0.000206527095658582755255648 * f;
00357
00358
             lff = 0.000206527095658582755255648;
             lfg = 0;
00359
00360
             lg = 0.0003614224174025198216973841 * g;
00361
             lgg = 0.0003614224174025198216973841;
00362
            break;
00363
          case 3:
00364
            1f = (0.000206527095658582755255648 + 0.000354046449700427580438254 * f) *
00365
            \begin{array}{c} 0.000191775160254398272737387 \ \star \ g \ \star \ g; \\ 1ff = 0.000206527095658582755255648 \ + \ 0.000708092899400855160876508 \ \star \ f; \end{array}
00366
00367
             lfg = 0.0003835503205087965454747749 * g;
00368
             lg = (0.000361422417402519821697384 + 0.000383550320508796545474775 \star f) \star f
00369
00370
                 q;
             lgg = 0.000361422417402519821697384 + 0.000383550320508796545474775 * f;
00371
00372
00373
          default:
            errorKill(
00374
                 "You need to specify a correct order in the weak-field expansion.");
00375
00376
00377
00378
          JMM[0] = lf + lff * Quad[0] +
00379
                    udata[3 + pp] * (2 * 1fg * udata[pp] + 1gg * udata[3 + pp]);
          JMM[6] =
00380
              lff * udata[pp] * udata[1 + pp] + lfg * udata[1 + pp] * udata[3 + pp] +
00381
               lfg * udata[pp] * udata[4 + pp] + lgg * udata[3 + pp] * udata[4 + pp];
00382
          JMM[7] = lf + lff * Quad[1] +
00383
00384
                   udata[4 + pp] * (2 * lfg * udata[1 + pp] + lgg * udata[4 + pp]);
00385
           JMM[12] =
               lff * udata[pp] * udata[2 + pp] + lfg * udata[2 + pp] * udata[3 + pp] +
00386
               lfg * udata[pp] * udata[5 + pp] + lgg * udata[3 + pp] * udata[5 + pp];
00387
          00388
00389
                     lfg * udata[1 + pp] * udata[5 + pp] +
00390
00391
                     lgg * udata[4 + pp] * udata[5 + pp];
          JMM[14] = 1f + 1ff * Quad[2] +
00392
          udata[5 + pp] * (2 * lfg * udata[2 + pp] + lgg * udata[5 + pp]);

JMM[18] = lg + lfg * (Quad[0] - Quad[3 + 0]) +
00393
00394
          (-lff + lgg) * udata[pp] * udata[3 + pp];

JMM[19] = -(udata[3 + pp] * (lff * udata[1 + pp] + lfg * udata[4 + pp])) + udata[pp] * (lfg * udata[1 + pp] + lgg * udata[4 + pp]);
00395
00396
00397
          00398
00399
          00400
00401
00403
00404
          JMM[25] = lg + lfg * (Quad[1] - Quad[4 + 0]) +
          00405
00406
                     udata[1 + pp] * (lfg * udata[2 + pp] + lgg * udata[5 + pp]);
00407
00408
          JMM[27] = lgg * udata[pp] * udata[1 + pp] +
                     lff * udata[3 + pp] * udata[4 + pp] -
00409
00410
                     lfg * (udata[1 + pp] * udata[3 + pp] + udata[pp] * udata[4 + pp]);
00411
          JMM[28] = -lf + lgg * Quad[1] +
          Udata[4 + pp] * (-2 * lfg * udata[1 + pp] + lff * udata[4 + pp]);

JMM[30] = udata[2 + pp] * (lfg * udata[pp] + lgg * udata[3 + pp]) -

(lff * udata[pp] + lfg * udata[3 + pp]) * udata[5 + pp];

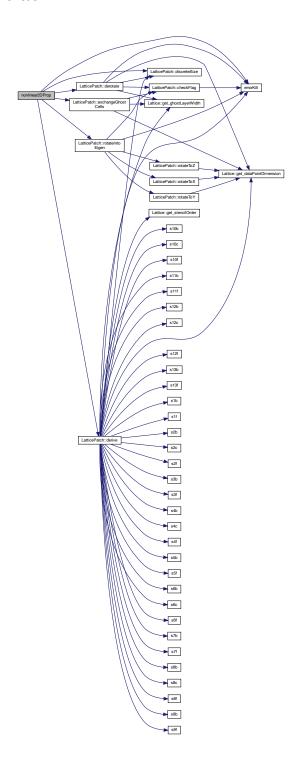
JMM[31] = udata[2 + pp] * (lfg * udata[1 + pp] + lgg * udata[4 + pp]) -
00412
00413
00414
00415
          (lff * udata[1 + pp] + lfg * udata[4 + pp]) * udata[5 + pp];

JMM[32] = lg + lfg * (Quad[2] - Quad[5 + 0]) +
00416
00417
                     (-lff + lgg) * udata[2 + pp] * udata[5 + pp];
00418
          00419
00420
                     lfg * (udata[2 + pp] * udata[3 + pp] + udata[pp] * udata[5 + pp]);
00421
00422
          JMM[34] =
00423
              lgg * udata[1 + pp] * udata[2 + pp]
               lff * udata[4 + pp] * udata[5 + pp] -
00424
          lff * (udata[2 + pp] * udata[4 + pp] + udata[1 + pp] * udata[5 + pp]);
JMM[35] = -lf + lgg * Quad[2] +
00425
00426
                     udata[5 + pp] * (-2 * lfg * udata[2 + pp] + lff * udata[5 + pp]);
00427
00428
00429
          //#pragma distribute_point
00430
           //#pragma unroll_and_jam
          for (int i = 0; i < 6; i++) {
  for (int j = i + 1; j < 6; j++) {</pre>
00431
00432
```

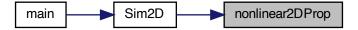
```
JMM[i * 6 + j] = JMM[j * 6 + i];
00434
00435
                           h[0] = 0;
00436
                           h[1] = dxData[pp] * JMM[30] + dxData[1 + pp] * JMM[31] + dxData[2 + pp] * JMM[32] + dxData[3 + pp] * JMM[33] + dxData[4 + pp] * JMM[34] + dxData[5 + pp] * (-1 + JMM[35]);
00437
00438
                           h[2] = -(dxData[pp] * JMM[24]) - dxData[1 + pp] * JMM[25] - dxData[2 + pp] * JMM[26] - dxData[3 + pp] * JMM[27] +
00440
00441
                                                 dxData[4 + pp] * (1 - JMM[28]) - dxData[5 + pp] * JMM[29];
00442
00443
                           h[3] = 0;
                           h[4] = dxData[2 + pp];
00444
                           00445
00446
00447
00448
                            h[1] += 0;
00449
                           h[1] - 0,
h[2] += dyData[pp] * JMM[18] + dyData[1 + pp] * JMM[19] +
dyData[2 + pp] * JMM[20] + dyData[3 + pp] * (-1 + JMM[21]) +
dyData[4 + pp] * JMM[22] + dyData[5 + pp] * JMM[23];
00450
00452
00453
                            h[3] += -dyData[2 + pp];
00454
                            h[4] += 0;
                           h[5] += dyData[pp];
h[0] -= h[3] * JMM[3] + h[4] * JMM[4] + h[5] * JMM[5];
h[1] -= h[3] * JMM[9] + h[4] * JMM[10] + h[5] * JMM[11];
00455
00456
00457
                             h[2] = h[3] * JMM[15] + h[4] * JMM[16] + h[5] * JMM[17];
                           00459
00460
00461
00462
00463
                                       h[2] * (JMM[2] * JMM[6] - (1 + JMM[0]) * JMM[8]) +
h[1] * (1 - JMM[2] * JMM[12] + JMM[14] + JMM[0] * (1 + JMM[14])) +
00464
00465
                                        h[0] * (JMM[8] * JMM[12] - JMM[6] * (1 + JMM[14]));
00466
                           dudata[pp + 2] =
  h[2] * (1 - JMM[1] * JMM[6] + JMM[7] + JMM[0] * (1 + JMM[7])) +
  h[1] * (JMM[1] * JMM[12] - (1 + JMM[0]) * JMM[13]) +
  h[0] * (-((1 + JMM[7]) * JMM[12]) + JMM[6] * JMM[13]);
00467
00468
00469
00471
                           pseudoDenom =
                                     -((1 + JMM[7]) * (-1 + JMM[2] * JMM[12])) +
(JMM[2] * JMM[6] - JMM[8]) * JMM[13] + JMM[14] + JMM[7] * JMM[14] +
00472
00473
                                       \[ \langle \text{ \text{Connected} \] \times \text{Connected} \] \times \[ \text{Connected} \] \
00474
00475
                           dudata[pp + 0] /= pseudoDenom;
dudata[pp + 1] /= pseudoDenom;
00476
00477
                           dudata[pp + 2] /= pseudoDenom;
dudata[pp + 3] = h[3];
dudata[pp + 4] = h[4];
00478
00479
00480
                           dudata[pp + 5] = h[5];
00481
00482
00483
                      return;
00484 }
```

References LatticePatch::buffData, LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::discreteSize(), errorKill(), LatticePatch::exchangeGhostCells(), and LatticePatch::rotateIntoEigen().

Referenced by Sim2D().



Here is the caller graph for this function:



6.28.2.6 nonlinear3DProp()

```
void nonlinear3DProp (
    LatticePatch * data,
    N_Vector u,
    N_Vector udot,
    int * c )
```

nonlinear 3D HE propagation

HE propagation function for 3D.

```
Definition at line 538 of file TimeEvolutionFunctions.cpp.
```

```
00538
00539
        sunrealtype *dxData = data->buffData[1 - 1];
00540
00541
        sunrealtype *dyData = data->buffData[2 - 1];
00542
        sunrealtype *dzData = data->buffData[3 - 1];
00543
00544
         /\star Under the hood call of point-to-point or collective communication \star/
00545
        // Point-to-Point:
00546
00547
             data->exchangeGhostCells(1);
00548
             data->rotateIntoEigen(1);
00549
             data->derive(1);
00550
             data->derotate(1,dxData);
00551
             data->exchangeGhostCells(2);
             data->rotateIntoEigen(2);
00552
00553
             data->derive(2);
00554
             data->derotate(2, dyData);
00555
             data->exchangeGhostCells(3);
00556
             data->rotateIntoEigen(3);
00557
             data->derive(3);
00558
             data->derotate(3,dzData);
00559
00560
        // Collective:
00561
00562
        data->exchangeGhostCells3D();
00563
        data->rotateIntoEigen3D();
00564
        data->derive(1);
00565
        data->derotate(1, dxData);
00566
        data->derive(2);
00567
        data->derotate(2, dyData);
00568
        data->derive(3);
00569
00570
        data->derotate(3, dzData);
00571
00572
        sunrealtype f = NAN, g = NAN; sunrealtype lf = NAN, lff = NAN, lfg = NAN, lg = NAN, lgg = NAN;
00574
        array<sunrealtype, 36> JMM;
00575
        array<sunrealtype, 6> Quad;
        array<sunrealtype, 6> h;
sunrealtype pseudoDenom = NAN;
00576
00577
        sunrealtype *udata = nullptr, *dudata = nullptr;
udata = NV_DATA_P(u);
00578
00579
00580
        dudata = NV_DATA_P(udot);
```

```
int totalNP = data->discreteSize();
        //#pragma distribute_point
00582
00583
         //#pragma unroll_and_jam
        for (int pp = 0; pp < totalNP * 6; pp += 6) {
    // 1</pre>
00584
00585
           f = 0.5 * ((Quad[0] = udata[pp] * udata[pp]) +
00586
                       (Quad[1] = udata[pp + 1] * udata[pp + 1]) +
                        (Quad[2] = udata[pp + 2] * udata[pp + 2]) -
00588
00589
                        (Quad[3] = udata[pp + 3] * udata[pp + 3]) -
00590
                        (Quad[4] = udata[pp + 4] * udata[pp + 4]) -
          (Quad[5] = udata[pp + 3] * udata[pp + 4]) *

(Quad[5] = udata[pp + 5] * udata[pp + 5]);

g = udata[pp] * udata[pp + 3] + udata[pp + 1] * udata[pp + 4] +
00591
00592
00593
              udata[pp + 2] * udata[pp + 5];
00594
           // 2
00595
           switch (*c) {
00596
           case 0:
            1f = 0:
00597
             lff = 0;
00598
             lfg = 0;
00600
             lg = 0;
             lgg = 0;
00601
00602
             break;
00603
          case 2:
            lf = 0.000354046449700427580438254 * f * f +
00604
                 0.000191775160254398272737387 * g * g;
00605
             lff = 0.0007080928994008551608765075 * f;
             1fg = 0.0003835503205087965454747749 * g;
00607
00608
             1g = 0.0003835503205087965454747749 * f * g;
00609
             lgg = 0.0003835503205087965454747749 * f;
00610
            break:
00611
           case 1:
00612
             1f = 0.000206527095658582755255648 * f;
             lff = 0.000206527095658582755255648;
00613
             lfg = 0;
00614
00615
             lg = 0.0003614224174025198216973841 * g;
             lgg = 0.0003614224174025198216973841;
00616
00617
            break;
           case 3:
00619
             lf = (0.000206527095658582755255648 + 0.000354046449700427580438254 * f) *
00620
             \begin{array}{c} 0.000191775160254398272737387 \ \star \ g \ \star \ g; \\ 1ff = 0.000206527095658582755255648 \ + \ 0.000708092899400855160876508 \ \star \ f; \end{array}
00621
00622
             lfg = 0.0003835503205087965454747749 * g;
00623
             lg = (0.000361422417402519821697384 + 0.000383550320508796545474775 * f) *
00624
00625
00626
             lgg = 0.000361422417402519821697384 + 0.000383550320508796545474775 * f;
00627
             break;
00628
           default:
            errorKill(
00629
                 "You need to specify a correct order in the weak-field expansion.");
00630
00631
           // 3
00632
00633
           JMM[0] = lf + lff * Quad[0] +
00634
                    udata[3 + pp] * (2 * lfg * udata[pp] + lgg * udata[3 + pp]);
           JMM[6] =
00635
               lff * udata[pp] * udata[1 + pp] + lfg * udata[1 + pp] * udata[3 + pp] +
00636
               lfg * udata[pp] * udata[4 + pp] + lgg * udata[3 + pp] * udata[4 + pp];
           JMM[7] = lf + lff * Quad[1] +
00638
00639
                    udata[4 + pp] * (2 * lfg * udata[1 + pp] + lgg * udata[4 + pp]);
00640
           .TMM [121 =
           lff * udata[pp] * udata[2 + pp] + lfg * udata[2 + pp] * udata[3 + pp] +
lfg * udata[pp] * udata[5 + pp] + lgg * udata[3 + pp] * udata[5 + pp];

