HEWES : Heisenberg-Euler Weak-Field Expansion Simulator

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Chapter 1

HEWES – Heisenberg-Euler Weak-Field Expansion Simulator

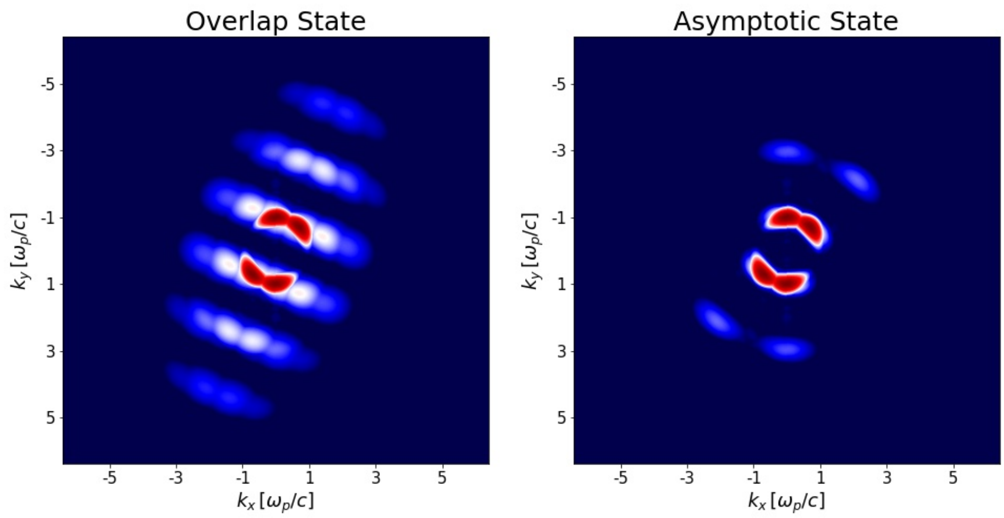


Figure 1.1 Harmonic Generation

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 `paper` 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 `outputDirectory`.
- 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.

- 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 name of the files written to the output directory is of the form `{step_number}_{process_number}`.
- 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.
  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.txt`file 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 unphysical 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. 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 dependend 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 written to csv files. 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 is created where the csv files are written into. The timestep filename is given in the form `yy-mm-dd_hh-MM-ss`.
There are six columns, corresponding to the six components of the electromagnetic field: $`E_x`$, $`E_y`$, $`E_z`$, $`B_x`$, $`B_y`$, $`B_z`$. Each row corresponds to one lattice point.
Every process writes to its own csv file, the ending of which (after an underscore) corresponds to the process number, as described above. This is not an elegant solution, but the best portable way that also works fast. On the other hand, it requires some postprocessing to read-in the files in order. A Python `module` taking care of this is provided.
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:

```
z=1                          z=2                          z=3             z=4
                                                          ...             ...
x                            x

1 | 0   4   8 12             1 |16  20  24  28
2 | 1   5   9 13             2 |17  21  25  29
3 | 2   6  10 14             3 |18  22  26  30
4 | 3   7  11 15             4 |19  23  27  31
   ------------->               ------------->
    1   2   3   4    y           1   2   3   4    y
```

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

- Arnau Pons Domenech
- Hartmut Ruhl (hartmut.ruhl@physik.uni-muenchen.de)
- Andreas Lindner (and.lindner@physik.uni-muenchen.de)
- Baris Ölmez (b.oelmez@physik.uni-muenchen.de)

Chapter 2

Hierarchical Index

2.1 Class Hierarchy

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

Chapter 3

Data Structure Index

3.1 Data Structures

Here are the data structures with brief descriptions:

Chapter 4

File Index

4.1 File List

Here is a list of all files with brief descriptions:

Chapter 5

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

phase shift in z-direction, ϕ_z

- sunrealtype x0x

  center of pulse in x-direction, x_0
- sunrealtype x0y

  center of pulse in y-direction, y_0
- sunrealtype x0z

  center of pulse in z-direction, z_0
- sunrealtype phig

  pulse width Φ_g

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 88 of file ICSetters.h.

5.1.2 Constructor & Destructor Documentation

5.1.2.1 Gauss1D()

```
Gauss1D::Gauss1D (
            vector< sunrealtype > k = {1, 0, 0},
            vector< sunrealtype > p = {0, 0, 1},
            vector< sunrealtype > xo = {0, 0, 0},
            sunrealtype phig_ = 1.01,
            vector< 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 122 of file ICSetters.cpp.

```
                                          {
    kx = k[0];      /** - wavevectors \f$ k_x \f$ */
    ky = k[1];      /** - \f$ k_y \f$ */
    kz = k[2];      /** - \f$ k_z \f$ normalized to \f$ 1/\lambda \f$*/
    px = p[0];      /** - amplitude (polarization) in x-direction */
    py = p[1];      /** - amplitude (polarization) in y-direction */
    pz = p[2];      /** - amplitude (polarization) in z-direction */
    phix = phi[0]; /** - phase shift in x-direction */
    phiy = phi[1]; /** - phase shift in y-direction */
    phiz = phi[2]; /** - phase shift in z-direction */
    phig = phig_;  /** - width */
    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*/
}
```

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()

```
void Gauss1D::addToSpace (
            sunrealtype x,
            sunrealtype y,
            sunrealtype z,
            sunrealtype * pTo6Space ) const
```

function for the actual implementation in space

Gauss1D implementation in space

Definition at line 141 of file ICSetters.cpp.

```
                                                          {
    const sunrealtype wavelength =
        sqrt(kx * kx + ky * ky + kz * kz); /* \f$ 1/\lambda \f$ */
    x = x - x0x; /* x-coordinate minus shift from origin */
    y = y - x0y; /* y-coordinate minus shift from origin */
    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$ */
    const sunrealtype envelopeAmp =
        exp(-(x * x + y * y + z * z) / phig / phig); /* enveloping Gauss shape */
    // Gaussian wave definition
    const array<sunrealtype, 3> E{
        {                                            /* E-field vector */
         px * cos(kScalarX - phix) * envelopeAmp,    /* \f$ E_x \f$ */
         py * cos(kScalarX - phiy) * envelopeAmp,    /* \f$ E_y \f$ */
         pz * cos(kScalarX - phiz) * envelopeAmp}}; /* \f$ E_z \f$ */
    // Put E-field into space
    pTo6Space[0] += E[0];
    pTo6Space[1] += E[1];
    pTo6Space[2] += E[2];
    // 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;
}
```

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 91 of file ICSetters.h.

Referenced by addToSpace(), and Gauss1D().

5.1.4.2 ky

`sunrealtype Gauss1D::ky [private]`

wavenumber k_y

Definition at line 93 of file ICSetters.h.

Referenced by addToSpace(), and Gauss1D().

5.1.4.3 kz

`sunrealtype Gauss1D::kz [private]`

wavenumber k_z

Definition at line 95 of file ICSetters.h.

Referenced by addToSpace(), and Gauss1D().

5.1.4.4 phig

`sunrealtype Gauss1D::phig [private]`

pulse width Φ_g

Definition at line 115 of file ICSetters.h.

Referenced by addToSpace(), and Gauss1D().

5.1.4.5 phix

`sunrealtype Gauss1D::phix [private]`

phase shift in x-direction, ϕ_x

Definition at line 103 of file ICSetters.h.

Referenced by addToSpace(), and Gauss1D().

5.1.4.6 phiy

`sunrealtype Gauss1D::phiy [private]`

phase shift in y-direction, ϕ_y

Definition at line 105 of file ICSetters.h.

Referenced by addToSpace(), and Gauss1D().

5.1.4.7 phiz

`sunrealtype Gauss1D::phiz [private]`

phase shift in z-direction, ϕ_z

Definition at line 107 of file ICSetters.h.

Referenced by addToSpace(), and Gauss1D().

5.1.4.8 px

`sunrealtype Gauss1D::px [private]`

polarization & amplitude in x-direction, p_x

Definition at line 97 of file ICSetters.h.

Referenced by addToSpace(), and Gauss1D().

5.1.4.9 py

```
sunrealtype Gauss1D::py [private]
```

polarization & amplitude in y-direction, p_y

Definition at line 99 of file ICSetters.h.

Referenced by addToSpace(), and Gauss1D().

5.1.4.10 pz

```
sunrealtype Gauss1D::pz [private]
```

polarization & amplitude in z-direction, p_z

Definition at line 101 of file ICSetters.h.

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 109 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 111 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 113 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) z_g
- 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 $g(z) = \tan^{-1}(z_g/z_r)$
- beam curvature $R(z) = z_g\,(1+(z_r/z_g)^2)$ obtained via the chosen parameters

Definition at line 142 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 169 of file ICSetters.cpp.

```
                                                                        {
    dis = dis_;                    /** - center it approaches */
    axis = axis_;                  /** - direction form where it comes */
    Amp = Amp_;                    /** - amplitude */
    phip = phip_;                  /** - polarization rotation from TE-mode */
    w0 = w0_;                      /** - taille */
    zr = zr_;                      /** - Rayleigh length */
    Ph0 = Ph0_;                    /** - beam center */
    PhA = PhA_;                    /** - 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
}
```

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

5.2.3 Member Function Documentation

5.2.3.1 addToSpace()

```
void Gauss2D::addToSpace (
            sunrealtype x,
            sunrealtype y,
            sunrealtype z,
            sunrealtype * pTo6Space ) const
```

function for the actual implementation in space

Definition at line 185 of file ICSetters.cpp.

```
                                                        {
    //\f$ \vec{x} = \vec{x}_0-\vec{dis} \f$ // coordinates minus distance to
    //origin
    x -= dis[0];
    y -= dis[1];
    // z-=dis[2];
    z = NAN;
    //  \f$ z_g = \vec{x}\cdot\vec{e}_g \f$ projection on propagation axis
    const sunrealtype zg =
        x * axis[0] + y * axis[1]; //+z*axis[2];  // =z-z0 -> propagation
                                   //direction, minus origin
    // \f$ r = \sqrt{\vec{x}^2 -z_g^2} \f$ -> pythagoras of radius minus
    // 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$
    const sunrealtype wz = w0 * sqrt(1 + (zg * zg / zr / zr)); // waist at position z
    // \f$ g(z) = atan(z_g/z_r) \f$
    const sunrealtype gz = atan(zg / zr); // Gouy phase
    // \f$ R(z) = z_g*(1+(z_r/z_g)^2) \f$
    sunrealtype Rz = NAN; // beam curvature
    if (zg != 0)
      Rz = zg * (1 + (zr * zr / zg / zg));
    else
      Rz = 1e308;
    // wavenumber \f$ k = 2\pi/\lambda \f$
    const sunrealtype k = 2 * numbers::pi / lambda;
    // \f$ \Phi_F = kr^2/(2*R(z))+g(z)-kz_g \f$
    const sunrealtype PhF =
        -k * r * r / (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$ -
    // CVode is a diva, no chance to remove the square in the second exponential
    // -> h too small
    const sunrealtype G2D = sqrt(w0 / wz) * exp(-r * r / wz / wz) *
                       exp(-(zg - Ph0) * (zg - Ph0) / PhA / PhA) *
                       cos(PhF); // gauss shape
    // \f$ c_\alpha =\vec{e}_x\cdot\vec{axis} \f$
    // projection components; do like this for CVode convergence -> otherwise
    // results in machine error values for non-existant field components if
    // axis[0] and axis[1] are given
    const sunrealtype ca =
```

```
    axis[0]; // x-component of propagation axis which is given as parameter
const sunrealtype sa = sqrt(1 - ca * ca); // no z-component for 2D propagation
// E-field to space: polarization in xy-plane (A2) is projection of
// z-polarization (A1) on x- and y-directions
pTo6Space[0] += sa * (G2D * A2);
pTo6Space[1] += -ca * (G2D * A2);
pTo6Space[2] += G2D * A1;
// B-field -> negative derivative wrt polarization shift of E-field
pTo6Space[3] += -sa * (G2D * A1);
pTo6Space[4] += ca * (G2D * A1);
pTo6Space[5] += G2D * A2;
}
```

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 162 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 164 of file ICSetters.h.

Referenced by addToSpace(), and Gauss2D().

5.2.4.3 Amp

`sunrealtype Gauss2D::Amp [private]`

amplitude A

Definition at line 149 of file ICSetters.h.

Referenced by Gauss2D().

5.2.4.4 axis

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

normalized propagation axis

Definition at line 147 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 145 of file ICSetters.h.

Referenced by addToSpace(), and Gauss2D().

5.2.4.6 lambda

`sunrealtype Gauss2D::lambda [private]`

wavelength λ

Definition at line 166 of file ICSetters.h.

Referenced by addToSpace(), and Gauss2D().

5.2.4.7 Ph0

`sunrealtype Gauss2D::Ph0 [private]`

center of beam Φ_0

Definition at line 158 of file ICSetters.h.

Referenced by addToSpace(), and Gauss2D().

5.2.4.8 PhA

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

length of beam Φ_A

Definition at line 160 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 152 of file ICSetters.h.

Referenced by Gauss2D().

5.2.4.10 w0

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

taille ω_0

Definition at line 154 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 156 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 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 (z-axis)
- sunrealtype A2

    amplitude projection on xy-plane
- sunrealtype lambda

    wavelength λ

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) z_g
- 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 $g(z) = \tan^{-1}(z_g/z_r)$
- beam curvature $R(z) = z_g\,(1+(z_r/z_g)^2)$ obtained via the chosen parameters

Definition at line 194 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 241 of file ICSetters.cpp.

```
                                                       {
    dis = dis_;     /** - center it approaches */
    axis = axis_;   /** - direction from where it comes */
    Amp = Amp_;     /** - amplitude */
    // pol=pol_;
    phip = phip_;   /** - polarization rotation form TE-mode */
    w0 = w0_;       /** - taille */
    zr = zr_;       /** - Rayleigh length */
    Ph0 = Ph0_;     /** - beam center */
    PhA = PhA_;     /** - beam length */
    lambda = numbers::pi * w0 * w0 / zr;
    A1 = Amp * cos(phip);
    A2 = Amp * sin(phip);
}
```

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

5.3.3 Member Function Documentation

5.3.3.1 addToSpace()

```
void Gauss3D::addToSpace (
            sunrealtype x,
            sunrealtype y,
            sunrealtype z,
            sunrealtype * pTo6Space ) const
```

function for the actual implementation in space

Gauss3D implementation in space

Definition at line 261 of file ICSetters.cpp.

```
                                                         {
    x -= dis[0];
    y -= dis[1];
    z -= dis[2];
    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));
    const sunrealtype gz = atan(zg / zr);
    sunrealtype Rz = NAN;
    if (zg != 0)
      Rz = zg * (1 + (zr * zr / zg / zg));
    else
      Rz = 1e308;
    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);
    const sunrealtype ca = axis[0];
    const sunrealtype sa = sqrt(1 - ca * ca);
    pTo6Space[0] += sa * (G3D * A2);
    pTo6Space[1] += -ca * (G3D * A2);
    pTo6Space[2] += G3D * A1;
    pTo6Space[3] += -sa * (G3D * A1);
    pTo6Space[4] += ca * (G3D * A1);
    pTo6Space[5] += G3D * A2;
}
```

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 216 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 218 of file ICSetters.h.

Referenced by addToSpace(), and Gauss3D().

5.3.4.3 Amp

`sunrealtype Gauss3D::Amp [private]`

amplitude A

Definition at line 201 of file ICSetters.h.

Referenced by Gauss3D().

5.3.4.4 axis

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

normalized propagation axis

Definition at line 199 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 197 of file ICSetters.h.

Referenced by addToSpace(), and Gauss3D().

5.3.4.6 lambda

`sunrealtype Gauss3D::lambda [private]`

wavelength λ

Definition at line 220 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 212 of file ICSetters.h.

Referenced by addToSpace(), and Gauss3D().

5.3.4.8 PhA

`sunrealtype Gauss3D::PhA [private]`

length of beam Φ_A

Definition at line 214 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 204 of file ICSetters.h.

Referenced by Gauss3D().

5.3.4.10 w0

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

taille ω_0

Definition at line 208 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 210 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 25 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 26 of file SimulationFunctions.h.

Referenced by main().

5.4.2.2 p

`vector<sunrealtype> gaussian1D::p`

amplitude & polarization vector

Definition at line 27 of file SimulationFunctions.h.

Referenced by main().

5.4.2.3 phi

`vector<sunrealtype> gaussian1D::phi`

phase shift

Definition at line 30 of file SimulationFunctions.h.

Referenced by main().

5.4.2.4 phig

```
sunrealtype gaussian1D::phig
```

width

Definition at line 29 of file SimulationFunctions.h.

Referenced by main().

5.4.2.5 x0

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

shift from origin

Definition at line 28 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 34 of file SimulationFunctions.h.

5.5.2 Field Documentation

5.5.2.1 amp

```
sunrealtype gaussian2D::amp
```

amplitude

Definition at line 37 of file SimulationFunctions.h.

5.5.2.2 axis

```
vector<sunrealtype> gaussian2D::axis
```

direction to center

Definition at line 36 of file SimulationFunctions.h.

5.5.2.3 ph0

```
sunrealtype gaussian2D::ph0
```

beam center

Definition at line 41 of file SimulationFunctions.h.

5.5.2.4 phA

```
sunrealtype gaussian2D::phA
```

beam length

Definition at line 42 of file SimulationFunctions.h.

5.5.2.5 phip

```
sunrealtype gaussian2D::phip
```

polarization rotation

Definition at line 38 of file SimulationFunctions.h.

5.5.2.6 w0

```
sunrealtype gaussian2D::w0
```

taille

Definition at line 39 of file SimulationFunctions.h.

5.5.2.7 x0

```
vector<sunrealtype> gaussian2D::x0
```

center

Definition at line 35 of file SimulationFunctions.h.

5.5.2.8 zr

```
sunrealtype gaussian2D::zr
```

Rayleigh length

Definition at line 40 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 46 of file SimulationFunctions.h.

5.6.2 Field Documentation

5.6.2.1 amp

`sunrealtype gaussian3D::amp`

amplitude

Definition at line 49 of file SimulationFunctions.h.

5.6.2.2 axis

`vector<sunrealtype> gaussian3D::axis`

direction to center

Definition at line 48 of file SimulationFunctions.h.

5.6.2.3 ph0

`sunrealtype gaussian3D::ph0`

beam center

Definition at line 53 of file SimulationFunctions.h.

5.6.2.4 phA

`sunrealtype gaussian3D::phA`

beam length

Definition at line 54 of file SimulationFunctions.h.

5.6.2.5 phip

```
sunrealtype gaussian3D::phip
```

polarization rotation

Definition at line 50 of file SimulationFunctions.h.

5.6.2.6 w0

```
sunrealtype gaussian3D::w0
```

taille

Definition at line 51 of file SimulationFunctions.h.

5.6.2.7 x0

```
vector<sunrealtype> gaussian3D::x0
```

center

Definition at line 47 of file SimulationFunctions.h.

5.6.2.8 zr

```
sunrealtype gaussian3D::zr
```

Rayleigh length

Definition at line 52 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 238 of file ICSetters.h.

5.7.2 Member Function Documentation

5.7.2.1 add()

```
void ICSetter::add (
            sunrealtype x,
            sunrealtype y,
            sunrealtype z,
            sunrealtype * pTo6Space )
```

function to fill the lattice space with initial field values

Add all initial field values to the lattice space

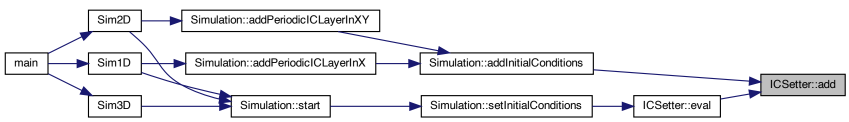
Definition at line 302 of file ICSetters.cpp.