JMM[13] = lff * udata[1 + pp] * udata[2 + pp] +
00641
00642
00643
                      lfg * udata[2 + pp] * udata[4 + pp] +
00644
00645
                      lfg * udata[1 + pp] * udata[5 + pp]
00646
                      lgg * udata[4 + pp] * udata[5 + pp];
          00647
00648
00649
                      (-lff + lgg) * udata[pp] * udata[3 + pp];
          00651
00652
00653
00654
           JMM[21] = -lf + lgg * Quad[0] +
00655
                     udata[3 + pp] * (-2 * lfg * udata[pp] + lff * udata[3 + pp]);
00656
           00657
00658
           JMM[25] = 1g + 1fg * (Quad[1] - Quad[4 + 0]) +
00659
           JMM[26] = -(udata[4 + pp] * udata[4 + pp];

JMM[26] = -(udata[4 + pp] * (lff * udata[2 + pp] + lfg * udata[5 + pp])) +

udata[1 + pp] * (lfg * udata[2 + pp] + lgg * udata[5 + pp]);
00660
00661
00662
           JMM[27] = lgg * udata[pp] * udata[1 + pp] +
00663
00664
                      lff * udata[3 + pp] * udata[4 + pp] -
           lfg * (udata[1 + pp] * udata[3 + pp] + udata[pp] * udata[4 + pp]);
JMM[28] = -lf + lgg * Quad[1] +
    udata[4 + pp] * (-2 * lfg * udata[1 + pp] + lff * udata[4 + pp]);
00665
00666
00667
```

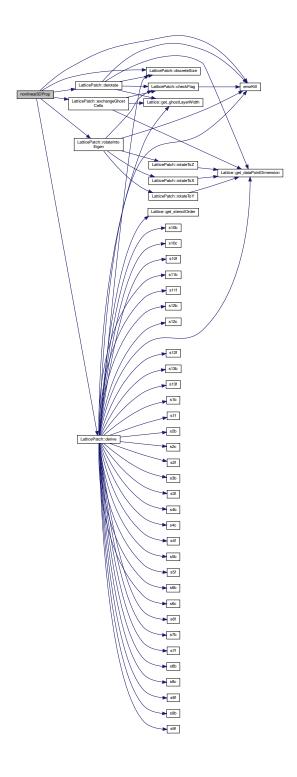
```
JMM[30] = udata[2 + pp] * (lfg * udata[pp] + lgg * udata[3 + pp]) -
                        (lff * udata[pp] + lfg * udata[3 + pp]) * udata[5 + pp];
00669
            00670
00671
00672
           00673
00675
                        lff * udata[3 + pp] * udata[5 + pp]
00676
                        lfg * (udata[2 + pp] * udata[3 + pp] + udata[pp] * udata[5 + pp]);
00677
            JMM[34] =
00678
                lgg * udata[1 + pp] * udata[2 + pp] +
            lff * udata[1 + pp] * udata[2 + pp] -
lff * (udata[2 + pp] * udata[5 + pp] -
lfg * (udata[2 + pp] * udata[4 + pp] + udata[1 + pp] * udata[5 + pp]);

JMM[35] = -lf + lgg * Quad[2] +
00679
00680
00681
00682
                       udata[5 + pp] * (-2 * lfg * udata[2 + pp] + lff * udata[5 + pp]);
00683
00684
            //#pragma distribute_point
            //#pragma unroll_and_jam
for (int i = 0; i < 6; i++) {</pre>
00685
00686
             for (int j = i + 1; j < 6; j++)
                JMM[i * 6 + j] = JMM[j * 6 + i];
00688
00689
              }
00690
           h[0] = 0:
00691
00692
           h[1] = dxData[pp] * JMM[30] + dxData[1 + pp] * JMM[31]
                    dxData[2 + pp] * JMM[32] + dxData[3 + pp] * JMM[33] + dxData[4 + pp] * JMM[34] + dxData[5 + pp] * (-1 + JMM[35]);
00694
           h[2] = -(dxData[pp] * JMM[24]) - dxData[1 + pp] * JMM[25] - dxData[2 + pp] * JMM[26] - dxData[3 + pp] * JMM[27] +
00695
00696
                    dxData[4 + pp] * (1 - JMM[28]) - dxData[5 + pp] * JMM[29];
00697
00698
           h[3] = 0;
00699
           h[4] = dxData[2 + pp];
00700
            h[5] = -dxData[1 + pp];
           h[0] += -(dyData[pp] * JMM[30]) - dyData[1 + pp] * JMM[31] - dyData[2 + pp] * JMM[32] - dyData[3 + pp] * JMM[33] - dyData[4 + pp] * JMM[34] + dyData[5 + pp] * (1 - JMM[35]);
00701
00702
00703
00704
           h[1] += 0;
           h[2] += dyData[pp] * JMM[18] + dyData[1 + pp] * JMM[19] +
                     dyData[2 + pp] * JMM[20] + dyData[3 + pp] * (-1 + JMM[21]) +
dyData[4 + pp] * JMM[22] + dyData[5 + pp] * JMM[23];
00706
00707
00708
           h[3] += -dyData[2 + pp];
           h[4] += 0;
00709
00710
           h[5] += dyData[pp];
00711
           h[0] += dzData[pp] * JMM[24] + dzData[1 + pp] * JMM[25] +
                     dzData[2 + pp] * JMM[26] + dzData[3 + pp] * JMM[27] +
00712
                     dzData[4 + pp] * (-1 + JMM[28]) + dzData[5 + pp] * JMM[29];
00713
           h[1] += -(dzData[pp] * JMM[18]) - dzData[1 + pp] * JMM[19] - dzData[2 + pp] * JMM[20] + dzData[3 + pp] * (1 - JMM[21]) - dzData[4 + pp] * JMM[22] - dzData[5 + pp] * JMM[23];
00714
00715
00716
00717
           h[2] += 0;
           h[3] += dzData[1 + pp];
00719
            h[4] += -dzData[pp];
00720
            h[5] += 0;
           h[0] = h[3] * JMM[3] + h[4] * JMM[4] + h[5] * JMM[5];

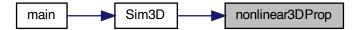
h[1] = h[3] * JMM[9] + h[4] * JMM[10] + h[5] * JMM[11];
00721
00722
00723
            h[2] = h[3] * JMM[15] + h[4] * JMM[16] + h[5] * JMM[17];
            dudata[pp + 0] =
00725
                h[2] * (-(JMM[2] * (1 + JMM[7])) + JMM[1] * JMM[8]) +
                h[1] * (JMM[2] * JMM[13] - JMM[1] * (1 + JMM[14])) +
h[0] * (1 - JMM[8] * JMM[13] + JMM[14] + JMM[7] * (1 + JMM[14]));
00726
00727
           dudata[pp + 1] =
00728
                h[2] * (JMM[2] * JMM[6] - (1 + JMM[0]) * JMM[8]) +
h[1] * (1 - JMM[2] * JMM[12] + JMM[14] + JMM[0] * (1 + JMM[14])) +
00729
00731
                h[0] * (JMM[8] * JMM[12] - JMM[6] * (1 + JMM[14]));
           00732
00733
                h[1] * (JMM[1] * JMM[12] - (1 + JMM[0]) * JMM[13]) + h[0] * (-((1 + JMM[7]) * JMM[12]) + JMM[6] * JMM[13]);
00734
00735
00736
           pseudoDenom =
                 -((1 + JMM[7]) * (-1 + JMM[2] * JMM[12])) +
(JMM[2] * JMM[6] - JMM[8]) * JMM[13] + JMM[14] + JMM[7] * JMM[14] +
00738
00739
                JMM[0] * (1 + JMM[7] - JMM[8] * JMM[13] + (1 + JMM[7]) * JMM[14]) -
                JMM[1] * (-(JMM[8] * JMM[12]) + JMM[6] * (1 + JMM[14]));
00740
           dudata[pp + 0] /= pseudoDenom;
00741
           dudata[pp + 1] /= pseudoDenom;
00742
00743
           dudata[pp + 2] /= pseudoDenom;
00744
            dudata[pp + 3] = h[3];
00745
            dudata[pp + 4] = h[4];
           dudata[pp + 5] = h[5];
00746
         1
00747
00748
         return;
```

References LatticePatch::buffData, LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::discreteSize(), errorKill(), LatticePatch::exchangeGhostCells(), and LatticePatch::rotateIntoEigen().

Referenced by Sim3D().



Here is the caller graph for this function:



6.29 TimeEvolutionFunctions.cpp

```
Go to the documentation of this file.
```

```
00002 /// @file TimeEvolutionFunctions.cpp
00003 /// @brief Implementation of functions to propagate
00004 /// data vectors in time according to Maxwell's equations,
00005 /// and various orders in the HE weak-field expansion
00007
00008 #include "TimeEvolutionFunctions.h"
00009
00010 #include <math.h>
00011
00012 /// CVode right-hand-side function (CVRhsFn)
00013 int TimeEvolution::f(sunrealtype t, N_Vector u, N_Vector udot, void *data_loc) {
       \ensuremath{//} Set recover pointer to provided lattice patch where the data resides
00014
00015
       LatticePatch *data = nullptr:
00016
       data = static_cast<LatticePatch *>(data_loc);
00017
00018
       // pointers for update circle
00019
       sunrealtype *udata = nullptr, *dudata = nullptr;
00020
       sunrealtype *originaluData = nullptr, *originalduData = nullptr;
00021
00022
       // Access NVECTOR_PARALLEL argument data with pointers
       udata = NV_DATA_P(u);
00023
00024
       dudata = NV_DATA_P(udot);
00025
00026
       // Store original data location of the patch
00027
       originaluData = data->uData;
00028
       originalduData = data->duData;
       // Point patch data to arguments of f
00029
00030
       data->uData = udata;
00031
       data->duData = dudata;
00032
00033
       // Time-evolve these arguments (the field data) with specific propagator below
00034
       TimeEvolver(data, u, udot, c);
00035
00036
       // Refer patch data back to original location
00037
       data->uData = originaluData;
       data->duData = originalduData;
00038
00039
00040
       return (0):
00041 }
00042
00043 /// only under-the-hood-callable Maxwell propagation in 1D \,
00044 // unused parameters 2-4 for compliance with CVRhsFn
\tt 00045 // same as the respective nonlinear function without nonlinear terms
00046 void linear1DProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c) {
00047
00048
       // pointers to temporal and spatial derivative data
00049
       sunrealtype *duData = data->duData;
00050
       sunrealtype *dxData = data->buffData[1 - 1];
00051
00052
       // sequence along any dimension:
       data->exchangeGhostCells(1); // exchange halos
00053
00054
       data->rotateIntoEigen(
00055
          1);
                       // -> rotate all data to prepare derivative operation
00056
       data->derive(1); // -> perform derivative on it
00057
       data->derotate(
00058
           1, dxData); // -> derotate derivative data to x-space for further use
00059
00060
       int totalNP = data->discreteSize();
00061
       int pp = 0;
```

```
00062 #pragma distribute_point
        for (int i = 0; i < totalNP; i++) {</pre>
00063
          pp = i * 6;
00064
00065
00066
          simple vacuum Maxwell equations for spatial deriative only in x-direction
00067
           temporal derivative is approximated by spatial derivative according to the
           numerical scheme with Jacobi=0 -> no polarization or magnetization terms
00069
00070
          duData[pp + 0] = 0;
          duData[pp + 1] = -dxData[pp + 5];
duData[pp + 2] = dxData[pp + 4];
00071
00072
          duData[pp + 3] = 0;
00073
          duData[pp + 4] = dxData[pp + 2];
00074
00075
          duData[pp + 5] = -dxData[pp + 1];
00076
00077 }
00078
00079 /// nonlinear 1D HE propagation
00080 void nonlinearlDProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c) {
00081
         / pointer to spatial derivative data sufficient, temporal derivative data
00082
        // provided with udot
00083
00084
        sunrealtype *dxData = data->buffData[1 - 1];
00085
00086
        // same sequence as in the linear case
        data->exchangeGhostCells(1);
00087
00088
        data->rotateIntoEigen(1);
00089
        data->derive(1);
00090
        data->derotate(1, dxData);
00091
00092
00093
        F and G are nonzero in the nonlinear case,
00094
        polarization and magnetization contributions in Jacobi matrix style
00095
        with derivatives of polarization and magnetization
00096
        w.r.t. E- and B-field
00097
        sunrealtype f = NAN, g = NAN; // em field invariants F, G sunrealtype lf = NAN, lff = NAN, lfg = NAN, lg = NAN,
00098
00100
                    lgg = NAN; // derivatives of Lagrangian w.r.t. field invariants
       array<sunrealtype, 36> JMM; // Jacobi matrix
array<sunrealtype, 6> Quad; // array to hold E^2 and B^2 components
array<sunrealtype, 6> h; // holding temporal derivatives of E and B components
// before operating (1+Z)^-1
00101
00102
00103
00104
00105
        sunrealtype pseudoDenom = NAN; // needed for inversion of 1+Z
        sunrealtype *udata = nullptr,
00106
00107
                    *dudata = nullptr; // pointers to data and temp. derivative data
00108
        udata = NV_DATA_P(u);
00109
        dudata = NV_DATA_P(udot);
        int totalNP = data->discreteSize(); // number of points in the patch
00110
        // #pragma omp parallel for private(...) reduction(...) -> unsafe due to
00111
        // reductions and many variables, how to deal with / reduction?
00112
00113
        //#pragma block_loop
00114
        //#pragma unroll_and_jam
00115
        //#pragma distribute_point
        00116
00117
00119
                                 for (int pp=ppB;pp<min(totalNP*6,ppB+6*6);pp+=6) {
00120
          /// Calculation of the Jacobi matrix
         00121
00122
00123
00124
00125
                      (Quad[3] = udata[pp + 3] * udata[pp + 3]) -
00126
                      (Quad[4] = udata[pp + 4] * udata[pp + 4]) -
                      (Quad[5] = udata[pp + 5] * udata[pp + 5]));
00127
          g = udata[pp] * udata[pp + 3] + udata[pp + 1] * udata[pp + 4] + udata[pp + 2] * udata[pp + 5];
00128
00129
00130
          // 2. Choose process/expansion order and assign derivative values of {\tt L}
00131
          // w.r.t. F, G
00132
          switch (*c) {
00133
          case 0:
00134
            1f = 0;
            lff = 0;
00135
            lfg = 0;
00136
            lg = 0;
00137
            lgg = 0;
00138
00139
            break;
00140
          case 2:
            lf = 0.000354046449700427580438254 * f * f +
00141
                0.000191775160254398272737387 * g * g;
00142
            lff = 0.0007080928994008551608765075 * f;
00143
            1fg = 0.0003835503205087965454747749 * g;
00144
00145
            lg = 0.0003835503205087965454747749 * f * g;
00146
            lgg = 0.0003835503205087965454747749 * f;
00147
            break;
          case 1:
00148
```

```
lf = 0.000206527095658582755255648 * f;
                     lff = 0.000206527095658582755255648;
00150
                    lfg = 0;
00151
00152
                     lg = 0.0003614224174025198216973841 * g;
                     lgg = 0.0003614224174025198216973841;
00153
00154
                    break:
                 case 3:
                     \texttt{lf} = (0.000206527095658582755255648 + 0.000354046449700427580438254 \star \texttt{f}) \; \star \; \texttt{f}
00156
00157
                    0.00191775160254398272737387 \star g \star g; \\ 1ff = 0.000206527095658582755255648 + 0.0007080928994008551608765075 \star f; \\
00158
00159
                     1fg = 0.0003835503205087965454747749 * g;
00160
00161
                     lg = (0.0003614224174025198216973841 +
                               0.0003835503205087965454747749 * f) *
00162
00163
00164
                     lgg = 0.0003614224174025198216973841 + 0.0003835503205087965454747749 * f;
00165
                    break:
00166
                 default:
                   errorKill(
00167
00168
                           "You need to specify a correct order in the weak-field expansion.");
00169
                  // 3. Assign Jacobi components
00170
00171
                 JMM[0] = lf + lff * Quad[0] +
00172
                                udata[3 + pp] * (2 * lfg * udata[pp] + lgg * udata[3 + pp]);
00173
                 JMM[6] =
                     lff * udata[pp] * udata[1 + pp] + lfg * udata[1 + pp] * udata[3 + pp] +
00174
00175
                        lfg * udata[pp] * udata[4 + pp] + lgg * udata[3 + pp] * udata[4 + pp];
00176
                 JMM[7] = lf + lff * Quad[1] +
00177
                                udata[4 + pp] * (2 * lfg * udata[1 + pp] + lgg * udata[4 + pp]);
00178
                 JMM[12] =
                       1ff * udata[pp] * udata[2 + pp] + lfg * udata[2 + pp] * udata[3 + pp] +
1fg * udata[pp] * udata[5 + pp] + lgg * udata[3 + pp] * udata[5 + pp];
00179
00180
                 JMM[13] = lff * udata[1 + pp] * udata[2 + pp] +
00181
                                   lfg * udata[2 + pp] * udata[4 + pp] +
00182
                                   lfg * udata[1 + pp] * udata[5 + pp] +
lgg * udata[4 + pp] * udata[5 + pp];
00183
00184
                 00185
00187
00188
                                   (-lff + lgg) * udata[pp] * udata[3 + pp];
                 00189
00190
                 00191
00192
                 JMM[21] = -1f + lgg * Quad[0] +
00193
00194
                                  udata[3 + pp] * (-2 * lfg * udata[pp] + lff * udata[3 + pp]);
                00195
00196
00197
00198
00199
00200
                                  udata[1 + pp] * (lfg * udata[2 + pp] + lgg * udata[5 + pp]);
00201
                 JMM[27] = lgg * udata[pp] * udata[1 + pp] +
                00202
00203
00204
00206
00207
                 00208
00209
00210
                                   (-lff + lgg) * udata[2 + pp] * udata[5 + pp];
00211
                 JMM[33] = lgg * udata[pp] * udata[2 + pp] +
00212
00213
                                  lff * udata[3 + pp] * udata[5 + pp] -
00214
                                 lfg * (udata[2 + pp] * udata[3 + pp] + udata[pp] * udata[5 + pp]);
                 JMM[34] =
00215
00216
                        lgg * udata[1 + pp] * udata[2 + pp] +
                        lfg * ddata[1 + pp] * ddata[2 + pp] -
lfg * (udata[2 + pp] * udata[4 + pp] + udata[1 + pp] * udata[5 + pp]);
00217
00219
                  JMM[35] = -1f + 1gg * Quad[2] +
00220
                                 udata[5 + pp] * (-2 * lfg * udata[2 + pp] + lff * udata[5 + pp]);
00221
                 //#pragma unroll_and_jam
00222
                 //#pragma distribute_point
                 for (int i = 0; i < 6; i++) {
  for (int j = i + 1; j < 6; j++) {</pre>
00223
00224
00225
                        JMM[i * 6 + j] = JMM[j * 6 + i];
00226
00227
                 ^{\prime} // 4. Final values for temporal derivatives of field values
00228
00229
                 h[0] = 0;
                 h[1] = dxData[pp] * JMM[30] + dxData[1 + pp] * JMM[31]
                             dxData[2+ pp] * JMM[32] + dxData[3 + pp] * JMM[33] + dxData[4 + pp] * JMM[34] + dxData[5 + pp] * (-1 + JMM[35]);
00231
00232
                h[2] = -(dxData[pp] * JMM[24]) - dxData[1 + pp] * JMM[25] - dxData[2 + pp] * JMM[26] - dxData[3 + pp] * JMM[27] + dxData[4 + pp] * (1 - JMM[28]) - dxData[5 + pp] * JMM[29];
00233
00234
00235
```

```
h[3] = 0;
            h[4] = dxData[2 + pp];
00237
            h[5] = -dxData[1 + pp];
00238
           00239
00240
00241
            // (1+Z)^{-1} applies only to E components
00243
            dudata[pp + 0] =
               h[2] * (-(JMM[2] * (1 + JMM[7])) + JMM[1] * JMM[8]) +
h[1] * (JMM[2] * JMM[13] - JMM[1] * (1 + JMM[14])) +
h[0] * (1 - JMM[8] * JMM[13] + JMM[14] + JMM[7] * (1 + JMM[14]));
00244
00245
00246
           dudata[pp + 1] =
    h[2] * (JMM[2] * JMM[6] - (1 + JMM[0]) * JMM[8]) +
    h[1] * (1 - JMM[2] * JMM[12] + JMM[14] + JMM[0] * (1 + JMM[14])) +
00247
00248
00249
00250
                h[0] * (JMM[8] * JMM[12] - JMM[6] * (1 + JMM[14]));
           dudata[pp + 2] =
  h[2] * (1 - JMM[1] * JMM[6] + JMM[7] + JMM[0] * (1 + JMM[7])) +
  h[1] * (JMM[1] * JMM[12] - (1 + JMM[0]) * JMM[13]) +
  h[0] * (-((1 + JMM[7]) * JMM[12]) + JMM[6] * JMM[13]);
00251
00252
00253
00255
           pseudoDenom =
                 -((1 + JMM[7]) * (-1 + JMM[2] * JMM[12])) +
(JMM[2] * JMM[6] - JMM[8]) * JMM[13] + JMM[14] + JMM[7] * JMM[14] +
00256
00257
                JMM[0] * (1 + JMM[7] - JMM[8] * JMM[13] + (1 + JMM[7]) * JMM[14]) - JMM[1] * (-(JMM[8] * JMM[12]) + JMM[6] * (1 + JMM[14]));
00258
00259
           dudata[pp + 0] /= pseudoDenom;
dudata[pp + 1] /= pseudoDenom;
00260
00262
            dudata[pp + 2] /= pseudoDenom;
           dudata[pp + 3] = h[3];
dudata[pp + 4] = h[4];
00263
00264
           dudata[pp + 5] = h[5];
00265
00266
00267
         return;
00268 }
00269
00270 /// only under-the-hood-callable Maxwell propagation in 2D
00271 // unused parameters 2-4 for compliance with {\tt CVRhsFn}
00272 // same as the respective nonlinear function without nonlinear terms
00273 void linear2DProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c) {
00274
00275
         sunrealtype *duData = data->duData;
00276
         sunrealtype *dxData = data->buffData[1 - 1];
         sunrealtype *dyData = data->buffData[2 - 1];
00277
00278
00279
         data->exchangeGhostCells(1);
00280
         data->rotateIntoEigen(1);
00281
         data->derive(1);
00282
         data->derotate(1, dxData);
00283
         data->exchangeGhostCells(2);
         data->rotateIntoEigen(2);
00284
00285
         data->derive(2);
00286
         data->derotate(2, dyData);
00287
00288
         int totalNP = data->discreteSize();
00289 int pp = 0;
00290 #pragma distribute_point
00291
         for (int i = 0; i < totalNP; i++) {</pre>
          pp = i * 6;
            duData[pp + 0] = dyData[pp + 5];
00293
           duData[pp + 1] = -dxData[pp + 5];
00294
           duData[pp + 2] = -dyData[pp + 3] + dxData[pp + 4];
00295
           duData[pp + 2] - -uybata[pp + 3]
duData[pp + 3] = -dyData[pp + 2];
duData[pp + 4] = dxData[pp + 2];
00296
00297
00298
           duData[pp + 5] = dyData[pp + 0] - dxData[pp + 1];
00299
00300 }
00301
00302 /// nonlinear 2D HE propagation
00303 void nonlinear2DProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c) {
00304
00305
         sunrealtype *dxData = data->buffData[1 - 1];
         sunrealtype *dyData = data->buffData[2 - 1];
00306
00307
00308
         data->exchangeGhostCells(1);
         data->rotateIntoEigen(1);
00309
00310
         data->derive(1);
00311
         data->derotate(1, dxData);
00312
         data->exchangeGhostCells(2);
00313
         data->rotateIntoEigen(2);
00314
         data->derive(2):
00315
         data->derotate(2, dyData);
00316
00317
         sunrealtype f = NAN, g = NAN;
00318
         sunrealtype lf = NAN, lff = NAN, lfg = NAN, lg = NAN, lgg = NAN;
00319
         array<sunrealtype, 36> JMM;
00320
         array<sunrealtype, 6> Quad;
         array<sunrealtype, 6> h;
00321
00322
         sunrealtype pseudoDenom = NAN;
```

```
sunrealtype *udata = nullptr, *dudata = nullptr;
        udata = NV_DATA_P(u);
00324
        dudata = NV_DATA_P(udot);
00325
        int totalNP = data->discreteSize();
00326
00327
        //#pragma distribute_point
00328
        //#pragma unroll_and_jam
        for (int pp = 0; pp < totalNP * 6; pp += 6) {</pre>
00330
00331
          f = 0.5 * ((Quad[0] = udata[pp] * udata[pp]) +
                       (Quad[1] = udata[pp + 1] * udata[pp + 1]) + (Quad[2] = udata[pp + 2] * udata[pp + 2]) -
00332
00333
00334
                       (Quad[3] = udata[pp + 3] * udata[pp + 3]) -
                       (Quad[4] = udata[pp + 4] * udata[pp + 4]) - (Quad[5] = udata[pp + 5] * udata[pp + 5]));
00335
00336
00337
          g = udata[pp] * udata[pp + 3] + udata[pp + 1] * udata[pp + 4] +
          udata[pp + 2] * udata[pp + 5];
00338
00339
00340
          switch (*c) {
00341
          case 0:
             lf = 0;
00342
00343
             lff = 0;
             lfg = 0;
00344
00345
             lg = 0;
             lgg = 0;
00346
00347
            break;
00348
          case 2:
00349
            1f = 0.000354046449700427580438254 * f * f +
                 0.000191775160254398272737387 * g * g;
00350
             1ff = 0.0007080928994008551608765075 * f:
00351
00352
             1fg = 0.0003835503205087965454747749 * g;
             lg = 0.0003835503205087965454747749 * f * g;
00353
00354
             lgg = 0.0003835503205087965454747749 * f;
00355
             break;
00356
           case 1:
00357
             lf = 0.000206527095658582755255648 * f;
             lff = 0.000206527095658582755255648;
00358
             lfg = 0;
00359
             lg = 0.0003614224174025198216973841 * g;
00360
             lgg = 0.0003614224174025198216973841;
00361
00362
             break;
00363
           case 3:
            1f = (0.000206527095658582755255648 + 0.000354046449700427580438254 * f) *
00364
00365
00366
                  0.000191775160254398272737387 * g * g;
             lff = 0.000206527095658582755255648 + 0.000708092899400855160876508 * f;
00367
             lfg = 0.0003835503205087965454747749 * g;
00368
00369
             00370
00371
             lgg = 0.000361422417402519821697384 + 0.000383550320508796545474775 * f;
00372
             break:
00373
          default:
00374
            errorKill(
00375
                 "You need to specify a correct order in the weak-field expansion.");
00376
00377
00378
          JMM[0] = lf + lff * Quad[0] +
                    udata[3 + pp] * (2 * lfg * udata[pp] + lgg * udata[3 + pp]);
00380
          lff * udata[pp] * udata[1 + pp] + lfg * udata[1 + pp] * udata[3 + pp] +
lfg * udata[pp] * udata[4 + pp] + lgg * udata[3 + pp] * udata[4 + pp];
JMM[7] = lf + lff * Quad[1] +
00381
00382
00383
                    udata[4 + pp] * (2 * lfg * udata[1 + pp] + lgg * udata[4 + pp]);
00384
00385
              lff * udata[pp] * udata[2 + pp] + lfg * udata[2 + pp] * udata[3 + pp] +
lfg * udata[pp] * udata[5 + pp] + lgg * udata[3 + pp] * udata[5 + pp];
00386
00387
00388
          JMM[13] = lff * udata[1 + pp] * udata[2 + pp] +
                     lfg * udata[2 + pp] * udata[4 + pp] +
00389
                      lfg * udata[1 + pp] * udata[5 + pp] +
00390
          lgg * udata[4 + pp] * udata[5 + pp];