```
                                             {
  for (const auto wave : planeWaves1D)
    wave.addToSpace(x, y, z, pTo6Space);
  for (const auto wave : planeWaves2D)
    wave.addToSpace(x, y, z, pTo6Space);
  for (const auto wave : planeWaves3D)
    wave.addToSpace(x, y, z, pTo6Space);
  for (const auto wave : gauss1Ds)
    wave.addToSpace(x, y, z, pTo6Space);
  for (const auto wave : gauss2Ds)
    wave.addToSpace(x, y, z, pTo6Space);
  for (const auto wave : gauss3Ds)
    wave.addToSpace(x, y, z, pTo6Space);
}
```

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 (
            vector< sunrealtype > k = {1, 0, 0},
            vector< sunrealtype > p = {0, 0, 1},
            vector< sunrealtype > xo = {0, 0, 0},
            sunrealtype phig_ = 1.01,
            vector< 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

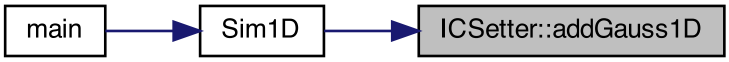
Definition at line 337 of file ICSetters.cpp.

```
                                                      {
  gauss1Ds.emplace_back(Gauss1D(k, p, xo, phig_, phi));
}
```

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_ = 1.0l,
            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

Add Gaussian waves in 2D to their container vector

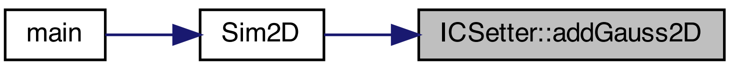
Definition at line 344 of file ICSetters.cpp.

```
                                                                        {
  gauss2Ds.emplace_back(
      Gauss2D(dis_, axis_, Amp_, phip_, w0_, zr_, Ph0_, PhA_));
}
```

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_ = 1.0l,
            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

Add Gaussian waves in 3D to their container vector

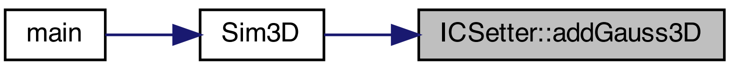
Definition at line 352 of file ICSetters.cpp.

```
00354                                                                         {
00355   gauss3Ds.emplace_back(
00356       Gauss3D(dis_, axis_, Amp_, phip_, w0_, zr_, Ph0_, PhA_));
00357 }
```

References gauss3Ds.

Referenced by Sim3D().

Here is the caller graph for this function:



5.7.2.5 addPlaneWave1D()

```
void ICSetter::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

Add plane waves in 1D to their container vector

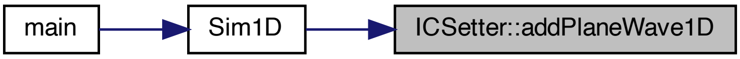
Definition at line 319 of file ICSetters.cpp.

```
00320                                                      {
00321   planeWaves1D.emplace_back(PlaneWave1D(k, p, phi));
00322 }
```

References planeWaves1D.

Referenced by Sim1D().

Here is the caller graph for this function:



5.7.2.6 addPlaneWave2D()

```
void ICSetter::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

Add plane waves in 2D to their container vector

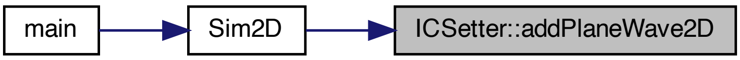
Definition at line 325 of file ICSetters.cpp.

```
00326                                                              {
00327   planeWaves2D.emplace_back(PlaneWave2D(k, p, phi));
00328 }
```

References planeWaves2D.

Referenced by Sim2D().

Here is the caller graph for this function:



5.7.2.7 addPlaneWave3D()

```
void ICSetter::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

Add plane waves in 3D to their container vector

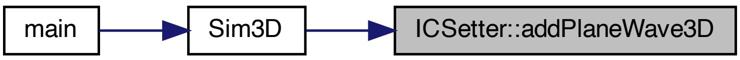
Definition at line 331 of file ICSetters.cpp.

```
00332                                                                     {
00333   planeWaves3D.emplace_back(PlaneWave3D(k, p, phi));
00334 }
```

References planeWaves3D.

Referenced by Sim3D().

Here is the caller graph for this function:



5.7.2.8 eval()

```
void ICSetter::eval (
            sunrealtype x,
            sunrealtype y,
            sunrealtype z,
            sunrealtype * pTo6Space )
```

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

Evaluate lattice point values to zero and add field values

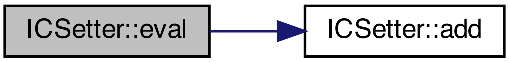
Definition at line 290 of file ICSetters.cpp.

```
00291                                                       {
00292   pTo6Space[0] = 0;
00293   pTo6Space[1] = 0;
00294   pTo6Space[2] = 0;
00295   pTo6Space[3] = 0;
00296   pTo6Space[4] = 0;
00297   pTo6Space[5] = 0;
00298   add(x, y, z, pTo6Space);
00299 }
```

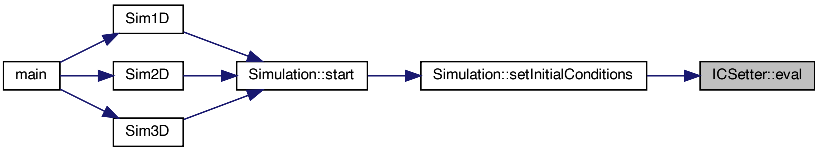
References add().

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 247 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 249 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 251 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 241 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 243 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 245 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

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 48 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

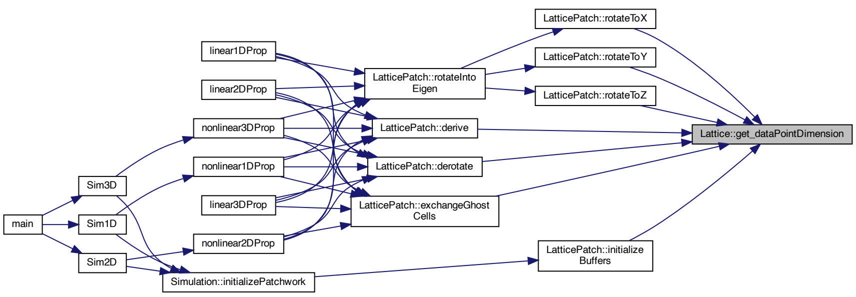
Definition at line 116 of file LatticePatch.h.

```
00116                                                   {
00117     return dataPointDimension;
00118   }
```

References dataPointDimension.

Referenced by LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::exchangeGhostCells(), LatticePatch::initializeBuffers(), LatticePatch::rotateToX(), LatticePatch::rotateToY(), 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 113 of file LatticePatch.h.

```
00113 { return dx; }
```

References dx.

5.8.3.3 get_dy()

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

getter function

Definition at line 114 of file LatticePatch.h.

```
00114 { return dy; }
```

References dy.

5.8.3.4 get_dz()

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

getter function

Definition at line 115 of file LatticePatch.h.

```
00115 { return dz; }
```

References dz.

5.8.3.5 get_ghostLayerWidth()

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

getter function

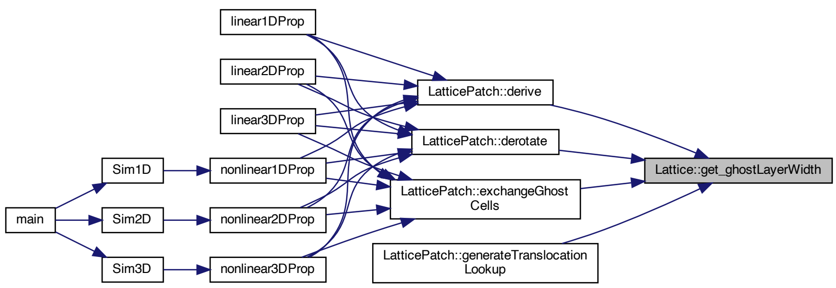
Definition at line 120 of file LatticePatch.h.

```
00120                                                                    {
00121     return ghostLayerWidth;
00122   }
```

References ghostLayerWidth.

Referenced by LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::exchangeGhostCells(), and LatticePatch::generateTranslocationLookup().

Here is the caller graph for this function:



5.8.3.6 get_stencilOrder()

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

getter function

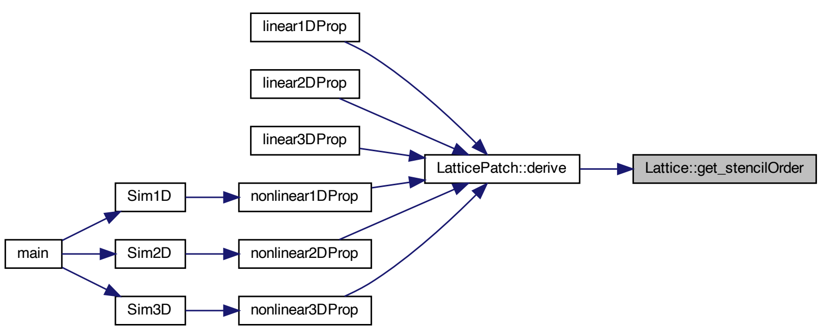
Definition at line 119 of file LatticePatch.h.

```
00119 { 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

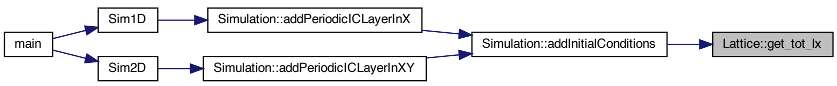
Definition at line 105 of file LatticePatch.h.

```
00105 { 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

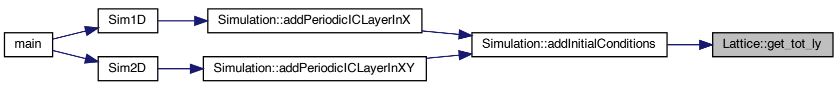
Definition at line 106 of file LatticePatch.h.

```
00106 { 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

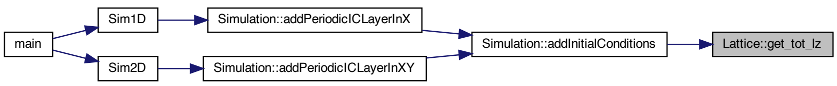
Definition at line 107 of file LatticePatch.h.

```
00107 { 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 112 of file LatticePatch.h.

```
00112 { 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 111 of file LatticePatch.h.

```
00111 { 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 108 of file LatticePatch.h.

```
00108 { 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 109 of file LatticePatch.h.

```
00109 { 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 110 of file LatticePatch.h.

```
00110 { return tot_nz; }
```

References tot_nz.

5.8.3.15 initializeCommunicator()

```
void Lattice::initializeCommunicator (
            const int nx,
            const int ny,
            const int nz,
            const bool per )
```

function to create and deploy the cartesian communicator

Initialize the cartesian communicator.

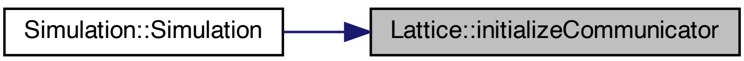
Definition at line 15 of file LatticePatch.cpp.

```
                                              {
    const int dims[3] = {nz, ny, nx};
    const int periods[3] = {static_cast<int>(per), static_cast<int>(per),
                            static_cast<int>(per)};
    // Create the cartesian communicator for MPI_COMM_WORLD
    MPI_Cart_create(MPI_COMM_WORLD, 3, dims, periods, 1, &comm);
    // Set MPI variables of the lattice
    MPI_Comm_size(comm, &(n_prc));
    MPI_Comm_rank(comm, &(my_prc));
    // Associate name to the communicator to identify it -> for debugging and
    // nicer error messages
    constexpr char lattice_comm_name[] = "Lattice";
    MPI_Comm_set_name(comm, lattice_comm_name);

    // Test if process naming is the same for both communicators
    /*
    int MYPRC;
    MPI_Comm_rank(MPI_COMM_WORLD,&MYPRC);
    cout«"\r"«my_prc«"\t"«MYPRC«endl;
    */
}
```

References comm, my_prc, and n_prc.

Referenced by Simulation::Simulation().

Here is the caller graph for this function:



5.8.3.16 setDiscreteDimensions()

```
void Lattice::setDiscreteDimensions (
            const sunindextype _nx,
            const sunindextype _ny,
            const sunindextype _nz )
```

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.

```
                                                         {
  // copy the given data for number of points
  tot_nx = _nx;
  tot_ny = _ny;
  tot_nz = _nz;
  // compute the resulting number of points and datapoints
  tot_noP = tot_nx * tot_ny * tot_nz;
  tot_noDP = dataPointDimension * tot_noP;
  // compute the new Delta, the physical resolution
  dx = tot_lx / tot_nx;
  dy = tot_ly / tot_ny;
  dz = tot_lz / tot_nz;
}
```

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()

```
void Lattice::setPhysicalDimensions (
            const sunrealtype _lx,
            const sunrealtype _ly,
            const sunrealtype _lz )
```

component function for resizing the physical size of the lattice

Set the physical size of the lattice.

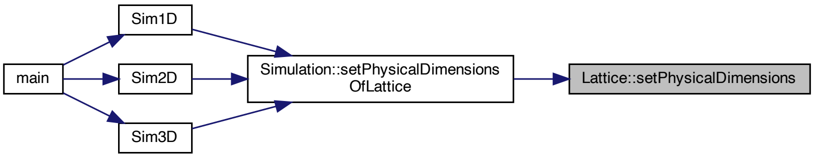
Definition at line 61 of file LatticePatch.cpp.

```
                                                       {
  tot_lx = _lx;
  tot_ly = _ly;
  tot_lz = _lz;
  // calculate physical distance between points
  dx = tot_lx / tot_nx;
  dy = tot_ly / tot_ny;
  dz = tot_lz / tot_nz;
  statusFlags |= FLatticeDimensionSet;
}
```

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 87 of file LatticePatch.h.

Referenced by LatticePatch::exchangeGhostCells(), Simulation::get_cart_comm(), initializeCommunicator(), Simulation::initializeCVODEobject(), 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 65 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 69 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 71 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 73 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 77 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 85 of file LatticePatch.h.

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

5.8.4.8 n_prc

```
int Lattice::n_prc
```

number of MPI processes

Definition at line 83 of file LatticePatch.h.

Referenced by initializeCommunicator().

5.8.4.9 profobj

```
SUNProfiler Lattice::profobj
```

SUNProfiler object.

Definition at line 96 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 79 of file LatticePatch.h.

Referenced by Lattice(), and setPhysicalDimensions().

5.8.4.11 stencilOrder

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

stencil order

Definition at line 75 of file LatticePatch.h.

Referenced by get_stencilOrder().

5.8.4.12 sunctx

```
SUNContext Lattice::sunctx
```

SUNContext object.

Definition at line 94 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 51 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 53 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 55 of file LatticePatch.h.

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

5.8.4.16 tot_noDP

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

number of lattice points times data dimension of each point

Definition at line 67 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 63 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 57 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 59 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 61 of file LatticePatch.h.

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

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

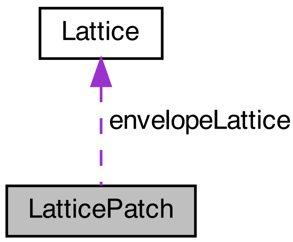
- src/LatticePatch.h
- src/LatticePatch.cpp

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
- void rotateIntoEigen (const int dir)

    function to rotate u into Z-matrix eigenraum
- 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 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_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

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 LIx

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

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

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

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

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

  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
- vector< sunrealtype > ghostCellRightToSend
- 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 139 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.

```
00078                             {
00079   // set default origin coordinates to (0,0,0)
00080   x0 = y0 = z0 = 0;
00081   // set default position in Lattice-Patchwork to (0,0,0)
00082   LIx = LIy = LIz = 0;
00083   // set default physical lentgth for lattice patch to (0,0,0)
00084   lx = ly = lz = 0;
00085   // set default discrete length for lattice patch to (0,1,1)
00086   /* This is done in this manner as even in 1D simulations require a 1 point
00087    * width */
00088   nx = 0;
00089   ny = nz = 1;
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;
00096 }
```

References LIx, LIy, LIz, 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.

```
00099                              {
00100   // Deallocate memory for solution vector
00101   if (statusFlags & FLatticePatchSetUp) {
00102     // Destroy data vectors
00103     N_VDestroy_Parallel(u);
00104     N_VDestroy_Parallel(du);
00105   }
00106 }
```

References du, FLatticePatchSetUp, statusFlags, and u.

5.9.3 Member Function Documentation

5.9.3.1 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 580 of file LatticePatch.cpp.