JMM[14] = lf + lff * Quad[2] +
00391
00392
          udata[5 + pp] * (2 * lfg * udata[2 + pp] + lgg * udata[5 + pp]);

JMM[18] = lg + lfg * (Quad[0] - Quad[3 + 0]) +
00393
00394
          (-lff + lgg) * udata[pp] * udata[3 + pp];

JMM[19] = -(udata[3 + pp] * (lff * udata[1 + pp] + lfg * udata[4 + pp])) +

udata[pp] * (lfg * udata[1 + pp] + lgg * udata[4 + pp]);
00395
00396
00397
          00398
00399
          00400
00401
00402
00403
00404
          \( \text{(-1ff + 1gg) * udata[1 + pp] * udata[4 + pp];} \)
\( \text{JMM[26]} = -(\text{udata[4 + pp] * (1ff * udata[2 + pp] + 1fg * udata[5 + pp])) + } \)
00405
00406
00407
                     udata[1 + pp] * (lfg * udata[2 + pp] + lgg * udata[5 + pp]);
          00408
00409
```

```
lfg * (udata[1 + pp] * udata[3 + pp] + udata[pp] * udata[4 + pp]);
            00411
00412
00413
00414
00415
00416
00417
00418
                         (-lff + lgg) * udata[2 + pp] * udata[5 + pp];
00419
            JMM[33] = lgg * udata[pp] * udata[2 + pp] +
                        lff * udata[3 + pp] * udata[5 + pp] -
lfg * (udata[2 + pp] * udata[3 + pp] + udata[pp] * udata[5 + pp]);
00420
00421
00422
            JMM[34] =
00423
                 lgg * udata[1 + pp] * udata[2 + pp] +
00424
                 lff * udata[4 + pp] * udata[5 + pp] -
            lfg * (udata[2 + pp] * udata[4 + pp] + udata[1 + pp] * udata[5 + pp]);
JMM[35] = -lf + lgg * Quad[2] +
00425
00426
00427
                        udata[5 + pp] * (-2 * lfg * udata[2 + pp] + lff * udata[5 + pp]);
00429
            //#pragma distribute_point
00430
            //#pragma unroll_and_jam
            for (int i = 0; i < 6; i++) {
  for (int j = i + 1; j < 6; j++) {
00431
00432
                JMM[i * 6 + j] = JMM[j * 6 + i];
00433
00434
              }
00435
00436
            h[0] = 0;
00437
            h[1] = dxData[pp] * JMM[30] + dxData[1 + pp] * JMM[31]
            dxData[2 + pp] * JMM[32] + dxData[3 + pp] * JMM[33] +
dxData[4 + pp] * JMM[34] + dxData[3 + pp] * JMM[35]);
h[2] = -(dxData[pp] * JMM[24]) - dxData[1 + pp] * JMM[25] -
dxData[2 + pp] * JMM[26] - dxData[3 + pp] * JMM[27] +
dxData[4 + pp] * (1 - JMM[28]) - dxData[5 + pp] * JMM[29];
00438
00439
00440
00441
00442
00443
            h[3] = 0;
            h[4] = dxData[2 + pp];
h[5] = -dxData[1 + pp];
00444
00445
            h[0] += -(dyData[pp] * JMM[30]) - dyData[1 + pp] * JMM[31] - dyData[2 + pp] * JMM[32] - dyData[3 + pp] * JMM[33] -
00446
00448
                      dyData[4 + pp] * JMM[34] + dyData[5 + pp] * (1 - JMM[35]);
00449
            h[1] += 0;
            h[2] += dyData[pp] * JMM[18] + dyData[1 + pp] * JMM[19] + dyData[2 + pp] * JMM[20] + dyData[3 + pp] * (-1 + JMM[21]) + dyData[4 + pp] * JMM[22] + dyData[5 + pp] * JMM[23];
00450
00451
00452
            h[3] += -dyData[2 + pp];
00453
            h[4] += 0;
00454
00455
            h[5] += dyData[pp];
            00456
00457
00458
            dudata[pp + 0] =
00459
                h[2] * (-(JMM[2] * (1 + JMM[7])) + JMM[1] * JMM[8]) +
h[1] * (JMM[2] * JMM[13] - JMM[1] * (1 + JMM[14])) +
h[0] * (1 - JMM[8] * JMM[13] + JMM[14] + JMM[7] * (1 + JMM[14]));
00460
00461
00462
00463
            dudata[pp + 1] =
                 h[2] * (JMM[2] * JMM[6] - (1 + JMM[0]) * JMM[8]) +
h[1] * (1 - JMM[2] * JMM[12] + JMM[14] + JMM[0] * (1 + JMM[14])) +
00464
00465
                 h[0] * (JMM[8] * JMM[12] - JMM[6] * (1 + JMM[14]));
            fl() * (OFM*[0] * OFM*[12],
dudata[pp + 2] =
  h[2] * (1 - JMM[1] * JMM[6] + JMM[7] + JMM[0] * (1 + JMM[7])) +
  h[1] * (JMM[1] * JMM[12] - (1 + JMM[0]) * JMM[13]) +
  h[0] * (-((1 + JMM[7]) * JMM[12]) + JMM[6] * JMM[13]);
00467
00468
00469
00470
00471
            pseudoDenom =
00472
                 -((1 + JMM[7]) * (-1 + JMM[2] * JMM[12]))
                  (JMM[2] * JMM[6] - JMM[8]) * JMM[13] + JMM[14] + JMM[7] * JMM[14] +
00473
00474
                 JMM[0] * (1 + JMM[7] - JMM[8] * JMM[13] + (1 + JMM[7]) * JMM[14]) -
                JMM[1] * (-(JMM[8] * JMM[12]) + JMM[6] * (1 + JMM[14]));
00475
            dudata[pp + 0] /= pseudoDenom;
00476
            dudata[pp + 1] /= pseudoDenom;
00477
            dudata[pp + 2] /= pseudoDenom;
00478
            dudata[pp + 3] = h[3];
00480
            dudata[pp + 4] = h[4];
00481
            dudata[pp + 5] = h[5];
00482
00483
         return;
00484 }
00486 /// only under-the-hood-callable Maxwell propagation in 3D
00487 // unused parameters 2-4 for compliance with CVRhsFn \,
00488 // same as the respective nonlinear function without nonlinear terms
00489 void linear3DProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c) {
00490
         sunrealtype *duData = data->duData;
         sunrealtype *dxData = data->buffData[1 - 1];
00492
         sunrealtype *dyData = data->buffData[2 - 1];
00493
00494
         sunrealtype *dzData = data->buffData[3 - 1];
00495
00496
         /* Under the hood call of point-to-point or collective communication */
```

```
00497
        // Point-to-Point:
00498
        data->exchangeGhostCells(1);
00499
        data->rotateIntoEigen(1);
00500
        data->derive(1);
00501
        data->derotate(1, dxData);
00502
        data->exchangeGhostCells(2);
00503
        data->rotateIntoEigen(2);
00504
        data->derive(2);
00505
        data->derotate(2, dyData);
00506
        data->exchangeGhostCells(3);
        data->rotateIntoEigen(3);
00507
00508
        data->derive(3);
00509
        data->derotate(3, dzData);
00510
00511
         // Collective:
00512
             data->exchangeGhostCells3D();
00513
00514
             data->rotateIntoEigen3D();
             data->derive(1);
00516
             data->derotate(1,dxData);
00517
             data->derive(2);
00518
             data->derotate(2,dyData);
00519
             data->derive(3);
00520
             data->derotate(3,dzData);
00521
00522
00523
        int totalNP = data->discreteSize();
00524
        int pp = 0;
00525 #pragma distribute_point
        for (int i = 0; i < totalNP; i++) {
   pp = i * 6;</pre>
00526
00527
          duData[pp + 0] = dyData[pp + 5] - dzData[pp + 4];
duData[pp + 1] = dzData[pp + 3] - dxData[pp + 5];
duData[pp + 2] = dxData[pp + 4] - dyData[pp + 3];
00528
00529
00530
          duData[pp + 3] = -dyData[pp + 2] + dzData[pp + 1];
duData[pp + 4] = -dzData[pp + 0] + dxData[pp + 2];
duData[pp + 5] = -dxData[pp + 1] + dyData[pp + 0];
00531
00532
00533
00534
00535 }
00536
00537 /// nonlinear 3D HE propagation
00538 void nonlinear3DProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c) {
00539
00540
        sunrealtype *dxData = data->buffData[1 - 1];
00541
        sunrealtype *dyData = data->buffData[2 - 1];
00542
        sunrealtype *dzData = data->buffData[3 - 1];
00543
00544
        /\star Under the hood call of point-to-point or collective communication \star/
00545
        // Point-to-Point:
00546
00547
             data->exchangeGhostCells(1);
00548
             data->rotateIntoEigen(1);
00549
             data->derive(1);
00550
             data->derotate(1, dxData);
00551
             data->exchangeGhostCells(2);
00552
             data->rotateIntoEigen(2);
             data->derive(2);
             data->derotate(2,dyData);
00554
00555
             data->exchangeGhostCells(3);
00556
             data->rotateIntoEigen(3);
00557
             data \rightarrow derive(3):
00558
             data->derotate(3,dzData);
00559
00560
        // Collective:
00561
00562
        data->exchangeGhostCells3D();
00563
        data->rotateIntoEigen3D();
00564
        data->derive(1):
00565
        data->derotate(1, dxData);
00566
        data->derive(2);
00567
        data->derotate(2, dyData);
00568
        data->derive(3);
00569
        data->derotate(3, dzData);
00570
00571
00572
        sunrealtype f = NAN, g = NAN;
00573
        sunrealtype lf = NAN, lff = NAN, lfg = NAN, lg = NAN, lgg = NAN;
00574
        array<sunrealtype, 36> JMM;
00575
        array<sunrealtype, 6> Quad;
00576
        array<sunrealtype, 6> h;
00577
        sunrealtype pseudoDenom = NAN;
00578
        sunrealtype *udata = nullptr, *dudata = nullptr;
00579
        udata = NV_DATA_P(u);
00580
        dudata = NV_DATA_P(udot);
00581
        int totalNP = data->discreteSize();
00582
        //#pragma distribute_point
00583
        //#pragma unroll and jam
```

```
for (int pp = 0; pp < totalNP * 6; pp += 6) {</pre>
00585
00586
         f = 0.5 * ((Quad[0] = udata[pp] * udata[pp]) +
                    (Quad[1] = udata[pp + 1] * udata[pp + 1]) +
00587
                    (Quad[2] = udata[pp + 2] * udata[pp + 2]) -
00588
                    (Quad[3] = udata[pp + 3] * udata[pp + 3]) -
00589
                    (Quad[4] = udata[pp + 4] * udata[pp + 4])
00591
                    (Quad[5] = udata[pp + 5] * udata[pp + 5]));
00592
         g = udata[pp] * udata[pp + 3] + udata[pp + 1] * udata[pp + 4] +
             udata[pp + 2] * udata[pp + 5];
00593
         // 2
00594
00595
         switch (*c) {
00596
         case 0:
00597
          1f = 0;
00598
           lff = 0;
           lfg = 0;
00599
           lg = 0;
00600
           lgg = 0;
00601
00602
           break;
00603
         case 2:
           lf = 0.000354046449700427580438254 * f * f +
00604
00605
               0.000191775160254398272737387 * g * g;
           1ff = 0.0007080928994008551608765075 * f:
00606
           lfg = 0.0003835503205087965454747749 * g;
00607
00608
           lg = 0.0003835503205087965454747749 * f * g;
           lgg = 0.0003835503205087965454747749 * f;
00610
00611
         case 1:
           lf = 0.000206527095658582755255648 * f;
00612
00613
           lff = 0.000206527095658582755255648;
           lfg = 0;
00614
00615
           lg = 0.0003614224174025198216973841 * g;
           lgg = 0.0003614224174025198216973841;
00616
00617
           break;
         case 3:
00618
           lf = (0.000206527095658582755255648 + 0.000354046449700427580438254 * f) *
00619
00620
           0.000191775160254398272737387 * g * g; \\ lff = 0.000206527095658582755255648 + 0.000708092899400855160876508 * f; \\
00622
00623
           lfg = 0.0003835503205087965454747749 * g;
           lg = (0.000361422417402519821697384 + 0.000383550320508796545474775 * f) *
00624
00625
               g;
           lgg = 0.000361422417402519821697384 + 0.000383550320508796545474775 * f;
00626
00627
           break;
00628
         default:
00629
           errorKill(
00630
               "You need to specify a correct order in the weak-field expansion.");
00631
          // 3
00632
         JMM[0] = lf + lff * Quad[0] +
00633
00634
                 udata[3 + pp] * (2 * lfg * udata[pp] + lgg * udata[3 + pp]);
00635
          JMM[6] =
00636
             lff * udata[pp] * udata[1 + pp] + lfg * udata[1 + pp] * udata[3 + pp] +
         lfg * udata[pp] * udata[4 + pp] + lgg * udata[3 + pp] * udata[4 + pp];