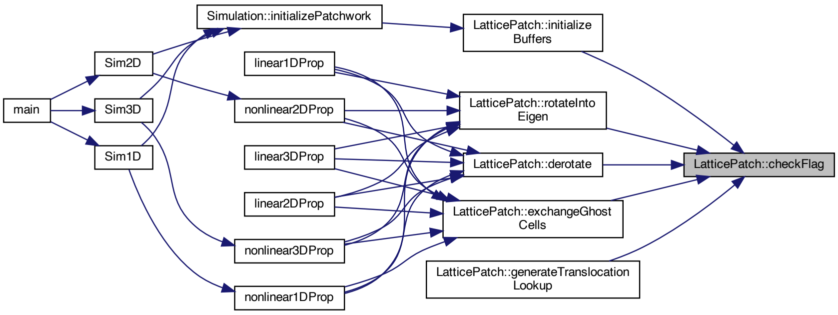
```
00580                                                   {
00581   if (!(statusFlags & flag)) {
00582     string errorMessage;
00583     switch (flag) {
00584     case FLatticePatchSetUp:
00585       errorMessage = "The Lattice patch was not set up please make sure to "
00586                      "initilize a Lattice topology";
00587       break;
00588     case TranslocationLookupSetUp:
00589       errorMessage = "The translocation lookup tables have not been generated, "
00590                      "please be sure to run generateTranslocationLookup()";
00591       break;
00592     case GhostLayersInitialized:
00593       errorMessage = "The space for the ghost layers has not been allocated, "
00594                      "please be sure to run initializeGhostLayer()";
00595       break;
00596     case BuffersInitialized:
00597       errorMessage = "The space for the buffers has not been allocated, please "
00598                      "be sure to run initializeBuffers()";
00599       break;
00600     default:
00601       errorMessage = "Uppss, you've made a non-standard error, sadly I can't "
00602                      "help you there";
00603       break;
00604     }
00605     errorKill(errorMessage);
00606   }
00607   return;
00608 }
```

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

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

Here is the call graph for this function:

Here is the caller graph for this function:



5.9.3.2 derive()

```
void LatticePatch::derive (
            const int dir )
```

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 611 of file LatticePatch.cpp.

```
00611                                         {
00612   // ghost layer width
00613   const int gLW = envelopeLattice->get_ghostLayerWidth();
00614   // dimensionality of data points -> 6
00615   const int dPD = envelopeLattice->get_dataPointDimension();
00616   // total width of patch in given direction including ghost layers at ends
00617   const int dirWidth = discreteSize(dir) + 2 * gLW;
00618   // width of patch only in given direction
00619   const int dirWidthO = discreteSize(dir);
00620   // size of plane perpendicular to given dimension
00621   const int perpPlainSize = discreteSize() / discreteSize(dir);
00622   // physical distance between points in that direction
00623   sunrealtype dxi = NAN;
00624   switch (dir) {
00625   case 1:
00626     dxi = dx;
00627     break;
00628   case 2:
00629     dxi = dy;
00630     break;
00631   case 3:
00632     dxi = dz;
00633     break;
00634   default:
00635     dxi = 1;
00636     errorKill("Tried to derive in the wrong direction");
00637     break;
00638   }
00639   // Derive according to chosen stencil accuracy order (which determines also
00640   // gLW)
00641   const int order = envelopeLattice->get_stencilOrder();
00642   switch (order) {
00643   case 1:
00644     for (int i = 0; i < perpPlainSize; i++) {
00645       for (int j = (i * dirWidth + gLW) * dPD;
00646            j < (i * dirWidth + gLW + dirWidthO) * dPD; j += dPD) {
00647         uAux[j + 0 - gLW * dPD] = s1b(&uAux[j + 0]) / dxi;
00648         uAux[j + 1 - gLW * dPD] = s1b(&uAux[j + 1]) / dxi;
00649         uAux[j + 2 - gLW * dPD] = s1f(&uAux[j + 2]) / dxi;
00650         uAux[j + 3 - gLW * dPD] = s1f(&uAux[j + 3]) / dxi;
00651         uAux[j + 4 - gLW * dPD] = s1f(&uAux[j + 4]) / dxi;
```

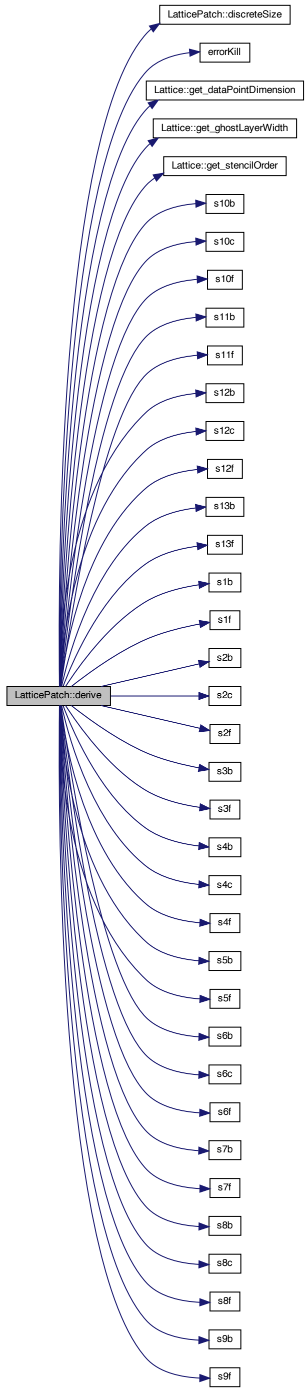
```
            uAux[j + 5 - gLW * dPD] = s1f(&uAux[j + 5]) / dxi;
          }
        }
        break;
      case 2:
        for (int i = 0; i < perpPlainSize; i++) {
          for (int j = (i * dirWidth + gLW) * dPD;
               j < (i * dirWidth + gLW + dirWidthO) * dPD; j += dPD) {
            uAux[j + 0 - gLW * dPD] = s2b(&uAux[j + 0]) / dxi;
            uAux[j + 1 - gLW * dPD] = s2b(&uAux[j + 1]) / dxi;
            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;
            uAux[j + 5 - gLW * dPD] = s2c(&uAux[j + 5]) / dxi;
          }
        }
        break;
      case 3:
        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] = s3b(&uAux[j + 0]) / dxi;
            uAux[j + 1 - gLW * dPD] = s3b(&uAux[j + 1]) / dxi;
            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 + 5]) / dxi;
          }
        }
        break;
      case 4:
        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] = s4b(&uAux[j + 0]) / dxi;
            uAux[j + 1 - gLW * dPD] = s4b(&uAux[j + 1]) / dxi;
            uAux[j + 2 - gLW * dPD] = s4f(&uAux[j + 2]) / dxi;
            uAux[j + 3 - gLW * dPD] = s4f(&uAux[j + 3]) / dxi;
            uAux[j + 4 - gLW * dPD] = s4c(&uAux[j + 4]) / dxi;
            uAux[j + 5 - gLW * dPD] = s4c(&uAux[j + 5]) / dxi;
          }
        }
        break;
      case 5:
        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] = s5b(&uAux[j + 0]) / dxi;
            uAux[j + 1 - gLW * dPD] = s5b(&uAux[j + 1]) / dxi;
            uAux[j + 2 - gLW * dPD] = s5f(&uAux[j + 2]) / dxi;
            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;
          }
        }
        break;
      case 6:
        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] = s6b(&uAux[j + 0]) / dxi;
            uAux[j + 1 - gLW * dPD] = s6b(&uAux[j + 1]) / dxi;
            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;
            uAux[j + 5 - gLW * dPD] = s6c(&uAux[j + 5]) / dxi;
          }
        }
        break;
      case 7:
        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] = s7b(&uAux[j + 0]) / dxi;
            uAux[j + 1 - gLW * dPD] = s7b(&uAux[j + 1]) / dxi;
            uAux[j + 2 - gLW * dPD] = s7f(&uAux[j + 2]) / dxi;
            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;
          }
        }
        break;
      case 8:
        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] = 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;
        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 + 5]) / dxi;
      }
    }
    break;
  case 9:
    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] = s9b(&uAux[j + 0]) / dxi;
        uAux[j + 1 - gLW * dPD] = s9b(&uAux[j + 1]) / dxi;
        uAux[j + 2 - gLW * dPD] = s9f(&uAux[j + 2]) / dxi;
        uAux[j + 3 - gLW * dPD] = s9f(&uAux[j + 3]) / dxi;
        uAux[j + 4 - gLW * dPD] = s9f(&uAux[j + 4]) / dxi;
        uAux[j + 5 - gLW * dPD] = s9f(&uAux[j + 5]) / dxi;
      }
    }
    break;
  case 10:
    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] = s10b(&uAux[j + 0]) / dxi;
        uAux[j + 1 - gLW * dPD] = s10b(&uAux[j + 1]) / dxi;
        uAux[j + 2 - gLW * dPD] = s10f(&uAux[j + 2]) / dxi;
        uAux[j + 3 - gLW * dPD] = s10f(&uAux[j + 3]) / dxi;
        uAux[j + 4 - gLW * dPD] = s10c(&uAux[j + 4]) / dxi;
        uAux[j + 5 - gLW * dPD] = s10c(&uAux[j + 5]) / dxi;
      }
    }
    break;
  case 11:
    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] = s11b(&uAux[j + 0]) / dxi;
        uAux[j + 1 - gLW * dPD] = s11b(&uAux[j + 1]) / dxi;
        uAux[j + 2 - gLW * dPD] = s11f(&uAux[j + 2]) / dxi;
        uAux[j + 3 - gLW * dPD] = s11f(&uAux[j + 3]) / dxi;
        uAux[j + 4 - gLW * dPD] = s11f(&uAux[j + 4]) / dxi;
        uAux[j + 5 - gLW * dPD] = s11f(&uAux[j + 5]) / dxi;
      }
    }
    break;
  case 12:
    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] = s12b(&uAux[j + 0]) / dxi;
        uAux[j + 1 - gLW * dPD] = s12b(&uAux[j + 1]) / dxi;
        uAux[j + 2 - gLW * dPD] = s12f(&uAux[j + 2]) / dxi;
        uAux[j + 3 - gLW * dPD] = s12f(&uAux[j + 3]) / dxi;
        uAux[j + 4 - gLW * dPD] = s12c(&uAux[j + 4]) / dxi;
        uAux[j + 5 - gLW * dPD] = s12c(&uAux[j + 5]) / dxi;
      }
    }
    break;
  case 13:
    // Iterate through all points in the plane perpendicular to the given
    // direction
    for (int i = 0; i < perpPlainSize; i++) {
      // 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) {
        /* Compute the stencil derivative for any of the six field components
         * with a ghostlayer width adjusted to the order of the finite
         * difference scheme */
        uAux[j + 0 - gLW * dPD] = s13b(&uAux[j + 0]) / dxi;
        uAux[j + 1 - gLW * dPD] = s13b(&uAux[j + 1]) / dxi;
        uAux[j + 2 - gLW * dPD] = s13f(&uAux[j + 2]) / dxi;
        uAux[j + 3 - gLW * dPD] = s13f(&uAux[j + 3]) / dxi;
        uAux[j + 4 - gLW * dPD] = s13f(&uAux[j + 4]) / dxi;
        uAux[j + 5 - gLW * dPD] = s13f(&uAux[j + 5]) / dxi;
      }
    }
    break;

  default:
    errorKill("Please set an existing stencil order");
    break;
  }
}
```

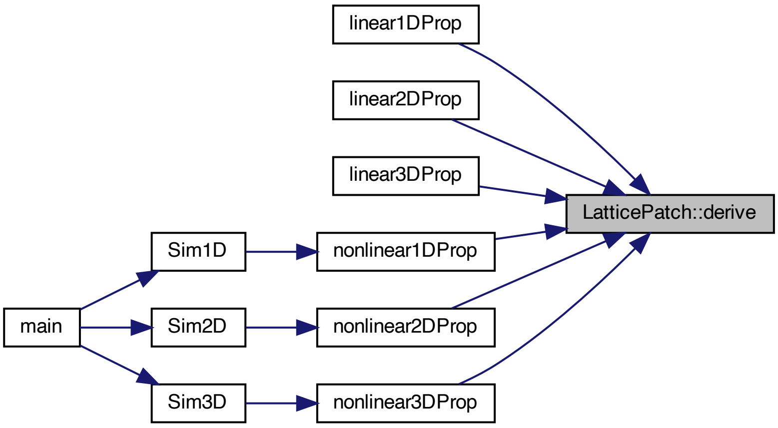
References discreteSize(), dx, dy, dz, envelopeLattice, errorKill(), Lattice::get_dataPointDimension(), Lattice::get_ghostLayerWidth(), Lattice::get_stencilOrder(), s10b(), s10c(), s10f(), s11b(), s11f(), s12b(), s12c(), s12f(), s13b(), s13f(), s1b(), s1f(), s2b(), s2c(), s2f(), s3b(), s3f(), s4b(), s4c(), s4f(), s5b(), s5f(), s6b(), s6c(), s6f(), s7b(), s7f(), s8b(), s8c(), s8f(), s9b(), s9f(), and uAux.

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:



5.9.3.3 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 394 of file LatticePatch.cpp.

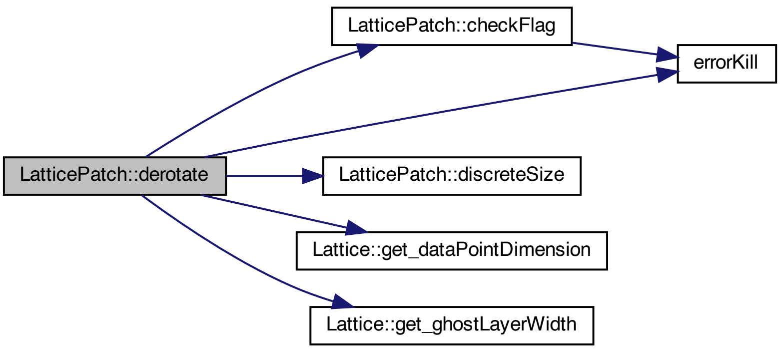
```
00394                                                         {
00395   // Check that the lattice as well as the translocation lookups have been set
00396   // up;
00397   checkFlag(FLatticePatchSetUp);
00398   checkFlag(TranslocationLookupSetUp);
00399   const int dPD = envelopeLattice->get_dataPointDimension();
00400   const int gLW = envelopeLattice->get_ghostLayerWidth();
00401   const int uSize = discreteSize();
00402   int ii = 0, target = 0;
00403   switch (dir) {
00404   case 1:
00405 #pragma ivdep
00406 #pragma omp simd
00407     for (int i = 0; i < uSize; i++) {
00408       // get correct indices in u and rotation space
00409       target = dPD * i;
00410       ii = dPD * (uTox[i] - gLW);
00411       buffOut[target + 0] = uAux[5 + ii];
00412       buffOut[target + 1] = (-uAux[ii] + uAux[2 + ii]) / 2.;
00413       buffOut[target + 2] = (uAux[1 + ii] - uAux[3 + ii]) / 2.;
00414       buffOut[target + 3] = uAux[4 + ii];
00415       buffOut[target + 4] = (uAux[1 + ii] + uAux[3 + ii]) / 2.;
00416       buffOut[target + 5] = (uAux[ii] + uAux[2 + ii]) / 2.;
00417     }
00418     break;
00419   case 2:
00420 #pragma omp simd
00421     for (int i = 0; i < uSize; i++) {
00422       target = dPD * i;
```

```
      ii = dPD * (uToy[i] - gLW);
      buffOut[target + 0] = (uAux[ii] - uAux[2 + ii]) / 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];
      buffOut[target + 5] = (uAux[ii] + uAux[2 + ii]) / 2.;
    }
    break;
  case 3:
#pragma omp simd
    for (int i = 0; i < uSize; i++) {
      target = dPD * i;
      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];
      buffOut[target + 3] = (uAux[1 + ii] + uAux[3 + ii]) / 2.;
      buffOut[target + 4] = (uAux[ii] + uAux[2 + ii]) / 2.;
      buffOut[target + 5] = uAux[4 + ii];
    }
    break;
  default:
    errorKill("Tried to derotate from the wrong direction");
    break;
  }
}
```

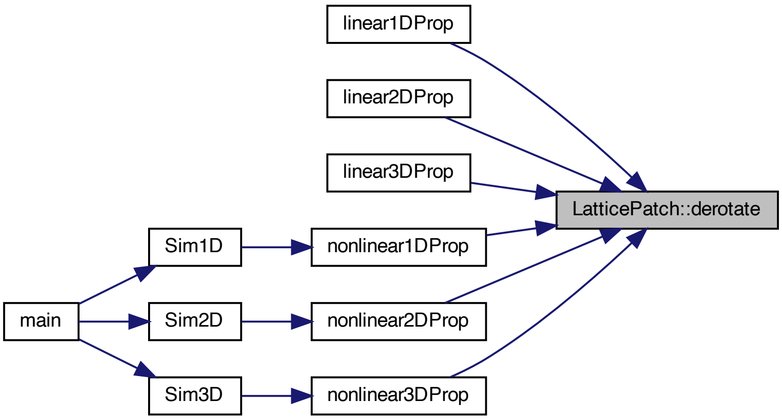
References checkFlag(), discreteSize(), envelopeLattice, errorKill(), FLatticePatchSetUp, Lattice::get_dataPointDimension(), Lattice::get_ghostLayerWidth(), TranslocationLookupSetUp, uAux, uTox, uToy, and uToz.

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

Here is the call graph for this function:



Here is the caller graph for this function:



5.9.3.4 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

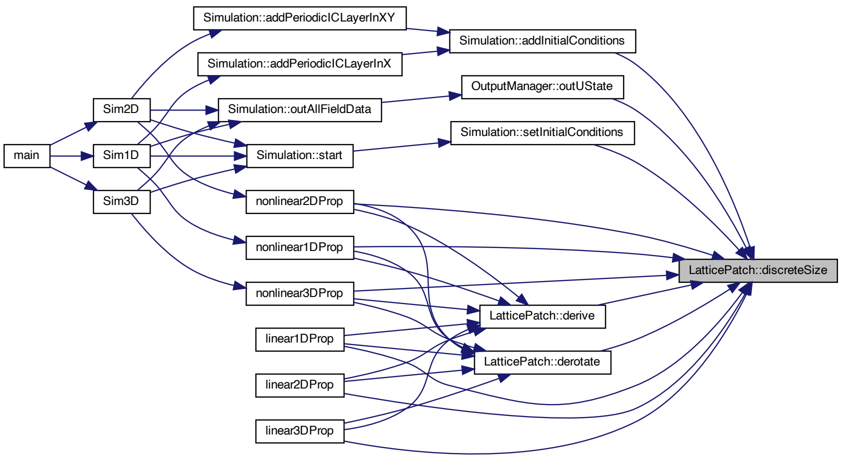
Definition at line 183 of file LatticePatch.cpp.

```
00183                                              {
00184   switch (dir) {
00185   case 0:
00186     return nx * ny * nz;
00187   case 1:
00188     return nx;
00189   case 2:
00190     return ny;
00191   case 3:
00192     return nz;
00193   // case 4: return uAux.size(); // for debugging
00194   default:
00195     return -1;
00196   }
00197 }
```

References nx, ny, and nz.

Referenced by Simulation::addInitialConditions(), derive(), derotate(), linear1DProp(), linear2DProp(), linear3DProp(), nonlinear1DProp(), nonlinear2DProp(), nonlinear3DProp(), OutputManager::outUState(), and Simulation::setInitialConditions().

Here is the caller graph for this function:



5.9.3.5 exchangeGhostCells()

```
void LatticePatch::exchangeGhostCells (
               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 467 of file LatticePatch.cpp.

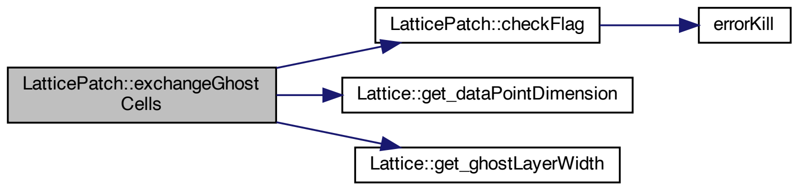
```
00467                                                         {
00468     // Check that the lattice has been set up
00469     checkFlag(FLatticeDimensionSet);
00470     checkFlag(FLatticePatchSetUp);
00471     // Variables to per dimension calculate the halo indices, and distance to
00472     // other side halo boundary
00473     int mx = 1, my = 1, mz = 1, distToRight = 1;
00474     const int gLW = envelopeLattice->get_ghostLayerWidth();
00475     // In the chosen direction m is set to ghost layer width while the others
00476     // remain to form the plane
00477     switch (dir) {
00478     case 1:
00479       mx = gLW;
00480       my = ny;
00481       mz = nz;
00482       distToRight = (nx - gLW);
00483       break;
00484     case 2:
00485       mx = nx;
00486       my = gLW;
00487       mz = nz;
00488       distToRight = nx * (ny - gLW);
00489       break;
00490     case 3:
00491       mx = nx;
00492       my = ny;
00493       mz = gLW;
00494       distToRight = nx * ny * (nz - gLW);
00495       break;
00496     }
00497     // total number of exchanged points
00498     const int dPD = envelopeLattice->get_dataPointDimension();
00499     const int exchangeSize = mx * my * mz * dPD;
00500     // provide size of the halos for ghost cells
```

```
  ghostCellLeft.resize(exchangeSize);
  ghostCellRight.resize(ghostCellLeft.size());
  ghostCellLeftToSend.resize(ghostCellLeft.size());
  ghostCellRightToSend.resize(ghostCellLeft.size());
  gCLData = &ghostCellLeft[0];
  gCRData = &ghostCellRight[0];
  statusFlags |= GhostLayersInitialized;

  // Initialize running index li for the halo buffers, and index ui of uData for
  // data transfer
  int li = 0, ui = 0;

  for (int iz = 0; iz < mz; iz++) {
    for (int iy = 0; iy < my; iy++) {
      // uData vector start index of halo data to be transferred
      // 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) * dPD;
      // copy left halo data from uData to buffer, transfer size is given by
      // x-length (not x-range) perhaps faster but more fragile C lib copy
      // operation (contained in cstring header)
      /*
      memcpy(&ghostCellLeftToSend[li],
             &uData[ui],
             sizeof(sunrealtype)*mx*dPD);
      // increase ui by the distance to vis-a-vis boundary and copy right halo
      data to buffer ui+=distToRight*dPD; memcpy(&ghostCellRightToSend[li],
             &uData[ui],
             sizeof(sunrealtype)*mx*dPD);
      */
      // 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;
      copy(&uData[ui], &uData[ui + mx * dPD], &ghostCellRightToSend[li]);

      // increase halo index by transferred items per y-iteration step
      // (x-length)
      li += mx * dPD;
    }
  }

  /* Send and receive the data to and from neighboring latticePatches */
  // Adjust direction to cartesian communicator
  int dim = 2; // default for dir==1
  if (dir == 2) {
    dim = 1;
  } else if (dir == 3) {
    dim = 0;
  }
  MPI_Request requests[2];
  int rank_source = 0, rank_dest = 0;
  MPI_Cart_shift(envelopeLattice->comm, dim, -1, &rank_source,
                 &rank_dest); // s.t. rank_dest is left & v.v.

  // nonblocking Isend/Irecv
  /*
  MPI_Isend(&ghostCellLeftToSend[0], exchangeSize, MPI_SUNREALTYPE, rank_dest,
  1, envelopeLattice->comm, &requests[0]); MPI_Irecv(&ghostCellRight[0],
  exchangeSize, MPI_SUNREALTYPE, rank_source, 1, envelopeLattice->comm,
  &requests[0]); MPI_Isend(&ghostCellRightToSend[0], exchangeSize,
  MPI_SUNREALTYPE, rank_source, 2, envelopeLattice->comm, &requests[1]);
  MPI_Irecv(&ghostCellLeft[0], exchangeSize, MPI_SUNREALTYPE, rank_dest, 2,
  envelopeLattice->comm, &requests[1]);

  MPI_Waitall(2, requests, MPI_STATUS_IGNORE);
  */

  // blocking Sendrecv:

  MPI_Sendrecv(&ghostCellLeftToSend[0], exchangeSize, MPI_SUNREALTYPE,
               rank_dest, 1, &ghostCellRight[0], exchangeSize, MPI_SUNREALTYPE,
               rank_source, 1, envelopeLattice->comm, MPI_STATUS_IGNORE);
  MPI_Sendrecv(&ghostCellRightToSend[0], exchangeSize, MPI_SUNREALTYPE,
               rank_source, 2, &ghostCellLeft[0], exchangeSize, MPI_SUNREALTYPE,
               rank_dest, 2, envelopeLattice->comm, MPI_STATUS_IGNORE);
}
```

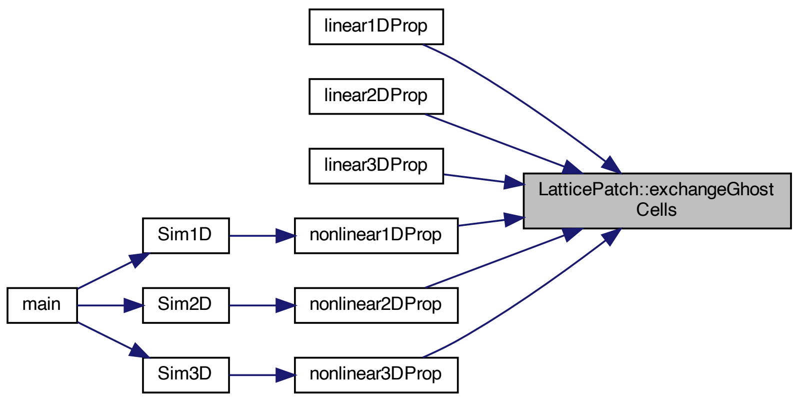
References checkFlag(), Lattice::comm, envelopeLattice, FLatticeDimensionSet, FLatticePatchSetUp, gCLData, gCRData, Lattice::get_dataPointDimension(), Lattice::get_ghostLayerWidth(), ghostCellLeft, ghostCellLeftToSend, ghostCellRight, ghostCellRightToSend, GhostLayersInitialized, nx, ny, nz, statusFlags,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



5.9.3.6 generateTranslocationLookup()

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

function to fill out the lookup tables

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

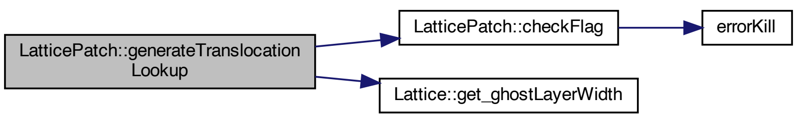
Definition at line 233 of file LatticePatch.cpp.

```
00233                                                     {
00234   // Check that the lattice has been set up
00235   checkFlag(FLatticeDimensionSet);
00236   // lenghts for auxilliary layers, including ghost layers
00237   const int gLW = envelopeLattice->get_ghostLayerWidth();
00238   const int mx = nx + 2 * gLW;
00239   const int my = ny + 2 * gLW;
00240   const int mz = nz + 2 * gLW;
00241   // sizes for lookup vectors
00242   // generate u->uAux
00243   uTox.resize(nx * ny * nz);
00244   uToy.resize(nx * ny * nz);
```

```
  uToz.resize(nx * ny * nz);
  // generate uAux->u with length including halo
  xTou.resize(mx * ny * nz);
  yTou.resize(nx * my * nz);
  zTou.resize(nx * ny * mz);
  // variables for cartesian position in the 3D discrete lattice
  int px = 0, py = 0, pz = 0;
  for (int i = 0; i < uToy.size(); i++) { // loop over all points in the patch
    // 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)
    uTox[i] = (px + gLW) + py * mx +
              pz * mx * ny; // unroll (de-flatten) cartesian dimension
    xTou[px + py * mx + pz * mx * ny] =
        i; // match cartesian point to u location
    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;
  }
  // same for ghost layer lookup tables
  lgcTox.resize(gLW * ny * nz);
  rgcTox.resize(gLW * ny * nz);
  for (int i = 0; i < lgcTox.size(); i++) {
    px = i % gLW;
    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;
  }
  lgcToy.resize(gLW * nx * nz);
  rgcToy.resize(gLW * nx * nz);
  for (int i = 0; i < lgcToy.size(); i++) {
    px = i % nx;
    py = (i / nx) % gLW;
    pz = (i / nx) / gLW;
    lgcToy[i] = py + pz * my + px * my * nz;
    rgcToy[i] = py + ny + gLW + pz * my + px * my * nz;
  }
  lgcToz.resize(gLW * nx * ny);
  rgcToz.resize(gLW * nx * ny);
  for (int i = 0; i < lgcToz.size(); i++) {
    px = i % nx;
    py = (i / nx) % ny;
    pz = (i / nx) / ny;
    lgcToz[i] = pz + px * mz + py * mz * nx;
    rgcToz[i] = pz + nz + gLW + px * mz + py * mz * nx;
  }
  statusFlags |= TranslocationLookupSetUp;
}
```

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.

Here is the call graph for this function:



5.9.3.7 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.

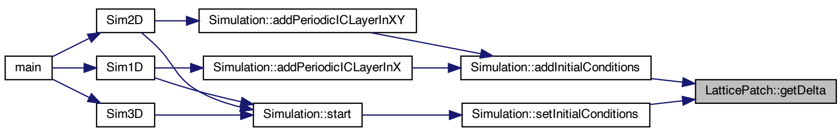
Definition at line 215 of file LatticePatch.cpp.
```
00215                                                        {
00216   switch (dir) {
00217   case 1:
00218     return dx;
00219   case 2:
00220     return dy;
00221   case 3:
00222     return dz;
00223   default:
00224     errorKill(
00225         "LatticePatch::getDelta function called with wrong dir parameter");
00226     return -1;
00227   }
00228 }
```

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

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

Here is the call graph for this function:

Here is the caller graph for this function:



5.9.3.8 initializeBuffers()

`void LatticePatch::initializeBuffers ( )`

initialize buffers to save derivatives

Create buffers to save derivative values, optimizing computational load.

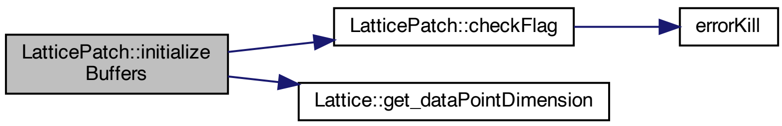
Definition at line 452 of file LatticePatch.cpp.
```
00452                                  {
00453   // Check that the lattice has been set up
```

```
    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);
    // Set pointers used for propagation functions
    buffData[0] = &buffX[0];
    buffData[1] = &buffY[0];
    buffData[2] = &buffZ[0];
    statusFlags |= BuffersInitialized;
}
```

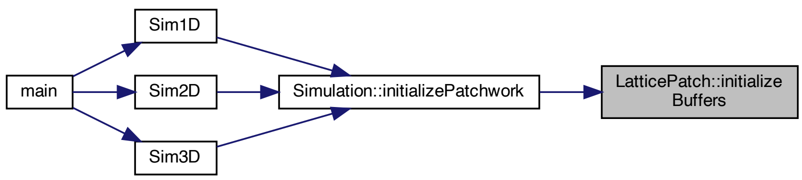
References buffData, BuffersInitialized, buffX, buffY, buffZ, checkFlag(), envelopeLattice, FLatticeDimensionSet, Lattice::get_dataPointDimension(), nx, ny, nz, and statusFlags.

Referenced by Simulation::initializePatchwork().

Here is the call graph for this function:



Here is the caller graph for this function:



5.9.3.9 initializeGhostLayer()

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

initialize ghost cells for halo exchange

5.9.3.10 origin()

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

function to get the origin of the patch

Return the physical origin of the patch in a dimension.

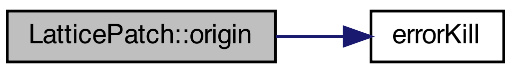
Definition at line 200 of file LatticePatch.cpp.

```
00200                                                     {
00201   switch (dir) {
00202   case 1:
00203     return x0;
00204   case 2:
00205     return y0;
00206   case 3:
00207     return z0;
00208   default:
00209     errorKill("LatticePatch::origin function called with wrong dir parameter");
00210     return -1;
00211   }
00212 }
```

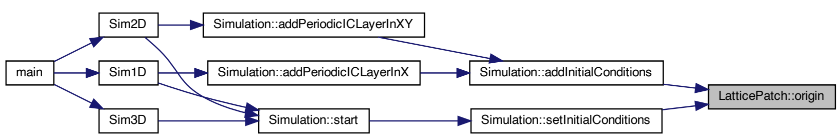
References errorKill(), x0, y0, and z0.

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

Here is the call graph for this function:



Here is the caller graph for this function:



5.9.3.11 rotateIntoEigen()

```
void LatticePatch::rotateIntoEigen (
            const int dir )
```

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

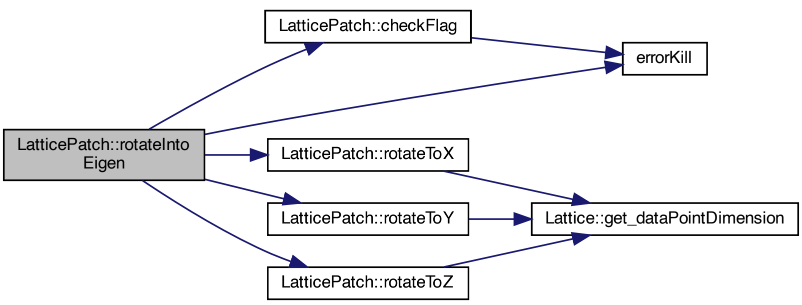
Definition at line 301 of file LatticePatch.cpp.

```
00301                                                       {
00302   // Check that the lattice, ghost layers as well as the translocation lookups
00303   // have been set up;
00304   checkFlag(FLatticePatchSetUp);
00305   checkFlag(TranslocationLookupSetUp);
00306   checkFlag(GhostLayersInitialized); // this check is only after call to
00307                                      // exchange ghost cells
00308   switch (dir) {
00309   case 1:
00310     rotateToX(uAuxData, gCLData, lgcTox);
00311     rotateToX(uAuxData, uData, uTox);
00312     rotateToX(uAuxData, gCRData, rgcTox);
00313     break;
00314   case 2:
00315     rotateToY(uAuxData, gCLData, lgcToy);
00316     rotateToY(uAuxData, uData, uToy);
00317     rotateToY(uAuxData, gCRData, rgcToy);
00318     break;
00319   case 3:
00320     rotateToZ(uAuxData, gCLData, lgcToz);
00321     rotateToZ(uAuxData, uData, uToz);
00322     rotateToZ(uAuxData, gCRData, rgcToz);
00323     break;
00324   default:
00325     errorKill("Tried to rotate into the wrong direction");
00326     break;
00327   }
00328 }
```

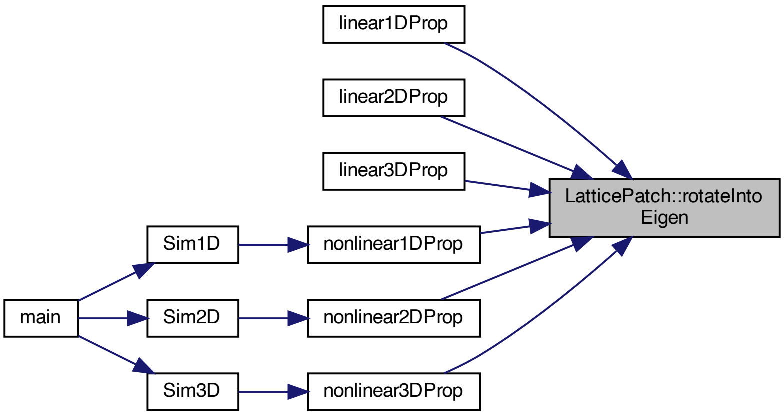
References checkFlag(), errorKill(), FLatticePatchSetUp, gCLData, gCRData, GhostLayersInitialized, lgcTox, lgcToy, lgcToz, rgcTox, rgcToy, rgcToz, rotateToX(), rotateToY(), rotateToZ(), TranslocationLookupSetUp, uAuxData, uData, uTox, uToy, and uToz.

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

Here is the call graph for this function:



Here is the caller graph for this function:



5.9.3.12 rotateToX()

```
void LatticePatch::rotateToX (
            sunrealtype * outArray,
            const sunrealtype * inArray,
            const vector< int > & lookup ) [inline], [private]
```

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

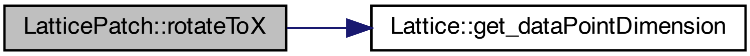
Definition at line 332 of file LatticePatch.cpp.

```
                                                                       {
  int ii = 0, target = 0;
#pragma ivdep
#pragma omp simd // safelen(6)
  for (int i = 0; i < lookup.size(); i++) {
    // get correct u-vector and spatial indices along previously defined lookup
    // tables
    target = envelopeLattice->get_dataPointDimension() * lookup[i];
    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];
    outArray[target + 3] = -inArray[2 + ii] + inArray[4 + ii];
    outArray[target + 4] = inArray[3 + ii];
    outArray[target + 5] = inArray[ii];
  }
}
```

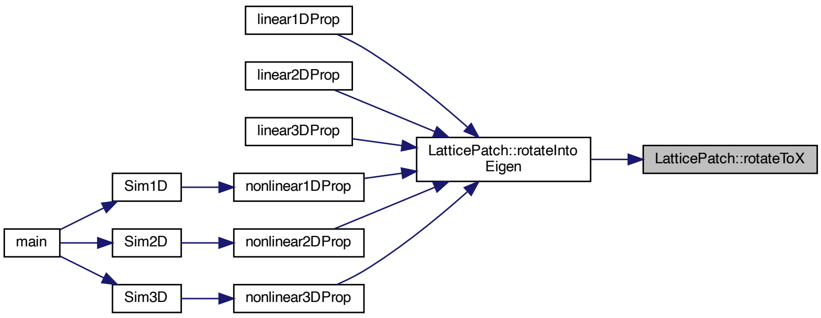
References envelopeLattice, and Lattice::get_dataPointDimension().

Referenced by rotateIntoEigen().

Here is the call graph for this function:



Here is the caller graph for this function:



5.9.3.13 rotateToY()

```
void LatticePatch::rotateToY (
            sunrealtype * outArray,
            const sunrealtype * inArray,
            const vector< int > & lookup )  [inline], [private]
```

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

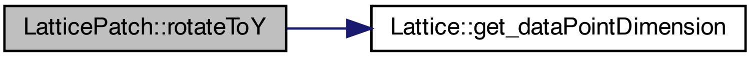
Definition at line 354 of file LatticePatch.cpp.