JMM[7] = lf + lff * Quad[1] +
00637
00638
                 udata[4 + pp] * (2 * lfg * udata[1 + pp] + lgg * udata[4 + pp]);
00639
             lff * udata[pp] * udata[2 + pp] + lfg * udata[2 + pp] * udata[3 + pp] +
00641
             lfg * udata[pp] * udata[5 + pp] + lgg * udata[3 + pp] * udata[5 + pp];
00642
00643
         JMM[13] = lff * udata[1 + pp] * udata[2 + pp] +
                   lfg * udata[2 + pp] * udata[4 + pp] +
00644
00645
                   lfg * udata[1 + pp] * udata[5 + pp] +
00646
                   lgg * udata[4 + pp] * udata[5 + pp];
         JMM[14] = lf + lff * Quad[2] +
00647
                   udata[5 + pp] * (2 * lfg * udata[2 + pp] + lgg * udata[5 + pp]);
00648
00649
         JMM[18] = lg + lfg * (Quad[0] - Quad[3 + 0]) +
00650
                   (-lff + lgg) * udata[pp] * udata[3 + pp];
         00651
00652
00654
00655
         JMM[21] = -lf + lgg * Quad[0] +
         00656
00657
00658
00659
                   (-lff + lgg) * udata[1 + pp] * udata[4 + pp];
00660
00661
         JMM[26] = -(udata[4 + pp] * (lff * udata[2 + pp] + lfg * udata[5 + pp])) +
00662
                   udata[1 + pp] * (lfg * udata[2 + pp] + lgg * udata[5 + pp]);
00663
         JMM[27] = lgg * udata[pp] * udata[1 + pp] +
                   lff * udata[3 + pp] * udata[4 + pp]
00664
                   lfg * (udata[1 + pp] * udata[3 + pp] + udata[pp] * udata[4 + pp]);
00665
         JMM[28] = -1f + lgg * Quad[1] +
00666
                  udata[4 + pp] * (-2 * lfg * udata[1 + pp] + lff * udata[4 + pp]);
00667
         00668
00669
00670
```

```
(lff * udata[1 + pp] + lfg * udata[4 + pp]) * udata[5 + pp];
                00672
00673
                00674
00675
00676
                JMM[34] =
00678
                      lgg * udata[1 + pp] * udata[2 + pp] +
                      lff * udata[4 + pp] * udata[5 + pp] -
lfg * (udata[2 + pp] * udata[4 + pp] + udata[1 + pp] * udata[5 + pp]);
00679
00680
                JMM[35] = -1f + lgg * Quad[2] +
00681
                               udata[5 + pp] * (-2 * lfg * udata[2 + pp] + lff * udata[5 + pp]);
00682
00683
                //#pragma distribute_point
00684
00685
                //#pragma unroll_and_jam
                for (int i = 0; i < 6; i++) {
  for (int j = i + 1; j < 6; j++) {
    JMM[i * 6 + j] = JMM[j * 6 + i];</pre>
00686
00687
00688
00689
00690
00691
                h[0] = 0;
                h[1] = dxData[pp] * JMM[30] + dxData[1 + pp] * JMM[31] +
00692
               dxData[2 + pp] * JMM[32] + dxData[3 + pp] * JMM[33] + dxData[4 + pp] * JMM[34] + dxData[5 + pp] * (-1 + JMM[35]);

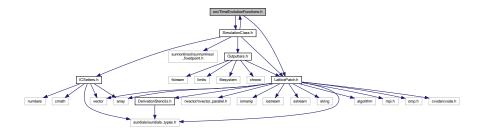
h[2] = -(dxData[pp] * JMM[24]) - dxData[1 + pp] * JMM[25] - dxData[2 + pp] * JMM[26] - dxData[3 + pp] * JMM[27] +
00693
00694
00695
00697
                           dxData[4 + pp] * (1 - JMM[28]) - dxData[5 + pp] * JMM[29];
00698
               h[3] = 0;
00699
                h[4] = dxData[2 + pp];
                h[5] = -dxData[1 + pp];
00700
               h[0] += -(dyData[pp] * JMM[30]) - dyData[1 + pp] * JMM[31] - dyData[2 + pp] * JMM[32] - dyData[3 + pp] * JMM[33] - dyData[4 + pp] * JMM[34] + dyData[5 + pp] * (1 - JMM[35]);
00701
00702
00703
00704
                h[1] += 0;
               h[2] += dyData[pp] * JMM[18] + dyData[1 + pp] * JMM[19] + dyData[2 + pp] * JMM[20] + dyData[3 + pp] * (-1 + JMM[21]) + dyData[4 + pp] * JMM[22] + dyData[5 + pp] * JMM[23];
00705
00706
00707
                h[3] += -dyData[2 + pp];
                h[4] += 0;
00709
00710
                h[5] += dyData[pp];
00711
                h[0] += dzData[pp] * JMM[24] + dzData[1 + pp] * JMM[25] +
               dzData[2 + pp] * JMM[26] + dzData[3 + pp] * JMM[27] + dzData[4 + pp] * (-1 + JMM[28]) + dzData[5 + pp] * JMM[29]; h[1] += -(dzData[pp] * JMM[18]) - dzData[1 + pp] * JMM[19] - dzData[2 + pp] * JMM[20] + dzData[3 + pp] * (1 - JMM[21]) - dzData[4 + pp] * JMM[22] - dzData[5 + pp] * JMM[23];
00712
00713
00714
00715
00716
00717
               h[2] += 0;
               h[3] += dzData[1 + pp];
h[4] += -dzData[pp];
00718
00719
00720
                h[5] += 0;
                h[0] -= h[3] * JMM[3] + h[4] * JMM[4] + h[5] * JMM[5];
h[1] -= h[3] * JMM[9] + h[4] * JMM[10] + h[5] * JMM[11];
h[2] -= h[3] * JMM[15] + h[4] * JMM[16] + h[5] * JMM[17];
00722
00723
               dudata[pp + 0] =
    h[2] * (-(JMM[2] * (1 + JMM[7])) + JMM[1] * JMM[8]) +
    h[1] * (JMM[2] * JMM[13] - JMM[1] * (1 + JMM[14])) +
    h[0] * (1 - JMM[8] * JMM[13] + JMM[14] + JMM[7] * (1 + JMM[14]));
00724
00725
00726
00727
                dudata[pp + 1] =
    h[2] * (JMM[2] * JMM[6] - (1 + JMM[0]) * JMM[8]) +
    h[1] * (1 - JMM[2] * JMM[12] + JMM[14] + JMM[0] * (1 + JMM[14])) +
00728
00729
00730
                      h[0] * (JMM[8] * JMM[12] - JMM[6] * (1 + JMM[14]));
00731
               h[0] * (OFM.[0] * OFM.[1] * JMM[0] * (1 + JMM[7]) +
h[2] * (1 - JMM[1] * JMM[6] + JMM[7] + JMM[0] * (1 + JMM[7])) +
h[1] * (JMM[1] * JMM[12] - (1 + JMM[0]) * JMM[13]) +
h[0] * (-((1 + JMM[7]) * JMM[12]) + JMM[6] * JMM[13]);
00732
00733
00734
00735
                pseudoDenom =
00736
                      -((1 + JMM[7]) * (-1 + JMM[2] * JMM[12])) +
(JMM[2] * JMM[6] - JMM[8]) * JMM[13] + JMM[14] + JMM[7] * JMM[14] +
JMM[0] * (1 + JMM[7] - JMM[8] * JMM[13] + (1 + JMM[7]) * JMM[14]) -
00737
00738
00739
                      JMM[1] * (-(JMM[8] * JMM[12]) + JMM[6] * (1 + JMM[14]));
00740
                dudata[pp + 0] /= pseudoDenom;
dudata[pp + 1] /= pseudoDenom;
00741
00742
               dudata[pp + 2] /= pseudoDenom;
dudata[pp + 3] = h[3];
dudata[pp + 4] = h[4];
00743
00744
00745
00746
                dudata[pp + 5] = h[5];
00747
00748
           return;
00749 }
```

6.30 src/TimeEvolutionFunctions.h File Reference

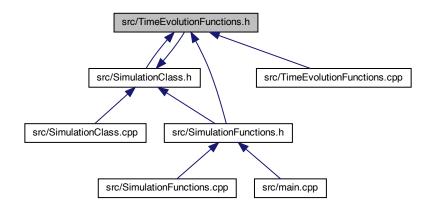
Functions to propagate data vectors in time according to Maxwell's equations, and various orders in the HE weak-field expansion.

```
#include "LatticePatch.h"
#include "SimulationClass.h"
```

Include dependency graph for TimeEvolutionFunctions.h:



This graph shows which files directly or indirectly include this file:



Data Structures

· class TimeEvolution

monostate TimeEvolution Class to propagate the field data in time in a given order of the HE weak-field expansion

Functions

- void linear1DProp (LatticePatch *data, N_Vector u, N_Vector udot, int *c)
 - Maxwell propagation function for 1D only for reference.
- void nonlinear1DProp (LatticePatch *data, N_Vector u, N_Vector udot, int *c)

HE propagation function for 1D.

• void linear2DProp (LatticePatch *data, N_Vector u, N_Vector udot, int *c)

Maxwell propagation function for 2D - only for reference.

void nonlinear2DProp (LatticePatch *data, N_Vector u, N_Vector udot, int *c)

HE propagation function for 2D.

void linear3DProp (LatticePatch *data, N_Vector u, N_Vector udot, int *c)

Maxwell propagation function for 3D - only for reference.

void nonlinear3DProp (LatticePatch *data, N_Vector u, N_Vector udot, int *c)

HE propagation function for 3D.

6.30.1 Detailed Description

Functions to propagate data vectors in time according to Maxwell's equations, and various orders in the HE weak-field expansion.

Definition in file TimeEvolutionFunctions.h.

6.30.2 Function Documentation

6.30.2.1 linear1DProp()

```
void linear1DProp (
    LatticePatch * data,
    N_Vector u,
    N_Vector udot,
    int * c )
```

Maxwell propagation function for 1D – only for reference.

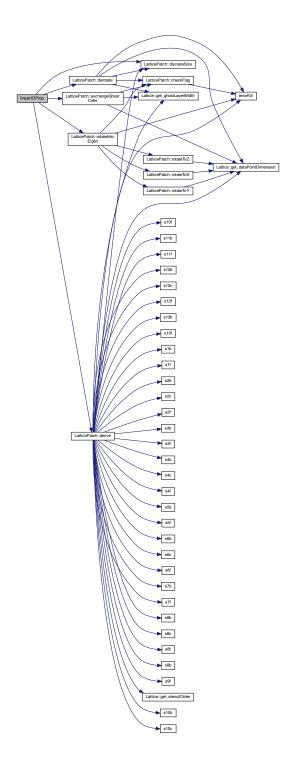
Maxwell propagation function for 1D – only for reference.

Definition at line 46 of file TimeEvolutionFunctions.cpp.

```
00046
00047
         // pointers to temporal and spatial derivative data
sunrealtype *duData = data->duData;
00048
00049
00050
         sunrealtype *dxData = data->buffData[1 - 1];
00051
00052
         // sequence along any dimension:
         data->exchangeGhostCells(1); // exchange halos
00053
00054
         data->rotateIntoEigen(
00055
             1);
                            // -> rotate all data to prepare derivative operation
         data->derive(1); // -> perform derivative on it
00056
00057
00058
              1, dxData); // -> derotate derivative data to x-space for further use
00059
00060
         int totalNP = data->discreteSize();
00061
         int pp = 0;
00062 #pragma distribute_point
00063
         for (int i = 0; i < totalNP; i++) {</pre>
00064
00065
00066
             simple vacuum Maxwell equations for spatial deriative only in x-direction
            temporal derivative is approximated by spatial derivative according to the numerical scheme with Jacobi=0 -> no polarization or magnetization terms
00067
00068
00069
00070
            duData[pp + 0] = 0;
           duData[pp + 1] = -dxData[pp + 5];
duData[pp + 2] = dxData[pp + 4];
duData[pp + 3] = 0;
00071
00072
00073
00074
           duData[pp + 4] = dxData[pp + 2];
00075
           duData[pp + 5] = -dxData[pp + 1];
```

```
00076 }
```

 $References\ Lattice Patch:: derive(),\ Lattice Patch:: derotate(),\ Latt$



6.30.2.2 linear2DProp()

```
void linear2DProp (
    LatticePatch * data,
    N_Vector u,
    N_Vector udot,
    int * c )
```

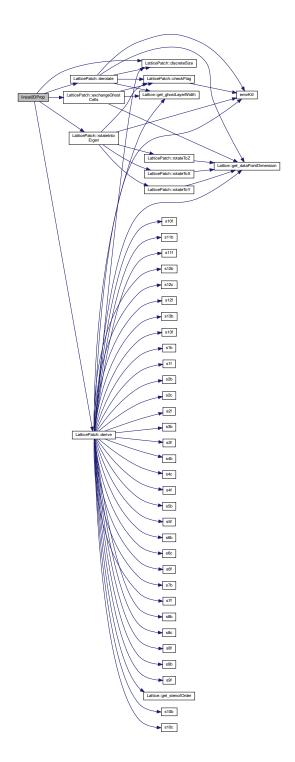
Maxwell propagation function for 2D – only for reference.

Maxwell propagation function for 2D – only for reference.

Definition at line 273 of file TimeEvolutionFunctions.cpp.

```
00273
00274
00275
         sunrealtype *duData = data->duData;
         sunrealtype *dxData = data->buffData[1 - 1];
00276
         sunrealtype *dyData = data->buffData[2 - 1];
00277
00278
00279
         data->exchangeGhostCells(1);
00280
         data->rotateIntoEigen(1);
00281
         data->derive(1);
00282
         data->derotate(1, dxData);
00283
         data->exchangeGhostCells(2);
         data->rotateIntoEigen(2);
00285
         data->derive(2);
00286
         data->derotate(2, dyData);
00287
         int totalNP = data->discreteSize();
00288
00289
         int pp = 0;
00290 #pragma distribute_point
00291
         for (int i = 0; i < totalNP; i++) {</pre>
          pp = i * 6;
duData[pp + 0] = dyData[pp + 5];
duData[pp + 1] = -dxData[pp + 5];
duData[pp + 2] = -dyData[pp + 3] + dxData[pp + 4];
duData[pp + 3] = -dyData[pp + 2];
duData[pp + 4] = dxData[pp + 2];
00292
00293
00294
00295
00296
00297
            duData[pp + 5] = dyData[pp + 0] - dxData[pp + 1];
00298
00299
00300 }
```

References LatticePatch::buffData, LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::discreteSize(), LatticePatch::duData, LatticePatch::exchangeGhostCells(), and LatticePatch::rotateIntoEigen().



6.30.2.3 linear3DProp()

```
N_Vector u,
N_Vector udot,
int * c )
```

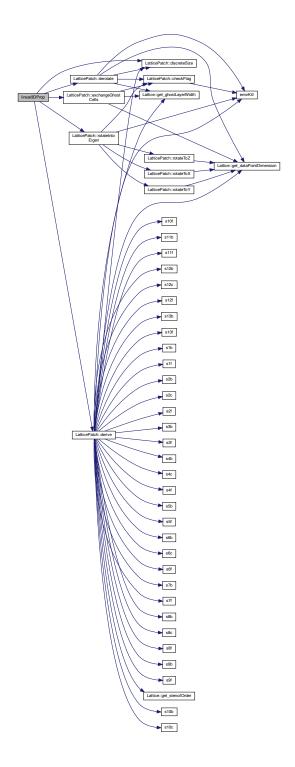
Maxwell propagation function for 3D – only for reference.

Maxwell propagation function for 3D – only for reference.

Definition at line 489 of file TimeEvolutionFunctions.cpp.

```
00490
00491
         sunrealtype *duData = data->duData;
00492
         sunrealtype *dxData = data->buffData[1 - 1];
sunrealtype *dyData = data->buffData[2 - 1];
00493
00494
         sunrealtype *dzData = data->buffData[3 - 1];
00495
00496
         /\star Under the hood call of point-to-point or collective communication \star/
00497
         // Point-to-Point:
00498
         data->exchangeGhostCells(1);
00499
         data->rotateIntoEigen(1);
00500
         data->derive(1);
00501
         data->derotate(1, dxData);
00502
         data->exchangeGhostCells(2);
00503
         data->rotateIntoEigen(2);
00504
         data->derive(2);
00505
         data->derotate(2, dyData);
00506
         data->exchangeGhostCells(3);
         data->rotateIntoEigen(3);
00508
         data->derive(3);
00509
         data->derotate(3, dzData);
00510
00511
         // Collective:
00512
00513
              data->exchangeGhostCells3D();
00514
              data->rotateIntoEigen3D();
00515
              data->derive(1);
00516
              data->derotate(1,dxData);
00517
             data->derive(2);
00518
             data->derotate(2,dvData);
00519
              data->derive(3);
00520
              data->derotate(3,dzData);
00521
00522
00523
         int totalNP = data->discreteSize();
00524
         int pp = 0;
00525 #pragma distribute_point
        for (int i = 0; i < totalNP; i++) {</pre>
           pp = i * 6;
00527
           duData[pp + 0] = dyData[pp + 5] - dzData[pp + 4];
duData[pp + 1] = dzData[pp + 3] - dxData[pp + 5];
duData[pp + 2] = dxData[pp + 4] - dyData[pp + 3];
duData[pp + 3] = -dyData[pp + 2] + dzData[pp + 1];
00528
00529
00530
00531
00532
           duData[pp + 4] = -dzData[pp + 0] + dxData[pp + 2];
00533
           duData[pp + 5] = -dxData[pp + 1] + dyData[pp + 0];
00534
00535 }
```

References LatticePatch::buffData, LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::discreteSize(), LatticePatch::duData, LatticePatch::exchangeGhostCells(), and LatticePatch::rotateIntoEigen().



6.30.2.4 nonlinear1DProp()

```
N_Vector u,
N_Vector udot,
int * c )
```

HE propagation function for 1D.

HE propagation function for 1D. Calculation of the Jacobi matrix

Definition at line 80 of file TimeEvolutionFunctions.cpp.

```
00081
00082
        // pointer to spatial derivative data sufficient, temporal derivative data
00083
        // provided with udot
        sunrealtype *dxData = data->buffData[1 - 1];
00084
00085
00086
        // same sequence as in the linear case
00087
        data->exchangeGhostCells(1);
00088
        data->rotateIntoEigen(1);
00089
        data->derive(1);
00090
        data->derotate(1, dxData);
00091
00092
00093
        F and G are nonzero in the nonlinear case,
00094
        polarization and magnetization contributions in Jacobi matrix style
00095
        with derivatives of polarization and magnetization % \left( {{\mathbf{p}}_{1}}\right) ={{\mathbf{p}}_{2}}
00096
        w.r.t. E- and B-field
00097
        sunrealtype f = NAN, g = NAN; // em field invariants F, G sunrealtype lf = NAN, lff = NAN, lfg = NAN, lg = NAN,
00098
00099
00100
                     lgg = NAN; // derivatives of Lagrangian w.r.t. field invariants
        array<sunrealtype, 36> JMM; // Jacobi matrix array<sunrealtype, 6> Quad; // array to hold E^2 and B^2 components array<sunrealtype, 6> h; // holding temporal derivatives of E and B components
00101
00102
00103
                                   // before operating (1+Z)^-1
00104
        sunrealtype pseudoDenom = NAN; // needed for inversion of 1+Z
00105
        00106
00107
        udata = NV_DATA_P(u);
dudata = NV_DATA_P(udot);
int totalNP = data->discreteSize(); // number of points in the patch
00108
00109
00110
00111
        // #pragma omp parallel for private(...) reduction(...) \rightarrow unsafe due to
00112
        // reductions and many variables, how to deal with / reduction?
00113
        //#pragma block_loop
00114
        //#pragma unroll_and_jam
00115
        //#pragma distribute_point
        for (int pp = 0; pp < totalNP * 6;</pre>
00116
             00117
00118
00119
                         11
                                 for(int pp=ppB;pp<min(totalNP*6,ppB+6*6);pp+=6){</pre>
          /// Calculation of the Jacobi matrix // 1. Calculate F and G
00120
00121
          f = 0.5 * ((Quad[0] = udata[pp] * udata[pp]) +
00122
          00123
00124
00125
00126
00127
00128
00129
00130
          // 2. Choose process/expansion order and assign derivative values of \ensuremath{\mathtt{L}}
00131
          // w.r.t. F, G
          switch (*c) {
case 0:
00132
00133
            lf = 0;
00134
            lff = 0;
lfg = 0;
00135
00136
00137
             lg = 0;
00138
             lgg = 0;
00139
            break;
00140
          case 2:
00141
            1f = 0.000354046449700427580438254 * f * f +
                 0.000191775160254398272737387 * g * g;
00142
             lff = 0.0007080928994008551608765075 * f;
00143
00144
            lfg = 0.0003835503205087965454747749 * g;
00145
            lg = 0.0003835503205087965454747749 * f * g;
             lgg = 0.0003835503205087965454747749 * f;
00146
00147
            break;
00148
          case 1:
00149
            1f = 0.000206527095658582755255648 * f;
00150
            lff = 0.000206527095658582755255648;
00151
            lfg = 0;
             lg = 0.0003614224174025198216973841 * g;
00152
            lgg = 0.0003614224174025198216973841;
00153
```

```
break;
00155
                  lf = (0.000206527095658582755255648 + 0.000354046449700427580438254 * f) *
00156
00157
                                 f +
                           0.000191775160254398272737387 * g * g;
00158
                   lff = 0.000206527095658582755255648 + 0.0007080928994008551608765075 * f;
00159
                   lfg = 0.0003835503205087965454747749 * g;
00160
                   lg = (0.0003614224174025198216973841 +
00161
00162
                            0.0003835503205087965454747749 * f) *
00163
                   lgg = 0.0003614224174025198216973841 + 0.0003835503205087965454747749 * f:
00164
00165
                   break:
               default:
00166
                  errorKill(
00167
00168
                         "You need to specify a correct order in the weak-field expansion.");
00169
                // 3. Assign Jacobi components
00170
               00171
00173
               JMM[6] =
                      lff * udata[pp] * udata[1 + pp] + lfg * udata[1 + pp] * udata[3 + pp] +
lfg * udata[pp] * udata[4 + pp] + lgg * udata[3 + pp] * udata[4 + pp];
00174
00175
               JMM[7] = lf + lff * Quad[1] +
00176
00177
                             udata[4 + pp] * (2 * lfg * udata[1 + pp] + lgg * udata[4 + pp]);
00178
               JMM[12] =
                    lff * udata[pp] * udata[2 + pp] + lfg * udata[2 + pp] * udata[3 + pp] +
lfg * udata[pp] * udata[5 + pp] + lgg * udata[3 + pp] * udata[5 + pp];
00179
00180
00181
               JMM[13] = lff * udata[1 + pp] * udata[2 + pp] +
                               lfg * udata[2 + pp] * udata[4 + pp] +
00182
00183
                                lfg * udata[1 + pp] * udata[5 + pp] +
               lgg * udata[4 + pp] * udata[5 + pp];

JMM[14] = lf + lff * Quad[2] +
00184
00185
               Udata[5 + pp] * (2 * lfg * udata[2 + pp] + lgg * udata[5 + pp]);

JMM[18] = lg + lfg * (Quad[0] - Quad[3 + 0]) +
00186
00187
               00188
00189
00190
               00191
00192
00193
                JMM[21] = -1f + lgg * Quad[0] +
               00194
00195
00196
00197
               (-lff + lgg) * udata[1 + pp] * udata[4 + pp];

JMM[26] = -(udata[4 + pp] * (lff * udata[2 + pp] + lfg * udata[5 + pp])) +
00198
00199
00200
                               udata[1 + pp] * (lfg * udata[2 + pp] + lgg * udata[5 + pp]);
               00201
00202
00203
00204
               00205
00206
00207
               00208
00209
00210
00211
                                (-lff + lgg) * udata[2 + pp] * udata[5 + pp];
00212
               JMM[33] = lgg * udata[pp] * udata[2 + pp] +
                               lff * udata[3 + pp] * udata[5 + pp] -
lfg * (udata[2 + pp] * udata[3 + pp] + udata[pp] * udata[5 + pp]);
00213
00214
00215
               JMM[34] =
00216
                      lgg * udata[1 + pp] * udata[2 + pp] +
                      lff * udata[4 + pp] * udata[5 + pp]
00217
00218
                      lfg * (udata[2 + pp] * udata[4 + pp] + udata[1 + pp] * udata[5 + pp]);
00219
               JMM[35] = -lf + lgg * Quad[2] +
00220
                              udata[5 + pp] * (-2 * lfg * udata[2 + pp] + lff * udata[5 + pp]);
               //#pragma unroll_and_jam
00221
00222
                //#pragma distribute_point
00223
                for (int i = 0; i < 6; i++) {
                   for (int j = i + 1; j < 6; j++)
00224
00225
                      JMM[i * 6 + j] = JMM[j * 6 + i];
00226
                  }
00227
00228
                // 4. Final values for temporal derivatives of field values
00229
               h[1] = dxData[pp] * JMM[30] + dxData[1 + pp] * JMM[31]
00230
                           dxData[2 + pp] * JMM[32] + dxData[3 + pp] * JMM[33] +
dxData[4 + pp] * JMM[34] + dxData[5 + pp] * (-1 + JMM[35]);
00231
00232
                h[2] = -(dxData[pp] * JMM[24]) - dxData[1 + pp] * JMM[25] - dxData[2 + pp] * JMM[26] - dxData[3 + pp] * JMM[27] - dxData[3 + p
00233
00234
                           dxData[4 + pp] * (1 - JMM[28]) - dxData[5 + pp] * JMM[29];
00235
00236
00237
               h[4] = dxData[2 + pp];
               h[5] = -dxData[1 + pp];
00238
               h(0) = h(3) * JMM(3) + h(4) * JMM(4) + h(5) * JMM(5);

h(1) = h(3) * JMM(9) + h(4) * JMM(10) + h(5) * JMM(11);
00239
00240
```

```
h[2] = h[3] * JMM[15] + h[4] * JMM[16] + h[5] * JMM[17];
                  // (1+Z)^-1 applies only to E components dudata[pp + 0] =
00242
00243
                  h[2] * (-(JMM[2] * (1 + JMM[7])) + JMM[1] * JMM[8]) +
h[1] * (JMM[2] * JMM[13] - JMM[1] * (1 + JMM[14])) +
h[0] * (1 - JMM[8] * JMM[13] + JMM[14] + JMM[7] * (1 + JMM[14]));
dudata[pp + 1] =
00244
00245
00246
                         h[2] * (JMM[2] * JMM[6] - (1 + JMM[0]) * JMM[8]) +
h[1] * (1 - JMM[2] * JMM[12] + JMM[14] + JMM[0] * (1 + JMM[14])) +
h[0] * (JMM[8] * JMM[12] - JMM[6] * (1 + JMM[14]));
00248
00249
00250
               dudata[pp + 2] =

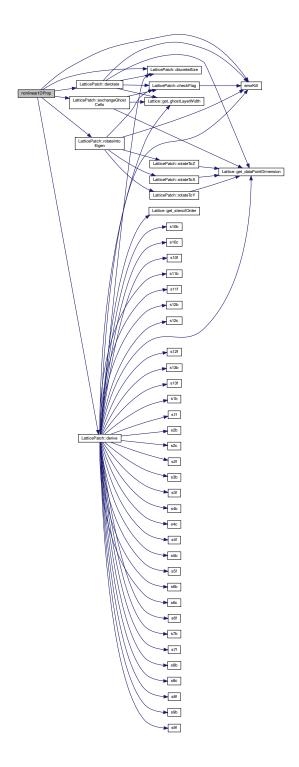
h[2] * (1 - JMM[1] * JMM[6] + JMM[7] + JMM[0] * (1 + JMM[7])) +

h[1] * (JMM[1] * JMM[12] - (1 + JMM[0]) * JMM[13]) +

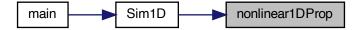
h[0] * (-((1 + JMM[7]) * JMM[12]) + JMM[6] * JMM[13]);
00251
00252
00253
00254
00255
               pseudoDenom =
                  -((1 + JMM[7]) * (-1 + JMM[2] * JMM[12])) +
(JMM[2] * JMM[6] - JMM[8]) * JMM[13] + JMM[14] + JMM[7] * JMM[14] +
JMM[0] * (1 + JMM[7] - JMM[8] * JMM[13] + (1 + JMM[7]) * JMM[14]) -
JMM[1] * (-(JMM[8] * JMM[12]) + JMM[6] * (1 + JMM[14]));
00256
00257
00258
                  dudata[pp + 0] /= pseudoDenom;
dudata[pp + 1] /= pseudoDenom;
00260
00261
                  dudata[pp + 2] /= pseudoDenom;
dudata[pp + 3] = h[3];
dudata[pp + 4] = h[4];
00262
00263
00264
00265
                  dudata[pp + 5] = h[5];
00266
00267
              return;
00268 }
```

References LatticePatch::buffData, LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::discreteSize(), errorKill(), LatticePatch::exchangeGhostCells(), and LatticePatch::rotateIntoEigen().

Referenced by Sim1D().



Here is the caller graph for this function:



6.30.2.5 nonlinear2DProp()

HE propagation function for 2D.

HE propagation function for 2D.

Definition at line 303 of file TimeEvolutionFunctions.cpp.