```
                                                              {
  int ii = 0, target = 0;
#pragma ivdep
#pragma omp simd
  for (int i = 0; i < lookup.size(); i++) {
    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];
    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];
  }
}
```

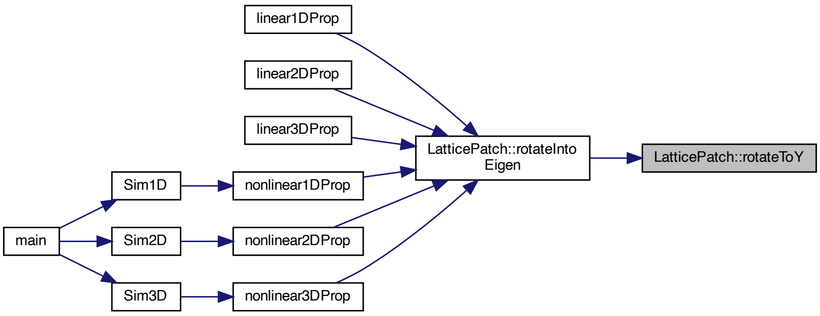
References envelopeLattice, and Lattice::get_dataPointDimension().

Referenced by rotateIntoEigen().

Here is the call graph for this function:



Here is the caller graph for this function:



5.9.3.14 rotateToZ()

```
void LatticePatch::rotateToZ (
            sunrealtype * outArray,
            const sunrealtype * inArray,
            const vector< int > & lookup ) [inline], [private]
```

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

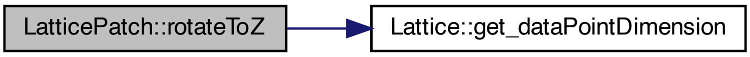
Definition at line 374 of file LatticePatch.cpp.

```
                                                                  {
  int ii = 0, target = 0;
#pragma ivdep
#pragma omp simd
  for (int i = 0; i < lookup.size(); i++) {
    target = envelopeLattice->get_dataPointDimension() * lookup[i];
    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];
    outArray[target + 5] = inArray[2 + ii];
  }
}
```

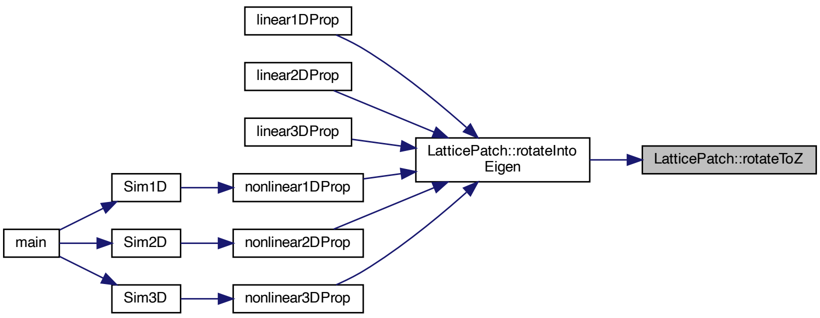
References envelopeLattice, and Lattice::get_dataPointDimension().

Referenced by rotateIntoEigen().

Here is the call graph for this function:



Here is the caller graph for this function:



5.9.4 Friends And Related Function Documentation

5.9.4.1 generatePatchwork

```
int generatePatchwork (
            const Lattice & envelopeLattice,
            LatticePatch & patchToMold,
            const int DLx,
            const int DLy,
            const int DLz )   [friend]
```

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();
    // Retrieve the data point dimension
    const int dPD = envelopeLattice.get_dataPointDimension();
    // MPI process/patch
    const int my_prc = envelopeLattice.my_prc;
    // Determine thicknes of the slice
```

```
    const sunindextype tot_NOXP = envelopeLattice.get_tot_nx(); // total points of lattice
    const sunindextype tot_NOYP = envelopeLattice.get_tot_ny();
    const sunindextype tot_NOZP = envelopeLattice.get_tot_nz();
    // position of the patch in the lattice of patches - process associated to
    // position
    const sunindextype LIx = my_prc % DLx;
    const sunindextype LIy = (my_prc / DLx) % DLy;
    const sunindextype LIz = (my_prc / DLx) / DLy;
    // Determine the number of points in the patch and first absolute points in
    // each dimension
    const sunindextype local_NOXP = tot_NOXP / DLx;
    const sunindextype local_NOYP = tot_NOYP / DLy;
    const sunindextype local_NOZP = tot_NOZP / DLz;
    // absolute positions of the first point in each dimension
    const sunindextype firstXPoint = local_NOXP * LIx;
    const sunindextype firstYPoint = local_NOYP * LIy;
    const sunindextype firstZPoint = local_NOZP * LIz;
    // total number of points in the patch
    const sunindextype local_NODP = dPD * local_NOXP * local_NOYP * local_NOZP;

    // Set patch up with above derived quantities
    patchToMold.dx = envelopeLattice.get_dx();
    patchToMold.dy = envelopeLattice.get_dy();
    patchToMold.dz = envelopeLattice.get_dz();
    patchToMold.x0 = firstXPoint * patchToMold.dx;
    patchToMold.y0 = firstYPoint * patchToMold.dy;
    patchToMold.z0 = firstZPoint * patchToMold.dz;
    patchToMold.LIx = LIx;
    patchToMold.LIy = LIy;
    patchToMold.LIz = LIz;
    patchToMold.nx = local_NOXP;
    patchToMold.ny = local_NOYP;
    patchToMold.nz = local_NOZP;
    patchToMold.lx = patchToMold.nx * patchToMold.dx;
    patchToMold.ly = patchToMold.ny * patchToMold.dy;
    patchToMold.lz = patchToMold.nz * patchToMold.dz;
    /* Create and allocate memory for parallel vectors with defined local and
     * global lenghts *
     * (-> CVode problem sizes Nlocal and N)
     * for field data and temporal derivatives and set extra pointers to them */
    patchToMold.u =
        N_VNew_Parallel(envelopeLattice.comm, local_NODP,
                        envelopeLattice.get_tot_noDP(), envelopeLattice.sunctx);
    patchToMold.uData = NV_DATA_P(patchToMold.u);
    patchToMold.du =
        N_VNew_Parallel(envelopeLattice.comm, local_NODP,
                        envelopeLattice.get_tot_noDP(), envelopeLattice.sunctx);
    patchToMold.duData = NV_DATA_P(patchToMold.du);
    // 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;
    const int s_min = min(s1, min(s2, s3));
    patchToMold.uAux.resize(s1 * s2 * s3 / s_min * (s_min + 2 * gLW) * dPD);
    patchToMold.uAuxData = &patchToMold.uAux[0];
    patchToMold.envelopeLattice = &envelopeLattice;
    // Set patch "name" to process number -> only for debugging
    // patchToMold.ID=my_prc;
    // set flag
    patchToMold.statusFlags = FLatticePatchSetUp;
    patchToMold.generateTranslocationLookup();
    return 0;
}
```

5.9.5 Field Documentation

5.9.5.1 buffData

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

pointer to spatial derivative data buffers

Definition at line 223 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 181 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 181 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 181 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 211 of file LatticePatch.h.

Referenced by ∼LatticePatch().

5.9.5.6 duData

`sunrealtype* LatticePatch::duData`

pointer to time-derivative data

Definition at line 217 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 166 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 168 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 170 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 172 of file LatticePatch.h.

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

5.9.5.11 gCLData

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

pointer to halo data

Definition at line 220 of file LatticePatch.h.

Referenced by exchangeGhostCells(), and rotateIntoEigen().

5.9.5.12 gCRData

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

pointer to halo data

Definition at line 220 of file LatticePatch.h.

Referenced by exchangeGhostCells(), and rotateIntoEigen().

5.9.5.13 ghostCellLeft

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

buffer for passing ghost cell data

Definition at line 185 of file LatticePatch.h.

Referenced by exchangeGhostCells().

5.9.5.14 ghostCellLeftToSend

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

buffer for passing ghost cell data

Definition at line 185 of file LatticePatch.h.

Referenced by exchangeGhostCells().

5.9.5.15 ghostCellRight

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

buffer for passing ghost cell data

Definition at line 185 of file LatticePatch.h.

Referenced by exchangeGhostCells().

5.9.5.16 ghostCellRightToSend

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

buffer for passing ghost cell data

Definition at line 186 of file LatticePatch.h.

Referenced by exchangeGhostCells().

5.9.5.17 ghostCells

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

buffer for passing ghost cell data

Definition at line 186 of file LatticePatch.h.

5.9.5.18 ghostCellsToSend

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

buffer for passing ghost cell data

Definition at line 186 of file LatticePatch.h.

5.9.5.19 ID

`int LatticePatch::ID`

ID of the LatticePatch, corresponds to process number.

Definition at line 207 of file LatticePatch.h.

5.9.5.20 lgcTox

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

ghost cell translocation lookup table

Definition at line 190 of file LatticePatch.h.

Referenced by generateTranslocationLookup(), and rotateIntoEigen().

5.9.5.21 lgcToy

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

ghost cell translocation lookup table

Definition at line 190 of file LatticePatch.h.

Referenced by generateTranslocationLookup(), and rotateIntoEigen().

5.9.5.22 lgcToz

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

ghost cell translocation lookup table

Definition at line 190 of file LatticePatch.h.

Referenced by generateTranslocationLookup(), and rotateIntoEigen().

5.9.5.23 LIx

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

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

Definition at line 148 of file LatticePatch.h.

Referenced by LatticePatch().

5.9.5.24 LIy

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

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

Definition at line 150 of file LatticePatch.h.

Referenced by LatticePatch().

5.9.5.25 LIz

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

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

Definition at line 152 of file LatticePatch.h.

Referenced by LatticePatch().

5.9.5.26 lx

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

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

Definition at line 154 of file LatticePatch.h.

Referenced by LatticePatch().

5.9.5.27 ly

`sunrealtype LatticePatch::ly [private]`

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

Definition at line 156 of file LatticePatch.h.

Referenced by LatticePatch().

5.9.5.28 lz

`sunrealtype LatticePatch::lz [private]`

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

Definition at line 158 of file LatticePatch.h.

Referenced by LatticePatch().

5.9.5.29 nx

`sunindextype LatticePatch::nx [private]`

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

Definition at line 160 of file LatticePatch.h.

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

5.9.5.30 ny

`sunindextype LatticePatch::ny [private]`

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

Definition at line 162 of file LatticePatch.h.

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

5.9.5.31 nz

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

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

Definition at line 164 of file LatticePatch.h.

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

5.9.5.32 rgcTox

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

ghost cell translocation lookup table

Definition at line 190 of file LatticePatch.h.

Referenced by generateTranslocationLookup(), and rotateIntoEigen().

5.9.5.33 rgcToy

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

ghost cell translocation lookup table

Definition at line 190 of file LatticePatch.h.

Referenced by generateTranslocationLookup(), and rotateIntoEigen().

5.9.5.34 rgcToz

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

ghost cell translocation lookup table

Definition at line 190 of file LatticePatch.h.

Referenced by generateTranslocationLookup(), and rotateIntoEigen().

5.9.5.35 statusFlags

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

char for checking flags

Definition at line 193 of file LatticePatch.h.

Referenced by checkFlag(), exchangeGhostCells(), generateTranslocationLookup(), initializeBuffers(), LatticePatch(), and ∼LatticePatch().

5.9.5.36 u

```
N_Vector LatticePatch::u
```

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

Definition at line 209 of file LatticePatch.h.

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

5.9.5.37 uAux

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

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

Definition at line 178 of file LatticePatch.h.

Referenced by derive(), and derotate().

5.9.5.38 uAuxData

```
sunrealtype* LatticePatch::uAuxData
```

pointer to auxiliary data vector

Definition at line 215 of file LatticePatch.h.

Referenced by rotateIntoEigen().

5.9.5.39 uData

```
sunrealtype* LatticePatch::uData
```

pointer to field data

Definition at line 213 of file LatticePatch.h.

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

5.9.5.40 uTox

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

translocation lookup table

Definition at line 175 of file LatticePatch.h.

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

5.9.5.41 uToy

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

translocation lookup table

Definition at line 175 of file LatticePatch.h.

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

5.9.5.42 uToz

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

translocation lookup table

Definition at line 175 of file LatticePatch.h.

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

5.9.5.43 x0

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

origin of the patch in physical space; x-coordinate

Definition at line 142 of file LatticePatch.h.

Referenced by LatticePatch(), and origin().

5.9.5.44 xTou

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

translocation lookup table

Definition at line 175 of file LatticePatch.h.

Referenced by generateTranslocationLookup().

5.9.5.45 y0

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

origin of the patch in physical space; y-coordinate

Definition at line 144 of file LatticePatch.h.

Referenced by LatticePatch(), and origin().

5.9.5.46 yTou

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

translocation lookup table

Definition at line 175 of file LatticePatch.h.

Referenced by generateTranslocationLookup().

5.9.5.47 z0

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

origin of the patch in physical space; z-coordinate

Definition at line 146 of file LatticePatch.h.

Referenced by LatticePatch(), and origin().

5.9.5.48 zTou

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

translocation lookup table

Definition at line 175 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 info
- void outUState (const int &state, const LatticePatch &latticePatch)
    output function for the whole lattice
- string getSimCode ()
    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
- int myPrc

    process ID

5.10.1 Detailed Description

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

Definition at line 27 of file Outputters.h.

5.10.2 Constructor & Destructor Documentation

5.10.2.1 OutputManager()

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

default constructor

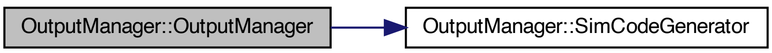
Directly generate the simCode at construction.

Definition at line 9 of file Outputters.cpp.

```
00009                           {
00010   simCode = SimCodeGenerator();
00011   MPI_Comm_rank(MPI_COMM_WORLD, &myPrc);
00012 }
```

References myPrc, 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 (
            const string & dir )
```

function that creates folder to save simulation info

Generate the folder to save the data to by one process: In the given directory it creates a direcory "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.

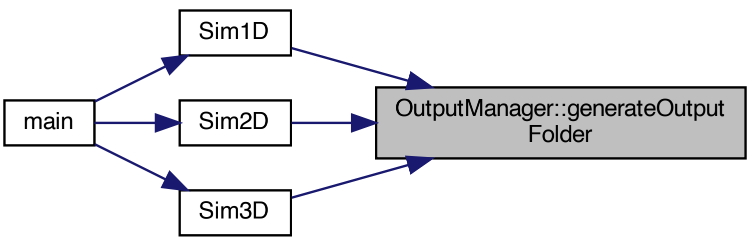
Definition at line 40 of file Outputters.cpp.

```
00040                                                        {
00041   // Do this only once for the first process
00042   if (myPrc == 0) {
00043     if (!fs::is_directory(dir))
00044       fs::create_directory(dir);
00045     if (!fs::is_directory(dir + "/SimResults"))
00046       fs::create_directory(dir + "/SimResults");
00047     if (!fs::is_directory(dir + "/SimResults/" + simCode))
00048       fs::create_directory(dir + "/SimResults/" + simCode);
00049   }
00050   // path variable for the output generation
00051   Path = dir + "/SimResults/" + simCode + "/";
00052 
00053   ifstream fin("main.cpp");
00054   ofstream fout(Path + "config.txt");
00055   string line;
00056   int begin=1000;
00057   for (int i = 1; !fin.eof(); i++) {
00058     getline(fin, line);
00059     if (line.starts_with("    //------------ B")) {
00060         begin=i;
00061     }
00062     if (i < begin) {
00063       continue;
00064     }
00065     fout « line « endl;
00066     if (line.starts_with("    //------------- E")) {
00067         break;
00068     }
00069   }
00070 
00071   return;
00072 }
```

References myPrc, Path, and simCode.

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

Here is the caller graph for this function:



5.10.3.2 getSimCode()

```
string OutputManager::getSimCode ( )
```

simCode getter function

Return the date+time simulation identifier for logging.

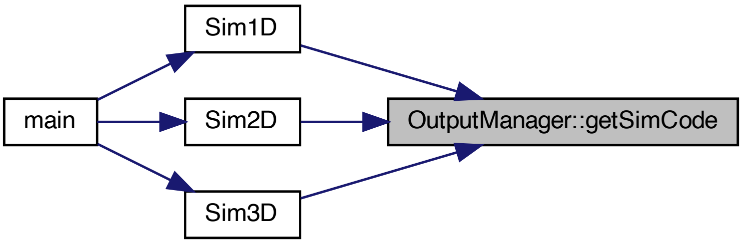
Definition at line 99 of file Outputters.cpp.

```
00099 { return simCode; }
```

References simCode.

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

Here is the caller graph for this function:



5.10.3.3 outUState()

```
void OutputManager::outUState (
            const int & state,
            const LatticePatch & latticePatch )
```

output function for the whole lattice

Write the field data to a csv file from each process (patch) with the field data into the simCode directory. The state (simulation step) denotes the prefix and the suffix after an underscore is given by the process/patch number

Definition at line 78 of file Outputters.cpp.

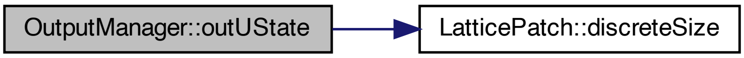
```
00078                                                                              {
00079   ofstream ofs;
00080   ofs.open(Path + to_string(state) + "_" + to_string(myPrc) + ".csv");
00081   // Set precision, number of digits for the values
00082   ofs « setprecision(numeric_limits<sunrealtype>::digits10);
00083
00084   // Walk through each lattice point
00085   for (int i = 0; i < latticePatch.discreteSize() * 6; i += 6) {
00086     // Six columns to contain the field data: Ex,Ey,Ez,Bx,By,Bz
00087     ofs « latticePatch.uData[i + 0] « "," « latticePatch.uData[i + 1] « ","
00088         « latticePatch.uData[i + 2] « "," « latticePatch.uData[i + 3] « ","
00089         « latticePatch.uData[i + 4] « "," « latticePatch.uData[i + 5]
00090         « endl;
00091   }
```

```
    ofs.close();

    return;
}
```

References LatticePatch::discreteSize(), myPrc, Path, and LatticePatch::uData.

Referenced by Simulation::outAllFieldData().

Here is the call graph for this function:



Here is the caller graph for this function:

5.10.3.4 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

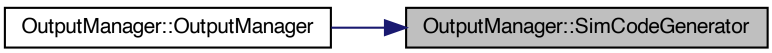
Definition at line 16 of file Outputters.cpp.