```
00303
00304
         sunrealtype *dxData = data->buffData[1 - 1];
sunrealtype *dyData = data->buffData[2 - 1];
00305
00306
00307
00308
         data->exchangeGhostCells(1);
00309
         data->rotateIntoEigen(1);
00310
         data->derive(1);
00311
         data->derotate(1, dxData);
00312
         data->exchangeGhostCells(2);
00313
         data->rotateIntoEigen(2);
00314
         data->derive(2);
00315
         data->derotate(2, dyData);
00316
         sunrealtype f = NAN, g = NAN; sunrealtype lf = NAN, lff = NAN, lfg = NAN, lg = NAN, lgg = NAN; array<sunrealtype, 36> JMM;
00317
00318
00319
00320
         array<sunrealtype, 6> Quad;
00321
         array<sunrealtype, 6> h;
00322
         sunrealtype pseudoDenom = NAN;
00323
         sunrealtype *udata = nullptr, *dudata = nullptr;
udata = NV_DATA_P(u);
00324
         dudata = NV_DATA_P(udot);
int totalNP = data->discreteSize();
00325
00326
00327
          //#pragma distribute_point
00328
          //#pragma unroll_and_jam
         for (int pp = 0; pp < totalNP * 6; pp += 6) {
    // 1</pre>
00329
00330
           00331
00332
00333
00334
                          (Quad[4] = udata[pp + 4] * udata[pp + 4]) -
00335
            (Quad[5] = udata[pp + 4] * udata[pp + 4]) -
(Quad[5] = udata[pp + 5] * udata[pp + 5]));

g = udata[pp] * udata[pp + 3] + udata[pp + 1] * udata[pp + 4] +
udata[pp + 2] * udata[pp + 5];
00336
00337
00338
            // 2
00339
00340
            switch (*c) {
            case 0:
lf = 0;
00341
00342
              lff = 0;
00343
00344
              lfg = 0;
00345
              lg = 0;
```

```
lgg = 0;
00347
            break;
00348
          case 2:
00349
            1f = 0.000354046449700427580438254 * f * f +
                 0.000191775160254398272737387 * g * g;
00350
             lff = 0.0007080928994008551608765075 * f;
00351
             lfg = 0.0003835503205087965454747749 * g;
             lg = 0.0003835503205087965454747749 * f
00353
00354
             lgg = 0.0003835503205087965454747749 * f;
00355
            break;
00356
          case 1:
            lf = 0.000206527095658582755255648 * f;
00357
00358
             lff = 0.000206527095658582755255648;
             lfg = 0;
00359
00360
             lg = 0.0003614224174025198216973841 * g;
00361
             lgg = 0.0003614224174025198216973841;
00362
            break;
00363
          case 3:
00364
            1f = (0.000206527095658582755255648 + 0.000354046449700427580438254 * f) *
00365
            \begin{array}{c} 0.000191775160254398272737387 \ \star \ g \ \star \ g; \\ 1ff = 0.000206527095658582755255648 \ + \ 0.000708092899400855160876508 \ \star \ f; \end{array}
00366
00367
             lfg = 0.0003835503205087965454747749 * g;
00368
             lg = (0.000361422417402519821697384 + 0.000383550320508796545474775 \star f) \star f
00369
00370
                 q;
             lgg = 0.000361422417402519821697384 + 0.000383550320508796545474775 * f;
00371
00372
00373
          default:
            errorKill(
00374
                 "You need to specify a correct order in the weak-field expansion.");
00375
00376
00377
00378
          JMM[0] = lf + lff * Quad[0] +
00379
                    udata[3 + pp] * (2 * 1fg * udata[pp] + 1gg * udata[3 + pp]);
          JMM[6] =
00380
              lff * udata[pp] * udata[1 + pp] + lfg * udata[1 + pp] * udata[3 + pp] +
00381
               lfg * udata[pp] * udata[4 + pp] + lgg * udata[3 + pp] * udata[4 + pp];
00382
          JMM[7] = lf + lff * Quad[1] +
00383
00384
                   udata[4 + pp] * (2 * lfg * udata[1 + pp] + lgg * udata[4 + pp]);
00385
           JMM[12] =
               lff * udata[pp] * udata[2 + pp] + lfg * udata[2 + pp] * udata[3 + pp] +
00386
               lfg * udata[pp] * udata[5 + pp] + lgg * udata[3 + pp] * udata[5 + pp];
00387
          00388
00389
                     lfg * udata[1 + pp] * udata[5 + pp] +
00390
00391
                     lgg * udata[4 + pp] * udata[5 + pp];
          JMM[14] = 1f + 1ff * Quad[2] +
00392
          udata[5 + pp] * (2 * lfg * udata[2 + pp] + lgg * udata[5 + pp]);

JMM[18] = lg + lfg * (Quad[0] - Quad[3 + 0]) +
00393
00394
          (-lff + lgg) * udata[pp] * udata[3 + pp];

JMM[19] = -(udata[3 + pp] * (lff * udata[1 + pp] + lfg * udata[4 + pp])) + udata[pp] * (lfg * udata[1 + pp] + lgg * udata[4 + pp]);
00395
00396
00397
          00398
00399
          00400
00401
00402
00403
00404
          JMM[25] = lg + lfg * (Quad[1] - Quad[4 + 0]) +
          00405
00406
                     udata[1 + pp] * (lfg * udata[2 + pp] + lgg * udata[5 + pp]);
00407
00408
          JMM[27] = lgg * udata[pp] * udata[1 + pp] +
                     lff * udata[3 + pp] * udata[4 + pp] -
00409
00410
                     lfg * (udata[1 + pp] * udata[3 + pp] + udata[pp] * udata[4 + pp]);
00411
          JMM[28] = -lf + lgg * Quad[1] +
          Udata[4 + pp] * (-2 * lfg * udata[1 + pp] + lff * udata[4 + pp]);

JMM[30] = udata[2 + pp] * (lfg * udata[pp] + lgg * udata[3 + pp]) -

(lff * udata[pp] + lfg * udata[3 + pp]) * udata[5 + pp];

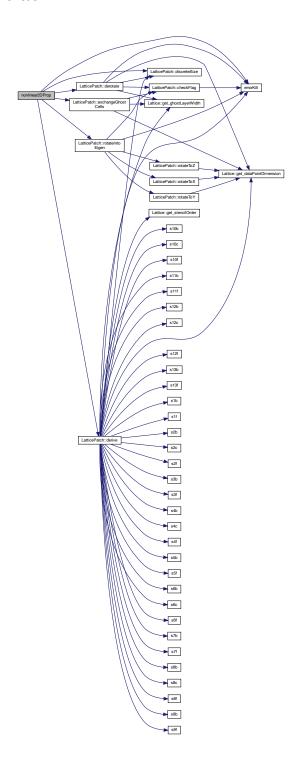
JMM[31] = udata[2 + pp] * (lfg * udata[1 + pp] + lgg * udata[4 + pp]) -
00412
00413
00414
00415
          (lff * udata[1 + pp] + lfg * udata[4 + pp]) * udata[5 + pp];

JMM[32] = lg + lfg * (Quad[2] - Quad[5 + 0]) +
00416
00417
                     (-lff + lgg) * udata[2 + pp] * udata[5 + pp];
00418
          00419
00420
                     lfg * (udata[2 + pp] * udata[3 + pp] + udata[pp] * udata[5 + pp]);
00421
00422
          JMM[34] =
00423
              lgg * udata[1 + pp] * udata[2 + pp]
               lff * udata[4 + pp] * udata[5 + pp] -
00424
          lff * (udata[2 + pp] * udata[4 + pp] + udata[1 + pp] * udata[5 + pp]);
JMM[35] = -lf + lgg * Quad[2] +
00425
00426
                     udata[5 + pp] * (-2 * lfg * udata[2 + pp] + lff * udata[5 + pp]);
00427
00428
00429
          //#pragma distribute_point
00430
           //#pragma unroll_and_jam
          for (int i = 0; i < 6; i++) {
  for (int j = i + 1; j < 6; j++) {</pre>
00431
00432
```

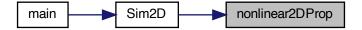
```
JMM[i * 6 + j] = JMM[j * 6 + i];
00434
00435
                           h[0] = 0;
00436
                           h[1] = dxData[pp] * JMM[30] + dxData[1 + pp] * JMM[31] + dxData[2 + pp] * JMM[32] + dxData[3 + pp] * JMM[33] + dxData[4 + pp] * JMM[34] + dxData[5 + pp] * (-1 + JMM[35]);
00437
00438
                           h[2] = -(dxData[pp] * JMM[24]) - dxData[1 + pp] * JMM[25] - dxData[2 + pp] * JMM[26] - dxData[3 + pp] * JMM[27] +
00440
00441
                                                 dxData[4 + pp] * (1 - JMM[28]) - dxData[5 + pp] * JMM[29];
00442
00443
                           h[3] = 0;
                           h[4] = dxData[2 + pp];
00444
                           00445
00446
00447
00448
                            h[1] += 0;
00449
                           h[1] - 0,
h[2] += dyData[pp] * JMM[18] + dyData[1 + pp] * JMM[19] +
dyData[2 + pp] * JMM[20] + dyData[3 + pp] * (-1 + JMM[21]) +
dyData[4 + pp] * JMM[22] + dyData[5 + pp] * JMM[23];
00450
00452
00453
                            h[3] += -dyData[2 + pp];
00454
                            h[4] += 0;
                           h[5] += dyData[pp];
h[0] -= h[3] * JMM[3] + h[4] * JMM[4] + h[5] * JMM[5];
h[1] -= h[3] * JMM[9] + h[4] * JMM[10] + h[5] * JMM[11];
00455
00456
00457
                             h[2] = h[3] * JMM[15] + h[4] * JMM[16] + h[5] * JMM[17];
                           00459
00460
00461
00462
00463
                                       h[2] * (JMM[2] * JMM[6] - (1 + JMM[0]) * JMM[8]) +
h[1] * (1 - JMM[2] * JMM[12] + JMM[14] + JMM[0] * (1 + JMM[14])) +
00464
00465
                                        h[0] * (JMM[8] * JMM[12] - JMM[6] * (1 + JMM[14]));
00466
                           dudata[pp + 2] =
  h[2] * (1 - JMM[1] * JMM[6] + JMM[7] + JMM[0] * (1 + JMM[7])) +
  h[1] * (JMM[1] * JMM[12] - (1 + JMM[0]) * JMM[13]) +
  h[0] * (-((1 + JMM[7]) * JMM[12]) + JMM[6] * JMM[13]);
00467
00468
00469
00471
                           pseudoDenom =
                                     -((1 + JMM[7]) * (-1 + JMM[2] * JMM[12])) +
(JMM[2] * JMM[6] - JMM[8]) * JMM[13] + JMM[14] + JMM[7] * JMM[14] +
00472
00473
                                       \[ \langle \text{ \text{Connected} \] \times \text{Connected} \] \times \[ \text{Connected} \] \
00474
00475
                           dudata[pp + 0] /= pseudoDenom;
dudata[pp + 1] /= pseudoDenom;
00476
00477
                           dudata[pp + 2] /= pseudoDenom;
dudata[pp + 3] = h[3];
dudata[pp + 4] = h[4];
00478
00479
00480
                           dudata[pp + 5] = h[5];
00481
00482
00483
                      return;
00484 }
```

References LatticePatch::buffData, LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::discreteSize(), errorKill(), LatticePatch::exchangeGhostCells(), and LatticePatch::rotateIntoEigen().

Referenced by Sim2D().



Here is the caller graph for this function:



6.30.2.6 nonlinear3DProp()

HE propagation function for 3D.

HE propagation function for 3D.

Definition at line 538 of file TimeEvolutionFunctions.cpp.

```
00538
00539
        sunrealtype *dxData = data->buffData[1 - 1];
00540
00541
        sunrealtype *dyData = data->buffData[2 - 1];
00542
        sunrealtype *dzData = data->buffData[3 - 1];
00543
00544
         /\star Under the hood call of point-to-point or collective communication \star/
00545
        // Point-to-Point:
00546
00547
             data->exchangeGhostCells(1);
00548
             data->rotateIntoEigen(1);
00549
             data->derive(1);
00550
             data->derotate(1,dxData);
00551
             data->exchangeGhostCells(2);
             data->rotateIntoEigen(2);
00552
00553
             data->derive(2);
00554
             data->derotate(2, dyData);
00555
             data->exchangeGhostCells(3);
00556
             data->rotateIntoEigen(3);
00557
             data->derive(3);
00558
             data->derotate(3,dzData);
00559
00560
        // Collective:
00561
00562
        data->exchangeGhostCells3D();
00563
        data->rotateIntoEigen3D();
00564
        data->derive(1);
00565
        data->derotate(1, dxData);
00566
        data->derive(2);
00567
        data->derotate(2, dyData);
00568
        data->derive(3);
00569
00570
        data->derotate(3, dzData);
00571
00572
        sunrealtype f = NAN, g = NAN; sunrealtype lf = NAN, lff = NAN, lfg = NAN, lg = NAN, lgg = NAN;
00574
        array<sunrealtype, 36> JMM;
00575
        array<sunrealtype, 6> Quad;
        array<sunrealtype, 6> h;
sunrealtype pseudoDenom = NAN;
00576
00577
        sunrealtype *udata = nullptr, *dudata = nullptr;
udata = NV_DATA_P(u);
00578
00579
00580
        dudata = NV_DATA_P(udot);
```

```
int totalNP = data->discreteSize();
        //#pragma distribute_point
00582
00583
         //#pragma unroll_and_jam
        for (int pp = 0; pp < totalNP * 6; pp += 6) {
    // 1</pre>
00584
00585
           f = 0.5 * ((Quad[0] = udata[pp] * udata[pp]) +
00586
                       (Quad[1] = udata[pp + 1] * udata[pp + 1]) +
00588
                        (Quad[2] = udata[pp + 2] * udata[pp + 2]) -
00589
                        (Quad[3] = udata[pp + 3] * udata[pp + 3]) -
00590
                        (Quad[4] = udata[pp + 4] * udata[pp + 4]) -
          (Quad[5] = udata[pp + 3] * udata[pp + 4]) *

(Quad[5] = udata[pp + 5] * udata[pp + 5]);

g = udata[pp] * udata[pp + 3] + udata[pp + 1] * udata[pp + 4] +
00591
00592
00593
              udata[pp + 2] * udata[pp + 5];
00594
           // 2
00595
           switch (*c) {
00596
           case 0:
            1f = 0:
00597
             lff = 0;
00598
             lfg = 0;
00600
             lg = 0;
             lgg = 0;
00601
00602
             break;
00603
          case 2:
            lf = 0.000354046449700427580438254 * f * f +
00604
                 0.000191775160254398272737387 * g * g;
00605
             lff = 0.0007080928994008551608765075 * f;
             1fg = 0.0003835503205087965454747749 * g;
00607
00608
             1g = 0.0003835503205087965454747749 * f * g;
00609
             lgg = 0.0003835503205087965454747749 * f;
00610
            break:
00611
           case 1:
00612
             1f = 0.000206527095658582755255648 * f;
             lff = 0.000206527095658582755255648;
00613
             lfg = 0;
00614
00615
             lg = 0.0003614224174025198216973841 * g;
             lgg = 0.0003614224174025198216973841;
00616
00617
             break;
           case 3:
00619
             lf = (0.000206527095658582755255648 + 0.000354046449700427580438254 * f) *
00620
             \begin{array}{c} 0.000191775160254398272737387 \ \star \ g \ \star \ g; \\ 1ff = 0.000206527095658582755255648 \ + \ 0.000708092899400855160876508 \ \star \ f; \end{array}
00621
00622
             lfg = 0.0003835503205087965454747749 * g;
00623
             lg = (0.000361422417402519821697384 + 0.000383550320508796545474775 * f) *
00624
00625
00626
             lgg = 0.000361422417402519821697384 + 0.000383550320508796545474775 * f;
00627
             break;
00628
           default:
            errorKill(
00629
                 "You need to specify a correct order in the weak-field expansion.");
00630
00631
           // 3
00632
00633
           JMM[0] = lf + lff * Quad[0] +
00634
                    udata[3 + pp] * (2 * lfg * udata[pp] + lgg * udata[3 + pp]);
           JMM[6] =
00635
               lff * udata[pp] * udata[1 + pp] + lfg * udata[1 + pp] * udata[3 + pp] +
00636
               lfg * udata[pp] * udata[4 + pp] + lgg * udata[3 + pp] * udata[4 + pp];
           JMM[7] = lf + lff * Quad[1] +
00638
00639
                    udata[4 + pp] * (2 * lfg * udata[1 + pp] + lgg * udata[4 + pp]);
00640
           .TMM [121 =
           lff * udata[pp] * udata[2 + pp] + lfg * udata[2 + pp] * udata[3 + pp] +
lfg * udata[pp] * udata[5 + pp] + lgg * udata[3 + pp] * udata[5 + pp];

JMM[13] = lff * udata[1 + pp] * udata[2 + pp] +
00641
00642
00643
                      lfg * udata[2 + pp] * udata[4 + pp] +
00644
00645
                      lfg * udata[1 + pp] * udata[5 + pp]
00646
                      lgg * udata[4 + pp] * udata[5 + pp];
          00647
00648
00649
                      (-lff + lgg) * udata[pp] * udata[3 + pp];
          00651
00652
00653
00654
           JMM[21] = -lf + lgg * Quad[0] +
00655
                     udata[3 + pp] * (-2 * lfg * udata[pp] + lff * udata[3 + pp]);
00656
           00657
00658
           JMM[25] = 1g + 1fg * (Quad[1] - Quad[4 + 0]) +
00659
           JMM[26] = -(udata[4 + pp] * udata[4 + pp];

JMM[26] = -(udata[4 + pp] * (lff * udata[2 + pp] + lfg * udata[5 + pp])) +

udata[1 + pp] * (lfg * udata[2 + pp] + lgg * udata[5 + pp]);
00660
00661
00662
           JMM[27] = lgg * udata[pp] * udata[1 + pp] +
00663
00664
                      lff * udata[3 + pp] * udata[4 + pp] -
           lfg * (udata[1 + pp] * udata[3 + pp] + udata[pp] * udata[4 + pp]);
JMM[28] = -lf + lgg * Quad[1] +
    udata[4 + pp] * (-2 * lfg * udata[1 + pp] + lff * udata[4 + pp]);
00665
00666
00667
```

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```
JMM[30] = udata[2 + pp] * (lfg * udata[pp] + lgg * udata[3 + pp]) -
                        (lff * udata[pp] + lfg * udata[3 + pp]) * udata[5 + pp];
00669
            00670
00671
00672
           (-lff + lgg) * udata[2 + pp] * udata[5 + pp];

JMM[33] = lgg * udata[pp] * udata[2 + pp] +
00673
00675
                        lff * udata[3 + pp] * udata[5 + pp]
00676
                        lfg * (udata[2 + pp] * udata[3 + pp] + udata[pp] * udata[5 + pp]);
00677
            JMM[34] =
00678
                 lgg * udata[1 + pp] * udata[2 + pp] +
            lff * udata[1 + pp] * udata[2 + pp] -
lff * udata[2 + pp] * udata[5 + pp] -
lfg * (udata[2 + pp] * udata[4 + pp] + udata[1 + pp] * udata[5 + pp]);

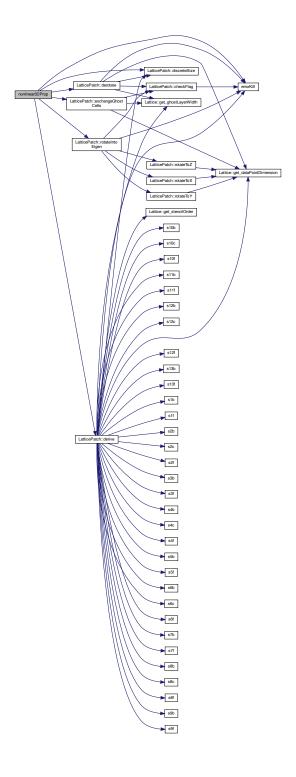
JMM[35] = -lf + lgg * Quad[2] +
00679
00680
00681
00682
                       udata[5 + pp] * (-2 * lfg * udata[2 + pp] + lff * udata[5 + pp]);
00683
00684
            //#pragma distribute_point
            //#pragma unroll_and_jam
for (int i = 0; i < 6; i++) {</pre>
00685
00686
             for (int j = i + 1; j < 6; j++)
                 JMM[i * 6 + j] = JMM[j * 6 + i];
00688
00689
              }
00690
           h[0] = 0:
00691
00692
           h[1] = dxData[pp] * JMM[30] + dxData[1 + pp] * JMM[31]
                    dxData[2 + pp] * JMM[32] + dxData[3 + pp] * JMM[33] + dxData[4 + pp] * JMM[34] + dxData[5 + pp] * (-1 + JMM[35]);
00694
           h[2] = -(dxData[pp] * JMM[24]) - dxData[1 + pp] * JMM[25] - dxData[2 + pp] * JMM[26] - dxData[3 + pp] * JMM[27] +
00695
00696
                    dxData[4 + pp] * (1 - JMM[28]) - dxData[5 + pp] * JMM[29];
00697
00698
           h[3] = 0;
00699
           h[4] = dxData[2 + pp];
00700
            h[5] = -dxData[1 + pp];
           h[0] += -(dyData[pp] * JMM[30]) - dyData[1 + pp] * JMM[31] - dyData[2 + pp] * JMM[32] - dyData[3 + pp] * JMM[33] - dyData[4 + pp] * JMM[34] + dyData[5 + pp] * (1 - JMM[35]);
00701
00702
00703
00704
           h[1] += 0;
           h[2] += dyData[pp] * JMM[18] + dyData[1 + pp] * JMM[19] +
                     dyData[2 + pp] * JMM[20] + dyData[3 + pp] * (-1 + JMM[21]) +
dyData[4 + pp] * JMM[22] + dyData[5 + pp] * JMM[23];
00706
00707
00708
           h[3] += -dyData[2 + pp];
           h[4] += 0;
00709
00710
           h[5] += dyData[pp];
00711
           h[0] += dzData[pp] * JMM[24] + dzData[1 + pp] * JMM[25] +
00712
                     dzData[2 + pp] * JMM[26] + dzData[3 + pp] * JMM[27] +
                     dzData[4 + pp] * (-1 + JMM[28]) + dzData[5 + pp] * JMM[29];
00713
           h[1] += -(dzData[pp] * JMM[18]) - dzData[1 + pp] * JMM[19] - dzData[2 + pp] * JMM[20] + dzData[3 + pp] * (1 - JMM[21]) - dzData[4 + pp] * JMM[22] - dzData[5 + pp] * JMM[23];
00714
00715
00716
00717
           h[2] += 0;
           h[3] += dzData[1 + pp];
00719
           h[4] += -dzData[pp];
00720
            h[5] += 0;
           h[0] = h[3] * JMM[3] + h[4] * JMM[4] + h[5] * JMM[5];

h[1] = h[3] * JMM[9] + h[4] * JMM[10] + h[5] * JMM[11];
00721
00722
00723
            h[2] = h[3] * JMM[15] + h[4] * JMM[16] + h[5] * JMM[17];
            dudata[pp + 0] =
00725
                h[2] * (-(JMM[2] * (1 + JMM[7])) + JMM[1] * JMM[8]) +
                h[1] * (JMM[2] * JMM[13] - JMM[1] * (1 + JMM[14])) +
h[0] * (1 - JMM[8] * JMM[13] + JMM[14] + JMM[7] * (1 + JMM[14]));
00726
00727
           dudata[pp + 1] =
00728
                h[2] * (JMM[2] * JMM[6] - (1 + JMM[0]) * JMM[8]) +
h[1] * (1 - JMM[2] * JMM[12] + JMM[14] + JMM[0] * (1 + JMM[14])) +
00729
00731
                 h[0] * (JMM[8] * JMM[12] - JMM[6] * (1 + JMM[14]));
           00732
00733
                h[1] * (JMM[1] * JMM[12] - (1 + JMM[0]) * JMM[13]) + h[0] * (-((1 + JMM[7]) * JMM[12]) + JMM[6] * JMM[13]);
00734
00735
00736
           pseudoDenom =
                 -((1 + JMM[7]) * (-1 + JMM[2] * JMM[12])) +
(JMM[2] * JMM[6] - JMM[8]) * JMM[13] + JMM[14] + JMM[7] * JMM[14] +
00738
00739
                 JMM[1] * (-(JMM[8] * JMM[12]) + JMM[6] * (1 + JMM[14]));
00740
           dudata[pp + 0] /= pseudoDenom;
00741
           dudata[pp + 1] /= pseudoDenom;
00742
00743
           dudata[pp + 2] /= pseudoDenom;
            dudata[pp + 3] = h[3];
dudata[pp + 4] = h[4];
00744
00745
           dudata[pp + 5] = h[5];
00746
00747
         1
00748
         return;
```

References LatticePatch::buffData, LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::discreteSize(), errorKill(), LatticePatch::exchangeGhostCells(), and LatticePatch::rotateIntoEigen().

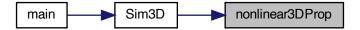
Referenced by Sim3D().

Here is the call graph for this function:



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Here is the caller graph for this function:



6.31 TimeEvolutionFunctions.h

Go to the documentation of this file.

```
00002 /// @file TimeEvolutionFunctions.h
00003 /// @brief Functions to propagate data vectors in time 00004 /// according to Maxwell's equations, and various
00005 /// orders in the HE weak-field expansion
00007
00008 #pragma once
00009
00010 #include "LatticePatch.h"
00011 #include "SimulationClass.h"
00013 /** @brief monostate TimeEvolution Class to propagate the field data in time in
00014 * a given order of the HE weak-field expansion */
00015 class TimeEvolution {
00016 public:
00017
       /// choice which processes of the weak field expansion are included
00018
       static int *c;
00019
00020
       /// Pointer to functions for differentiation and time evolution
00021
       static void (*TimeEvolver)(LatticePatch *, N_Vector, N_Vector, int *);
00022
       /// CVODE right hand side function (CVRhsFn) to provide IVP of the ODE
00023
00024
       static int f(sunrealtype t, N_Vector u, N_Vector udot, void *data_loc);
00025 };
00026
00027 /// Maxwell propagation function for 1D -- only for reference
00028 void linearlDProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c);
00029 /// HE propagation function for 1D
00030 void nonlinearIDProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c);
00031 /// Maxwell propagation function for 2D -- only for reference
00032 void linear2DProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c);
00033 /// HE propagation function for 2D \,
00034 void nonlinear2DProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c); 00035 /// Maxwell propagation function for 3D -- only for reference
00036 void linear3DProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c);
00037 /// HE propagation function for 3D
00038 void nonlinear3DProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c);
00039
```

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