```
00016                                         {
00017   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)};
00020   const auto tod = now - chrono::floor<chrono::days>(now);
00021   const chrono::hh_mm_ss hms{tod};
00022
00023   stringstream temp;
00024   temp « setfill('0') « setw(2)
00025        « static_cast<int>(ymd.year() - chrono::years(2000)) « "-"
00026        « setfill('0') « setw(2) « static_cast<unsigned>(ymd.month()) « "-"
00027        « setfill('0') « setw(2) « static_cast<unsigned>(ymd.day()) « "_"
00028        « setfill('0') « setw(2) « hms.hours().count() « "-" « setfill('0')
00029        « setw(2) « hms.minutes().count() « "-" « setfill('0') « setw(2)
00030        « hms.seconds().count();
```

```
  //« "_" « hms.subseconds().count(); // subseconds render the filename too
  //large
  return temp.str();
}
```

Referenced by OutputManager().

Here is the caller graph for this function:



5.10.4 Field Documentation

5.10.4.1 myPrc

`int OutputManager::myPrc [private]`

process ID

Definition at line 36 of file Outputters.h.

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

5.10.4.2 Path

`string OutputManager::Path [private]`

variable for the path to the output folder

Definition at line 34 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 32 of file Outputters.h.

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

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

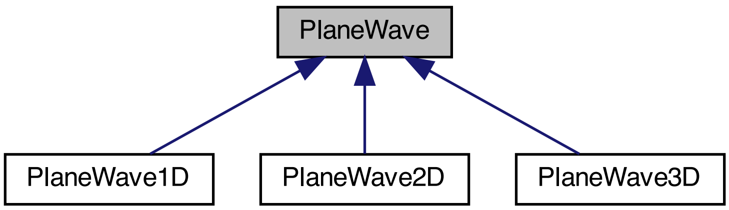
- src/Outputters.h
- src/Outputters.cpp

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, ϕ_x
- sunrealtype phiy

    phase shift in y-direction, ϕ_y
- sunrealtype phiz

    phase shift in z-direction, ϕ_z

5.11.1 Detailed Description

super-class for plane waves

They are given in the form $\vec{E} = \vec{E}_0 \, \cos\left(\vec{k}\cdot\vec{x} - \vec{\phi}\right)$

Definition at line 25 of file ICSetters.h.

5.11.2 Field Documentation

5.11.2.1 kx

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

wavenumber k_x

Definition at line 28 of file ICSetters.h.

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

5.11.2.2 ky

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

wavenumber k_y

Definition at line 30 of file ICSetters.h.

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

5.11.2.3 kz

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

wavenumber k_z

Definition at line 32 of file ICSetters.h.

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

5.11.2.4 phix

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

phase shift in x-direction, ϕ_x

Definition at line 40 of file ICSetters.h.

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

5.11.2.5 phiy

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

phase shift in y-direction, ϕ_y

Definition at line 42 of file ICSetters.h.

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

5.11.2.6 phiz

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

phase shift in z-direction, ϕ_z

Definition at line 44 of file ICSetters.h.

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

5.11.2.7 px

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

polarization & amplitude in x-direction, p_x

Definition at line 34 of file ICSetters.h.

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

5.11.2.8 py

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

polarization & amplitude in y-direction, p_y

Definition at line 36 of file ICSetters.h.

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

5.11.2.9 pz

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

polarization & amplitude in z-direction, p_z

Definition at line 38 of file ICSetters.h.

Referenced by PlaneWave1D::addToSpace(), PlaneWave2D::addToSpace(), PlaneWave3D::addToSpace(), PlaneWave1D::PlaneWave1D(), PlaneWave2D::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 18 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 19 of file SimulationFunctions.h.

Referenced by main().

5.12.2.2 p

`vector<sunrealtype> planewave::p`

amplitde & polarization vector

Definition at line 20 of file SimulationFunctions.h.

Referenced by main().

5.12.2.3 phi

`vector<sunrealtype> planewave::phi`

phase shift

Definition at line 21 of file SimulationFunctions.h.

Referenced by main().

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

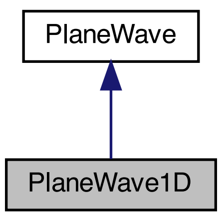
- src/SimulationFunctions.h

5.13 PlaneWave1D Class Reference

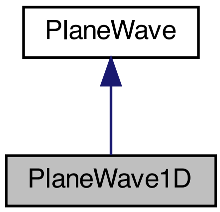
class for plane waves in 1D

`#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 48 of file ICSetters.h.

5.13.2 Constructor & Destructor Documentation

5.13.2.1 PlaneWave1D()

```
PlaneWave1D::PlaneWave1D (
            vector< sunrealtype > k = {1, 0, 0},
            vector< sunrealtype > p = {0, 0, 1},
            vector< 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_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.

```
                                                       {
    kx = k[0]; /** - wavevectors \f$ k_x \f$ */
    ky = k[1]; /** - \f$ k_y \f$ */
    kz = k[2]; /** - \f$ k_z \f$ normalized to \f$ 1/\lambda \f$ */
    // 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$ */
    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$ */
}
```

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

5.13.3 Member Function Documentation

5.13.3.1 addToSpace()

```
void PlaneWave1D::addToSpace (
            sunrealtype x,
            sunrealtype y,
            sunrealtype z,
            sunrealtype * pTo6Space ) const
```

function for the actual implementation in the lattice

PlaneWave1D implementation in space

Definition at line 27 of file ICSetters.cpp.

```
                                                                  {
    const sunrealtype wavelength =
        sqrt(kx * kx + ky * ky + kz * kz); /* \f$ 1/\lambda \f$ */
    const sunrealtype kScalarX = (kx * x + ky * y + kz * z) * 2 *
                       numbers::pi; /* \f$ 2\pi \ \vec{k} \cdot \vec{x} \f$ */
    // Plane wave definition
    const array<sunrealtype, 3> E{{                          /* E-field vector */
                         px * cos(kScalarX - phix),    /* \f$ E_x \f$ */
                         py * cos(kScalarX - phiy),    /* \f$ E_y \f$ */
                         pz * cos(kScalarX - phiz)}}; /* \f$ E_z \f$ */
    // Put E-field into space
    pTo6Space[0] += E[0];
    pTo6Space[1] += E[1];
    pTo6Space[2] += E[2];
    // and B-field
    pTo6Space[3] += (ky * E[2] - kz * E[1]) / wavelength;
```

```
00044     pTo6Space[4] += (kz * E[0] - kx * E[2]) / wavelength;
00045     pTo6Space[5] += (kx * E[1] - ky * E[0]) / wavelength;
00046 }
```

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

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

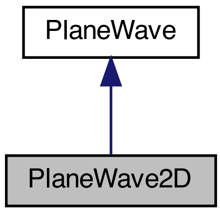
- src/ICSetters.h
- src/ICSetters.cpp

5.14 PlaneWave2D Class Reference

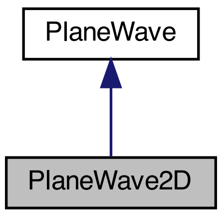
class for plane waves in 2D

`#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 60 of file ICSetters.h.

5.14.2 Constructor & Destructor Documentation

5.14.2.1 PlaneWave2D()

```
PlaneWave2D::PlaneWave2D (
            vector< sunrealtype > k = {1, 0, 0},
            vector< sunrealtype > p = {0, 0, 1},
            vector< 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 49 of file ICSetters.cpp.

```
                                                    {
    kx = k[0]; /** - wavevectors \f$ k_x \f$ */
    ky = k[1]; /** - \f$ k_y \f$ */
    kz = k[2]; /** - \f$ k_z \f$ normalized to \f$ 1/\lambda \f$*/
    // Amplitude bug: lower by factor 9
    px = p[0] / 9; /** - amplitude (polarization) in x-direction \f$ p_x \f$ */
    py = p[1] / 9; /** - amplitude (polarization) in y-direction \f$ p_y \f$ */
    pz = p[2] / 9; /** - 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$ */
}
```

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

5.14.3 Member Function Documentation

5.14.3.1 addToSpace()

```
void PlaneWave2D::addToSpace (
            sunrealtype x,
            sunrealtype y,
            sunrealtype z,
            sunrealtype * pTo6Space ) const
```

function for the actual implementation in the lattice

PlaneWave2D implementation in space

Definition at line 64 of file ICSetters.cpp.

```
                                                                    {
    const sunrealtype wavelength =
        sqrt(kx * kx + ky * ky + kz * kz); /* \f$ 1/\lambda \f$ */
    const sunrealtype kScalarX = (kx * x + ky * y + kz * z) * 2 *
                                 numbers::pi; /* \f$ 2\pi \ \vec{k} \cdot \vec{x} \f$ */
    // Plane wave definition
    const array<sunrealtype, 3> E{{                               /* E-field vector */
                                   px * cos(kScalarX - phix),   /* \f$ E_x \f$ */
                                   py * cos(kScalarX - phiy),   /* \f$ E_y \f$ */
                                   pz * cos(kScalarX - phiz)}}; /* \f$ E_z \f$ */
    // Put E-field into space
    pTo6Space[0] += E[0];
    pTo6Space[1] += E[1];
    pTo6Space[2] += E[2];
    // 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;
}
```

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

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

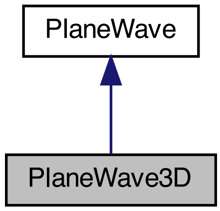
- src/ICSetters.h
- src/ICSetters.cpp

5.15 PlaneWave3D Class Reference

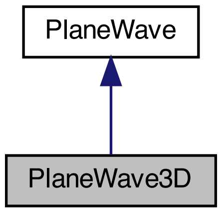
class for plane waves in 3D

`#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 72 of file ICSetters.h.

5.15.2 Constructor & Destructor Documentation

5.15.2.1 PlaneWave3D()

```
PlaneWave3D::PlaneWave3D (
            vector< sunrealtype > k = {1, 0, 0},
            vector< sunrealtype > p = {0, 0, 1},
            vector< sunrealtype > phi = {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 86 of file ICSetters.cpp.

```
                                                                  {
    kx = k[0];      /** - wavevectors \f$ k_x \f$ */
    ky = k[1];      /** - \f$ k_y \f$ */
    kz = k[2];      /** - \f$ k_z \f$ normalized to \f$ 1/\lambda \f$ */
    px = p[0];      /** - amplitude (polarization) in x-direction \f$ p_x \f$ */
    py = p[1];      /** - amplitude (polarization) in y-direction \f$ p_y \f$ */
    pz = p[2];      /** - 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$ */
}
```

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

5.15.3 Member Function Documentation

5.15.3.1 addToSpace()

```
void PlaneWave3D::addToSpace (
            sunrealtype x,
            sunrealtype y,
            sunrealtype z,
            sunrealtype * pTo6Space ) const
```

function for the actual implementation in space

PlaneWave3D implementation in space

Definition at line 100 of file ICSetters.cpp.

```
                                                                    {
    const sunrealtype wavelength =
        sqrt(kx * kx + ky * ky + kz * kz); /* \f$ 1/\lambda \f$ */
    const sunrealtype kScalarX = (kx * x + ky * y + kz * z) * 2 *
                       numbers::pi; /* \f$ 2\pi \ \vec{k} \cdot \vec{x} \f$ */
    // Plane wave definition
    const array<sunrealtype, 3> E{{/* E-field vector \f$ \vec{E}\f$*/
                         px * cos(kScalarX - phix),   /* \f$ E_x \f$ */
                         py * cos(kScalarX - phiy),   /* \f$ E_y \f$ */
                         pz * cos(kScalarX - phiz)}}; /* \f$ E_z \f$ */
    // Put E-field into space
    pTo6Space[0] += E[0];
    pTo6Space[1] += E[1];
    pTo6Space[2] += E[2];
    // 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;
}
```

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

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

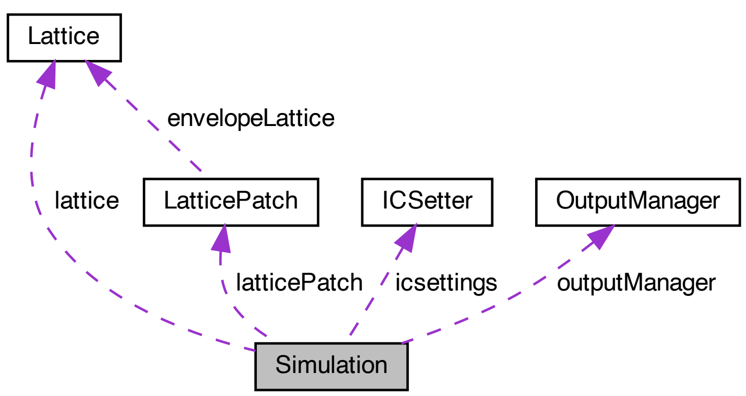
- src/ICSetters.h
- src/ICSetters.cpp

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 39 of file SimulationClass.h.

5.16.2 Constructor & Destructor Documentation

5.16.2.1 Simulation()

```
Simulation::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

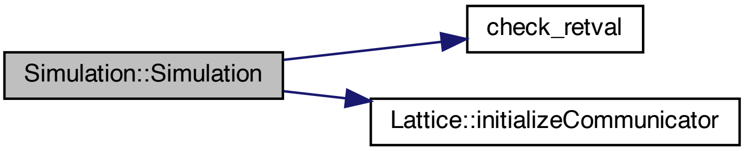
Along with the simulation object, create the cartesian communicator and SUNContext object

Definition at line 14 of file SimulationClass.cpp.

```
                                                         :
   lattice(StencilOrder){
  statusFlags = 0;
  t = 0;
  // Initialize the cartesian communicator
  lattice.initializeCommunicator(nx, ny, nz, periodicity);

  // Create the SUNContext object associated with the thread of execution
  int retval = 0;
  retval = SUNContext_Create(&lattice.comm, &lattice.sunctx);
  if (check_retval(&retval, "SUNContext_Create", 1, lattice.my_prc))
    MPI_Abort(lattice.comm, 1);
  // if (flag != CV_SUCCESS) { printf("SUNContext_Create failed, flag=%d.\n",
  // flag);
  //     MPI_Abort(lattice.comm, 1); }
}
```

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 ∼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.

```
00034                          {
00035   // Free solver memory
00036   if (statusFlags & CvodeObjectSetUp) {
00037     // PrintFinalStats(cvode_mem); // TODO write this function as in cvodes
00038     // cvAdvDiff_bnd.c SUNDIALS_MARK_FUNCTION_END(lattice.profobj);
00039     CVodeFree(&cvode_mem);
00040     SUNContext_Free(&lattice.sunctx);
00041   }
00042 }
```

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

5.16.3 Member Function Documentation

5.16.3.1 addInitialConditions()

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

functions to add initial periodic field configurations

Use parameters to add periodic IC layers.

Definition at line 185 of file SimulationClass.cpp.

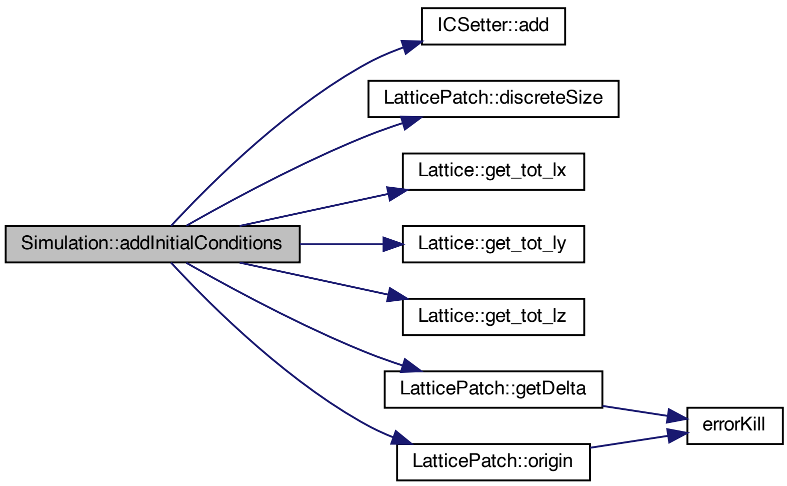
```
00186                          {
00187   const sunrealtype dx = latticePatch.getDelta(1);
00188   const sunrealtype dy = latticePatch.getDelta(2);
```

```
  const sunrealtype dz = latticePatch.getDelta(3);
  const int nx = latticePatch.discreteSize(1);
  const int ny = latticePatch.discreteSize(2);
  // Correct for demanded displacement, rest as for setInitialConditions
  const sunrealtype x0 = latticePatch.origin(1) + xm*lattice.get_tot_lx();
  const sunrealtype y0 = latticePatch.origin(2) + ym*lattice.get_tot_ly();
  const sunrealtype z0 = latticePatch.origin(3) + zm*lattice.get_tot_lz();
  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;
    icsettings.add(static_cast<sunrealtype>(px) * dx + x0,
                   static_cast<sunrealtype>(py) * dy + y0,
                   static_cast<sunrealtype>(pz) * dz + z0, &latticePatch.uData[i]);
  }
  return;
}
```

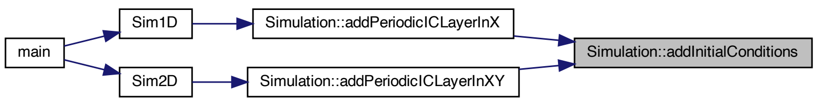
References ICSetter::add(), LatticePatch::discreteSize(), Lattice::get_tot_lx(), Lattice::get_tot_ly(), Lattice::get_tot_lz(), LatticePatch::getDelta(), icsettings, lattice, latticePatch, LatticePatch::origin(), and LatticePatch::uData.

Referenced by addPeriodicICLayerInX(), and addPeriodicICLayerInXY().

Here is the call graph for this function:



Here is the caller graph for this function:



5.16.3.2 addPeriodicICLayerInX()

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

function to add a periodic IC Layer in one dimension

Add initial conditions in one dimension.

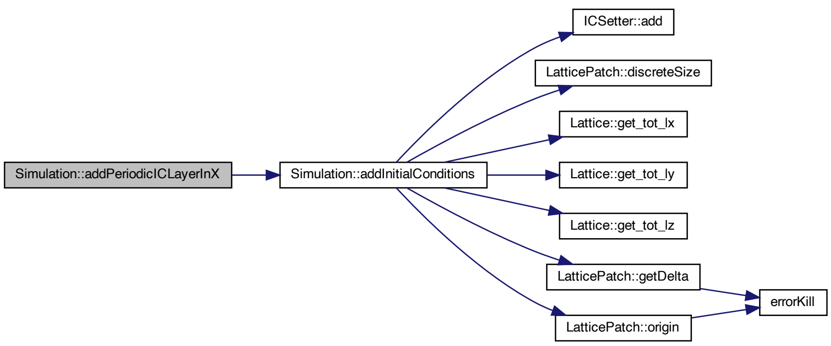
Definition at line 209 of file SimulationClass.cpp.

```
00209                                          {
00210    addInitialConditions(-1, 0, 0);
00211    addInitialConditions(1, 0, 0);
00212    return;
00213 }
```

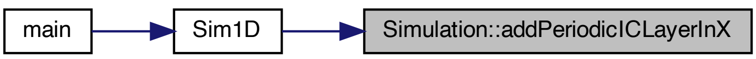
References addInitialConditions().

Referenced by Sim1D().

Here is the call graph for this function:



Here is the caller 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.

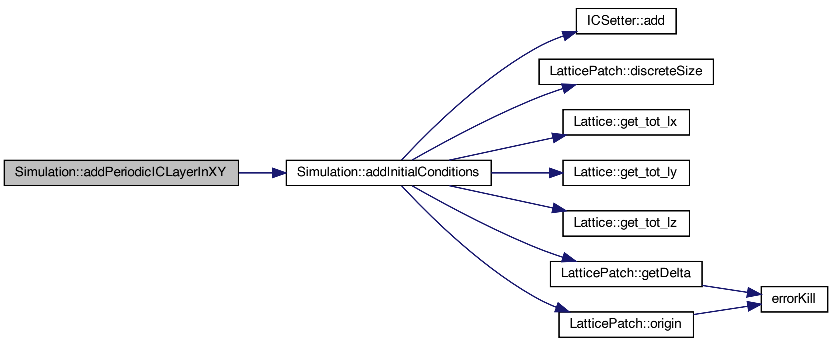
Definition at line 216 of file SimulationClass.cpp.

```
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 }
```

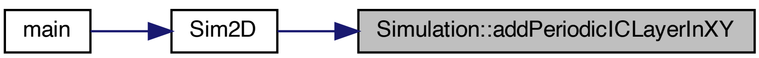
References addInitialConditions().

Referenced by Sim2D().

Here is the call graph for this function:



Here is the caller graph for this function:



5.16.3.4 advanceToTime()

```
void Simulation::advanceToTime (
            const sunrealtype & tEnd )
```

function to advance solution in time with CVODE

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

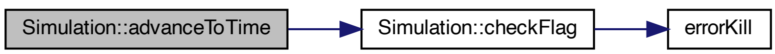
Definition at line 229 of file SimulationClass.cpp.

```
00229                                                   {
00230   checkFlag(SimulationStarted);
00231   int flag = 0;
00232   flag = CVode(cvode_mem, tEnd, latticePatch.u, &t,
00233                CV_NORMAL); // CV_NORMAL: internal steps to reach tEnd, then
00234                            // interpolate to return latticePatch.u, return time
00235                            // reached by the solver as t
00236   if (flag != CV_SUCCESS)
00237     printf("CVode failed, flag=%d.\n", flag);
00238 }
```

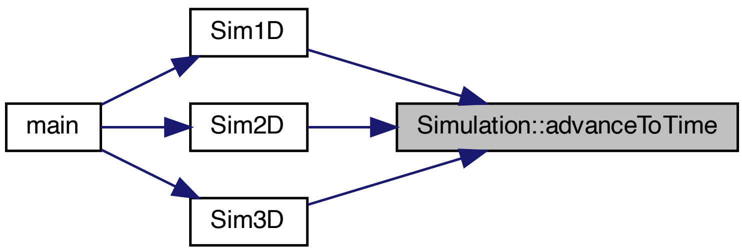
References checkFlag(), cvode_mem, latticePatch, SimulationStarted, t, and LatticePatch::u.

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

Here is the call graph for this function:



Here is the caller graph for this function:



5.16.3.5 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.

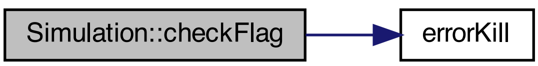
Definition at line 247 of file SimulationClass.cpp.

```
00247                                                  {
00248   if (!(statusFlags & flag)) {
00249     string errorMessage;
00250     switch (flag) {
00251     case LatticeDiscreteSetUp:
00252       errorMessage = "The discrete size of the Simulation has not been set up";
00253       break;
00254     case LatticePhysicalSetUp:
00255       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;
00260     case CvodeObjectSetUp:
00261       errorMessage = "The CVODE object has not been initialized";
00262       break;
00263     case SimulationStarted:
00264       errorMessage = "The Simulation has not been started";
00265       break;
00266     default:
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 }
```

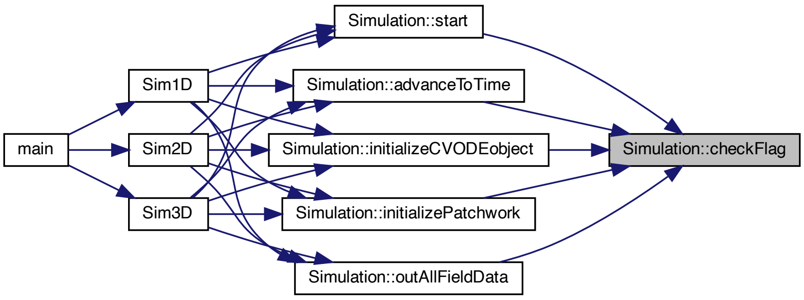
References CvodeObjectSetUp, errorKill(), LatticeDiscreteSetUp, LatticePatchworkSetUp, LatticePhysicalSetUp, SimulationStarted, and statusFlags.

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

Here is the call graph for this function:



Here is the caller graph for this function:



5.16.3.6 checkNoFlag()

```
void Simulation::checkNoFlag (
              unsigned int flag ) 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.

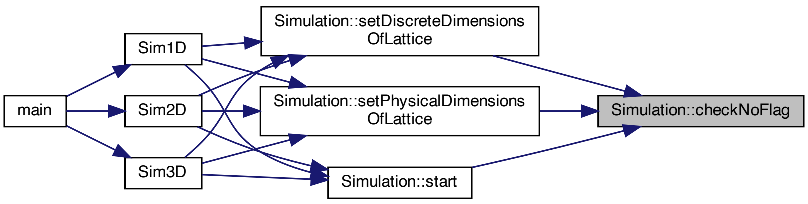
```
00277                                                    {
00278   if ((statusFlags & flag)) {
00279     string errorMessage;
00280     switch (flag) {
00281     case LatticeDiscreteSetUp:
00282       errorMessage =
00283           "The discrete size of the Simulation has already been set up";
00284       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       errorMessage = "The simulation has already started, some changes are no "
00297                      "longer possible";
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 }
```

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 63 of file SimulationClass.h.

```
00063 { return &lattice.comm; };
```

References Lattice::comm, and lattice.

5.16.3.8 initializeCVODEobject()

```
void Simulation::initializeCVODEobject (
            const sunrealtype reltol,
            const sunrealtype abstol )
```

function to initialize the CVODE object with all requirements

Configure CVODE.

Definition at line 74 of file SimulationClass.cpp.

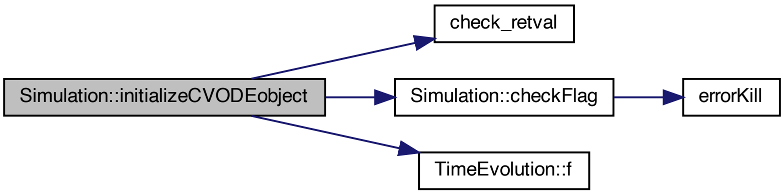
```
00075                                                    {
00076   checkFlag(SimulationStarted);
```

```

  // CVode settings return value
  int retval = 0;

  // Set the profiler
  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);
  //     MPI_Abort(lattice.comm, 1); }

  // SUNDIALS_MARK_FUNCTION_BEGIN(profobj);

  // Create CVODE object - returns a pointer to the cvode memory structure
  // with Adams method (Adams-Moulton formula) solver chosen for non-stiff ODE
  cvode_mem = CVodeCreate(CV_ADAMS, lattice.sunctx);

  // Specify user data and attach it to the main cvode memory block
  retval = CVodeSetUserData(
      cvode_mem,
      &latticePatch); // patch contains the user data as used in CVRhsFn
  if (check_retval(&retval, "CVodeSetUserData", 1, lattice.my_prc))
    MPI_Abort(lattice.comm, 1);
  // if (flag != CV_SUCCESS) { printf("CVodeSetUserData failed, flag=%d.\n",
  // flag);
  //     MPI_Abort(lattice.comm, 1); }

  // Initialize CVODE solver -> can only be called after start of simulation to
  // have data ready Provide required problem and solution specifications,
  // allocate internal memory, and initialize cvode
  retval = CVodeInit(cvode_mem, TimeEvolution::f, 0,
                     latticePatch.u); // allocate memory, CVRhsFn f, t_i=0, u
                                      // 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);
  //     MPI_Abort(lattice.comm, 1); }

  // Create fixed point nonlinear solver object (suitable for non-stiff ODE) and
  // attach it to CVode
  SUNNonlinearSolver NLS =
      SUNNonlinSol_FixedPoint(latticePatch.u, 0, lattice.sunctx);
  retval = CVodeSetNonlinearSolver(cvode_mem, NLS);
  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);
  //     MPI_Abort(lattice.comm, 1); }

  // Specify the maximum number of steps to be taken by the solver in its
  // attempt to reach the next output time
  retval = CVodeSetMaxNumSteps(cvode_mem, 10000);
  if (check_retval(&retval, "CVodeSetMaxNumSteps", 1, lattice.my_prc))
    MPI_Abort(lattice.comm, 1);
  // if (flag != CV_SUCCESS) { printf("CVodeSetMaxNumSteps failed, flag=%d.\n",
  // flag);
  //     MPI_Abort(lattice.comm, 1); }

  // Specify integration tolerances - a scalar relative tolerance and scalar
  // absolute tolerance
  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",
  // flag);
  //     MPI_Abort(lattice.comm, 1); }

  statusFlags |= CvodeObjectSetUp;
}
```

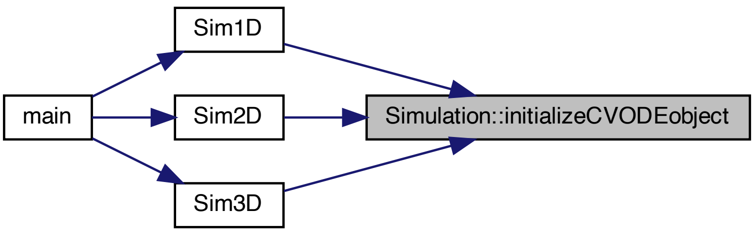
References check_retval(), checkFlag(), Lattice::comm, cvode_mem, CvodeObjectSetUp, TimeEvolution::f(), lattice, latticePatch, Lattice::my_prc, Lattice::profobj, SimulationStarted, statusFlags, Lattice::sunctx, and LatticePatch::u.

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()

```
void Simulation::initializePatchwork (
            const int nx,
            const int ny,
            const int nz )
```

function to initialize the Patchwork

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

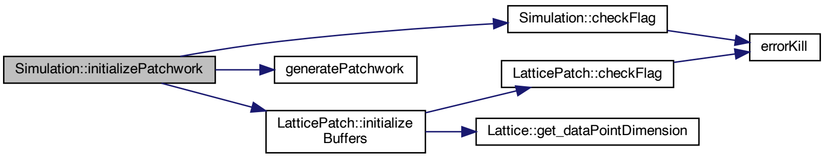
Definition at line 61 of file SimulationClass.cpp.

```
                          {
  checkFlag(LatticeDiscreteSetUp);
  checkFlag(LatticePhysicalSetUp);

  // Generate the patchwork
  generatePatchwork(lattice, latticePatch, nx, ny, nz);
  latticePatch.initializeBuffers();

  statusFlags |= LatticePatchworkSetUp;
}
```

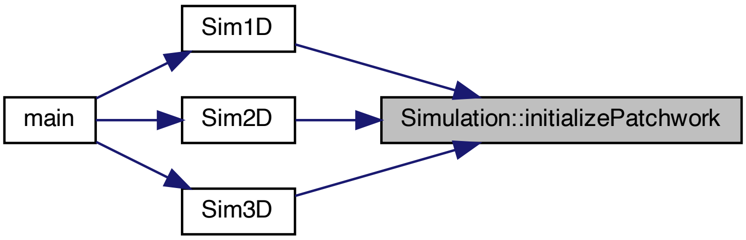
References checkFlag(), generatePatchwork(), LatticePatch::initializeBuffers(), lattice, LatticeDiscreteSetUp, latticePatch, LatticePatchworkSetUp, LatticePhysicalSetUp, and statusFlags.

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()

```
void Simulation::outAllFieldData (
            const int & state )
```

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

Write specified simulations steps to disk.

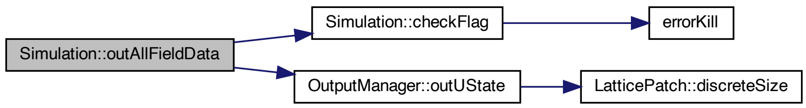
Definition at line 241 of file SimulationClass.cpp.

```
00241                                                     {
00242   checkFlag(SimulationStarted);
00243   outputManager.outUState(state, latticePatch);
00244 }
```

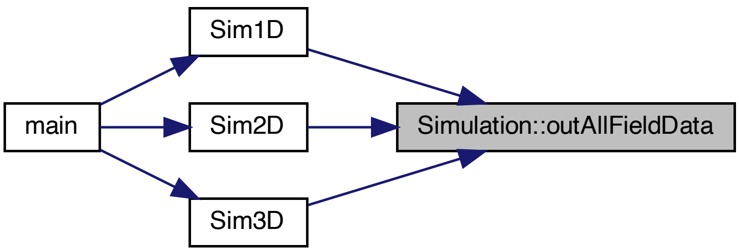
References checkFlag(), latticePatch, outputManager, OutputManager::outUState(), and SimulationStarted.

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()

```
void Simulation::setDiscreteDimensionsOfLattice (
            const sunindextype _tot_nx,
            const sunindextype _tot_ny,
            const sunindextype _tot_nz )
```

function to set discrete dimensions of the lattice

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

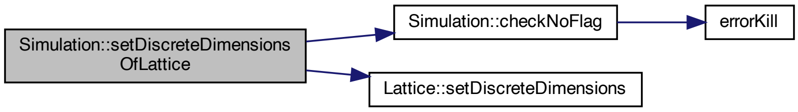
Definition at line 45 of file SimulationClass.cpp.

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

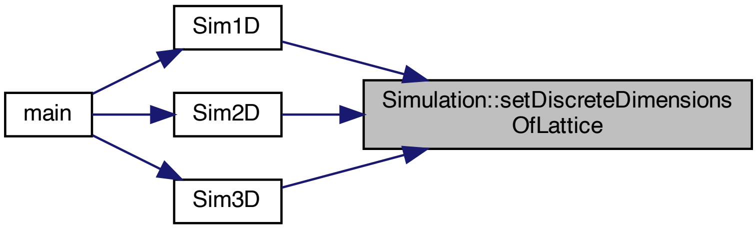
References checkNoFlag(), lattice, LatticeDiscreteSetUp, LatticePatchworkSetUp, Lattice::setDiscreteDimensions(), and statusFlags.

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

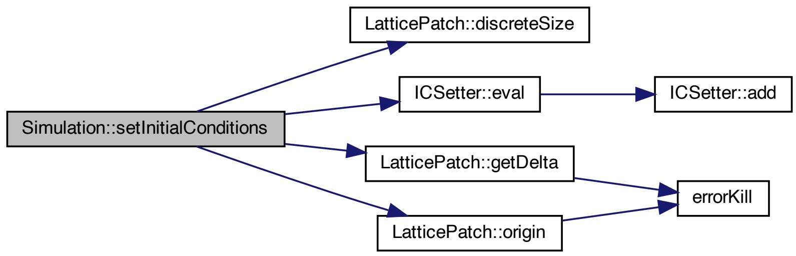
Definition at line 161 of file SimulationClass.cpp.

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

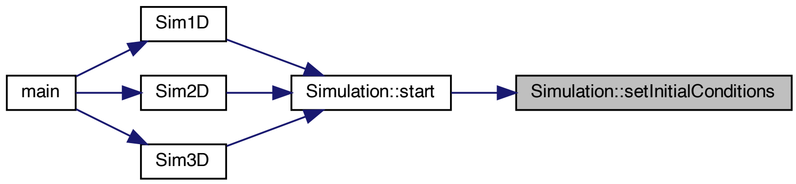
References LatticePatch::discreteSize(), ICSetter::eval(), LatticePatch::getDelta(), icsettings, latticePatch, LatticePatch::origin(), and LatticePatch::uData.

Referenced by start().

Here is the call graph for this function:



Here is the caller graph for this function:



5.16.3.13 setPhysicalDimensionsOfLattice()

```
void Simulation::setPhysicalDimensionsOfLattice (
            const sunrealtype lx,
            const sunrealtype ly,
            const sunrealtype lz )
```

function to set physical dimensions of the lattice

Set the physical dimensions with lenghts in micro meters.

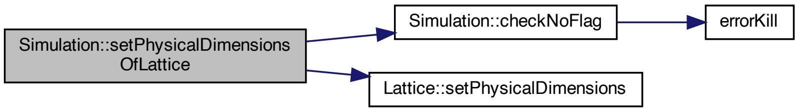
Definition at line 53 of file SimulationClass.cpp.

```
00054                                                       {
00055   checkNoFlag(LatticePatchworkSetUp);
00056   lattice.setPhysicalDimensions(lx, ly, lz);
00057   statusFlags |= LatticePhysicalSetUp;
00058 }
```

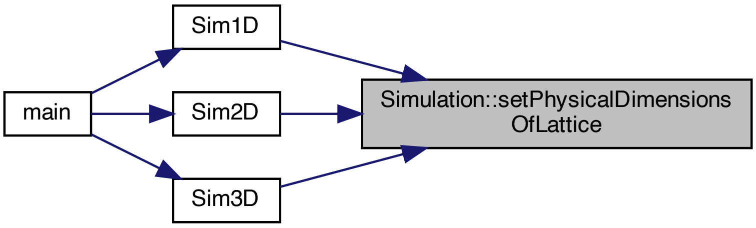
References checkNoFlag(), lattice, LatticePatchworkSetUp, LatticePhysicalSetUp, Lattice::setPhysicalDimensions(), and statusFlags.

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.

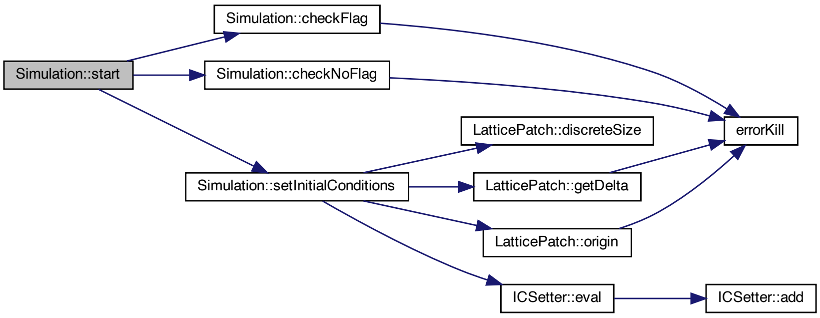
Definition at line 149 of file SimulationClass.cpp.

```
00149                        {
00150   checkFlag(LatticeDiscreteSetUp);
00151   checkFlag(LatticePhysicalSetUp);
00152   checkFlag(LatticePatchworkSetUp);
00153   checkNoFlag(SimulationStarted);
00154   checkNoFlag(CvodeObjectSetUp);
00155   setInitialConditions();
00156   statusFlags |= SimulationStarted;
00157 }
```

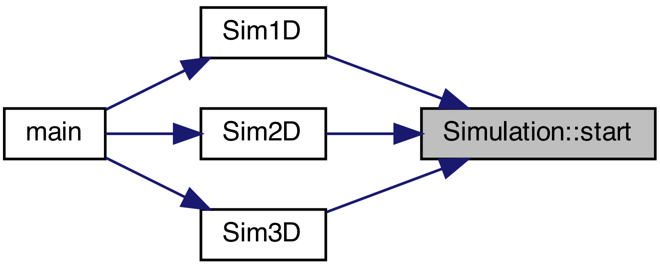
References checkFlag(), checkNoFlag(), CvodeObjectSetUp, LatticeDiscreteSetUp, LatticePatchworkSetUp, LatticePhysicalSetUp, setInitialConditions(), SimulationStarted, and statusFlags.

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 56 of file SimulationClass.h.

Referenced by advanceToTime(), initializeCVODEobject(), and ∼Simulation().

5.16.4.2 icsettings

`ICSetter Simulation::icsettings`

IC Setter object.

Definition at line 52 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 42 of file SimulationClass.h.

Referenced by addInitialConditions(), get_cart_comm(), initializeCVODEobject(), initializePatchwork(), setDiscreteDimensionsOfLattic
setPhysicalDimensionsOfLattice(), Simulation(), and ∼Simulation().

5.16.4.4 latticePatch

`LatticePatch Simulation::latticePatch [private]`

LatticePatch object.

Definition at line 44 of file SimulationClass.h.

Referenced by addInitialConditions(), advanceToTime(), initializeCVODEobject(), initializePatchwork(), outAllFieldData(), and setInitialConditions().

5.16.4.5 outputManager

`OutputManager Simulation::outputManager`

Output Manager object.

Definition at line 54 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 48 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 46 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 17 of file TimeEvolutionFunctions.h.

5.17.2 Member Function Documentation

5.17.2.1 f()

```
int TimeEvolution::f (
              sunrealtype t,
              N_Vector u,
              N_Vector udot,
              void * data_loc )  [static]
```

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

CVode right-hand-side function (CVRhsFn)

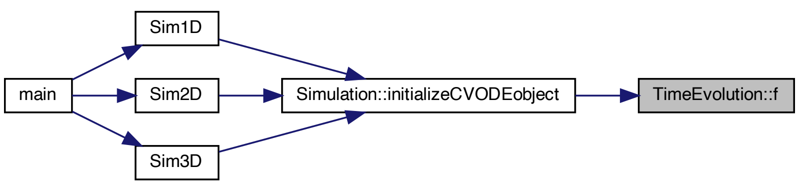
Definition at line 13 of file TimeEvolutionFunctions.cpp.

```
00013                                                                                   {
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
00023   udata = NV_DATA_P(u);
00024   dudata = NV_DATA_P(udot);
00025
00026   // Store original data location of the patch
00027   originaluData = data->uData;
00028   originalduData = data->duData;
00029   // Point patch data to arguments of f
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().

Here is the caller graph for this function:



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 20 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 23 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

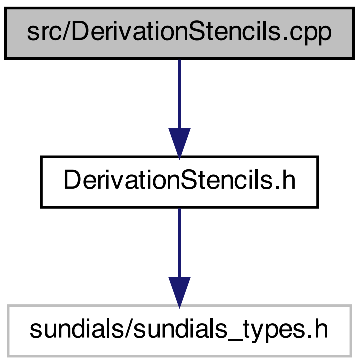
File Documentation

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.

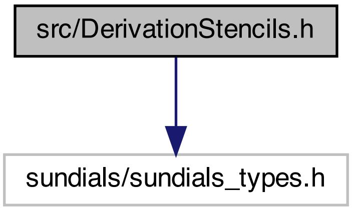
```
00001 ///////////////////////////////////////////////////
00002 /// @file DerivationStencils.cpp
00003 /// @brief Empty. All definitions in the header.
00004 //////////////////////////////////////////////////
00005 #include "DerivationStencils.h"
```

6.4 src/DerivationStencils.h File Reference

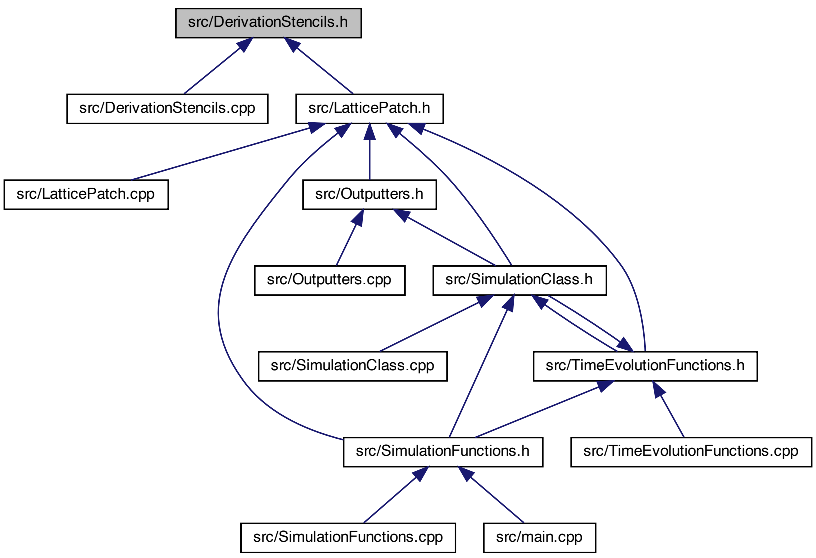
Definition of derivation stencils from order 1 to 13.

`#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]

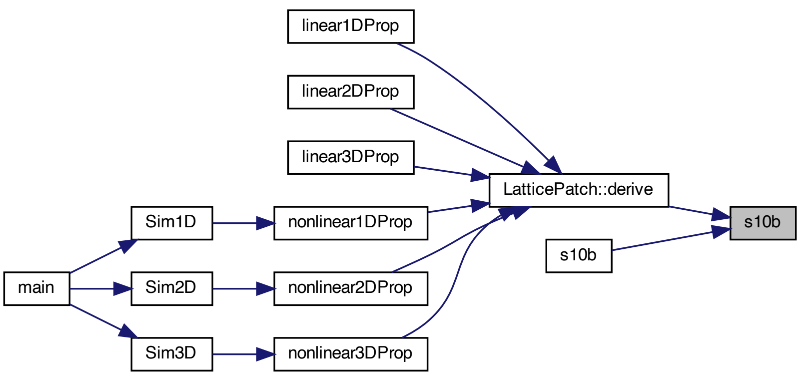
```
sunrealtype s10b (
            const sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 146 of file DerivationStencils.h.

```
00146                                                           {
00147   return 1.0 / 840.0 * udata[-4 * nx] - 1.0 / 63.0 * udata[-3 * nx] +
00148          3.0 / 28.0 * udata[-2 * nx] - 4.0 / 7.0 * udata[-1 * nx] -
00149          11.0 / 30.0 * udata[0] + 6.0 / 5.0 * udata[1 * nx] -
00150          1.0 / 2.0 * udata[2 * nx] + 4.0 / 21.0 * udata[3 * nx] -
00151          3.0 / 56.0 * udata[4 * nx] + 1.0 / 105.0 * udata[5 * nx] -
00152          1.0 / 1260.0 * udata[6 * nx];
00153 }
```

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

Here is the caller graph for this function:



6.4.2.2 s10b() [2/2]

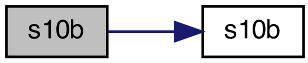
```
sunrealtype s10b (
              sunrealtype * udata ) [inline]
```

Definition at line 243 of file DerivationStencils.h.

```
00243 { return s10b(udata, 6); }
```

References s10b().

Here is the call graph for this function:



6.4.2.3 s10c() [1/2]

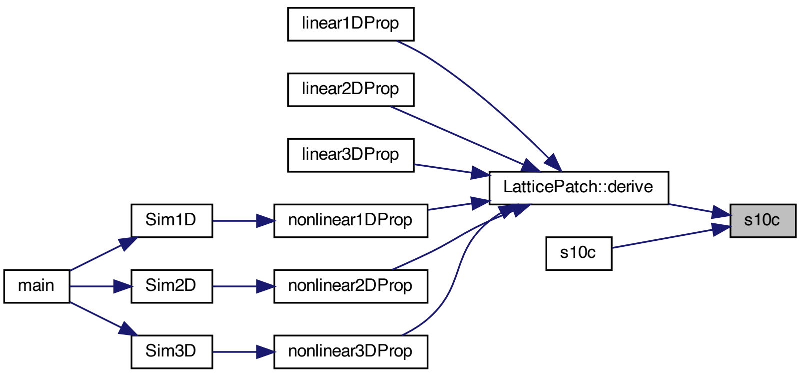
```
sunrealtype s10c (
              const sunrealtype * udata,
              int nx ) [inline]
```

Definition at line 139 of file DerivationStencils.h.

```
00139                                                            {
00140   return -1.0 / 1260.0 * udata[-5 * nx] + 5.0 / 504.0 * udata[-4 * nx] -
00141          5.0 / 84.0 * udata[-3 * nx] + 5.0 / 21.0 * udata[-2 * nx] -
00142          5.0 / 6.0 * udata[-1 * nx] + 0 + 5.0 / 6.0 * udata[1 * nx] -
00143          5.0 / 21.0 * udata[2 * nx] + 5.0 / 84.0 * udata[3 * nx] -
00144          5.0 / 504.0 * udata[4 * nx] + 1.0 / 1260.0 * udata[5 * nx];
00145 }
```

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

Here is the caller graph for this function:



6.4.2.4 s10c() [2/2]

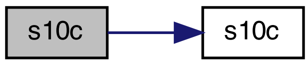
```
sunrealtype s10c (
            sunrealtype * udata )  [inline]
```

Definition at line 242 of file DerivationStencils.h.

```
00242 { return s10c(udata, 6); }
```

References s10c().

Here is the call graph for this function:



6.4.2.5 s10f() [1/2]

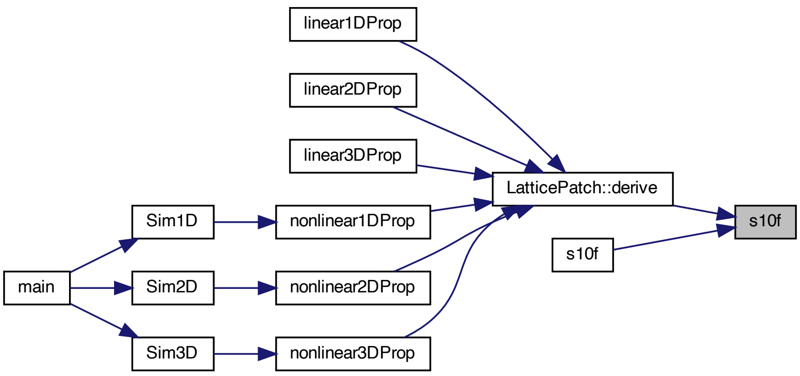
```
sunrealtype s10f (
            const sunrealtype * udata,
            int nx )  [inline]
```

Definition at line 131 of file DerivationStencils.h.

```
00131                                                   {
00132   return 1.0 / 1260.0 * udata[-6 * nx] - 1.0 / 105.0 * udata[-5 * nx] +
00133          3.0 / 56.0 * udata[-4 * nx] - 4.0 / 21.0 * udata[-3 * nx] +
00134          1.0 / 2.0 * udata[-2 * nx] - 6.0 / 5.0 * udata[-1 * nx] +
00135          11.0 / 30.0 * udata[0] + 4.0 / 7.0 * udata[1 * nx] -
00136          3.0 / 28.0 * udata[2 * nx] + 1.0 / 63.0 * udata[3 * nx] -
00137          1.0 / 840.0 * udata[4 * nx];
00138 }
```

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

Here is the caller graph for this function:



6.4.2.6 s10f() [2/2]

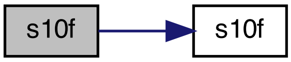
```
sunrealtype s10f (
            sunrealtype * udata )  [inline]
```

Definition at line 241 of file DerivationStencils.h.

```
00241 { return s10f(udata, 6); }
```

References s10f().

Here is the call graph for this function:



6.4.2.7 s11b() [1/2]

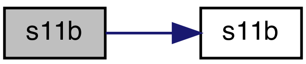
```
sunrealtype s11b (
            sunrealtype * udata )  [inline]
```

Definition at line 245 of file DerivationStencils.h.

```
00245 { return s11b(udata, 6); }
```

References s11b().

Here is the call graph for this function:



6.4.2.8 s11b() [2/2]

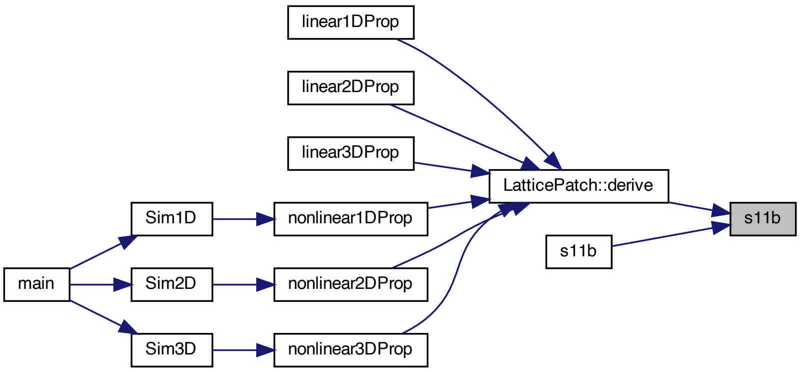
```
sunrealtype s11b (
            sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 162 of file DerivationStencils.h.

```
00162                                               {
00163   return -1.0 / 2310.0 * udata[-5 * nx] + 1.0 / 168.0 * udata[-4 * nx] -
00164          5.0 / 126.0 * udata[-3 * nx] + 5.0 / 28.0 * udata[-2 * nx] -
00165          5.0 / 7.0 * udata[-1 * nx] - 1.0 / 6.0 * udata[0] + udata[1 * nx] -
00166          5.0 / 14.0 * udata[2 * nx] + 5.0 / 42.0 * udata[3 * nx] -
00167          5.0 / 168.0 * udata[4 * nx] + 1.0 / 210.0 * udata[5 * nx] -
00168          1.0 / 2772.0 * udata[6 * nx];
00169 }
```

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

Here is the caller graph for this function:



6.4.2.9 s11f() [1/2]

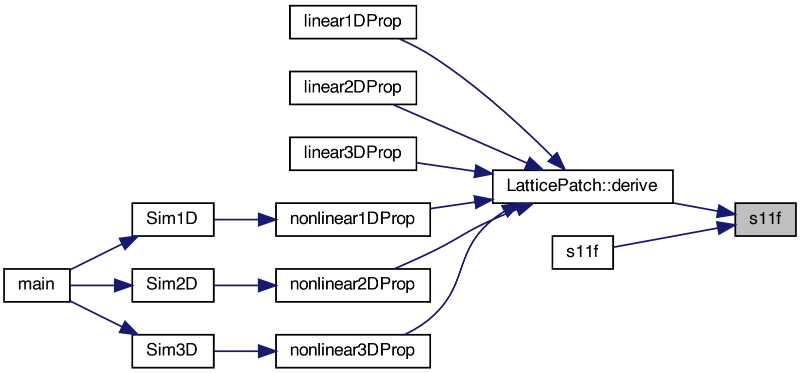
```
sunrealtype s11f (
            const sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 154 of file DerivationStencils.h.

```
00154                                                     {
00155   return 1.0 / 2772.0 * udata[-6 * nx] - 1.0 / 210.0 * udata[-5 * nx] +
00156          5.0 / 168.0 * udata[-4 * nx] - 5.0 / 42.0 * udata[-3 * nx] +
00157          5.0 / 14.0 * udata[-2 * nx] - 1.0 / 1.0 * udata[-1 * nx] +
00158          1.0 / 6.0 * udata[0] + 5.0 / 7.0 * udata[1 * nx] -
00159          5.0 / 28.0 * udata[2 * nx] + 5.0 / 126.0 * udata[3 * nx] -
00160          1.0 / 168.0 * udata[4 * nx] + 1.0 / 2310.0 * udata[5 * nx];
00161 }
```

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

Here is the caller graph for this function:



6.4.2.10 s11f() [2/2]

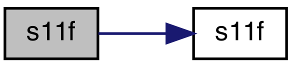
```
sunrealtype s11f (
            sunrealtype * udata )  [inline]
```

Definition at line 244 of file DerivationStencils.h.

```
00244 { 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]
```

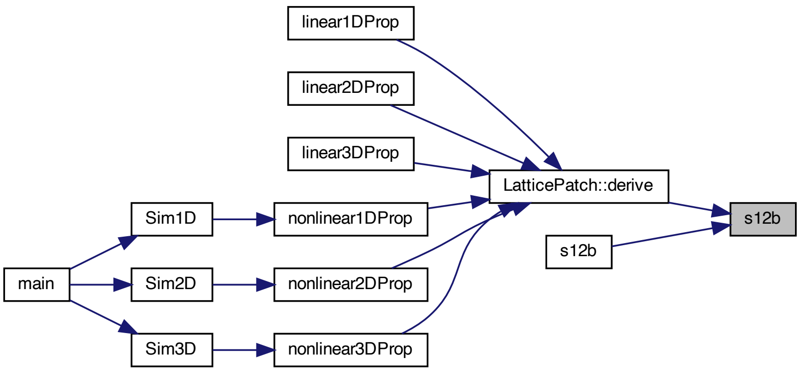
Definition at line 187 of file DerivationStencils.h.

```
00187                                                        {
```

```
00188   return -1.0 / 3960.0 * udata[-5 * nx] + 1.0 / 264.0 * udata[-4 * nx] -
00189          1.0 / 36.0 * udata[-3 * nx] + 5.0 / 36.0 * udata[-2 * nx] -
00190          5.0 / 8.0 * udata[-1 * nx] - 13.0 / 42.0 * udata[0] +
00191          7.0 / 6.0 * udata[1 * nx] - 1.0 / 2.0 * udata[2 * nx] +
00192          5.0 / 24.0 * udata[3 * nx] - 5.0 / 72.0 * udata[4 * nx] +
00193          1.0 / 60.0 * udata[5 * nx] - 1.0 / 396.0 * udata[6 * nx] +
00194          1.0 / 5544.0 * udata[7 * nx];
00195 }
```

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

Here is the caller graph for this function:



6.4.2.12 s12b() [2/2]

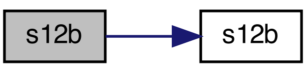
```
sunrealtype s12b (
            sunrealtype * udata )  [inline]
```

Definition at line 248 of file DerivationStencils.h.

```
00248 { return s12b(udata, 6); }
```

References s12b().

Here is the call graph for this function:



6.4.2.13 s12c() [1/2]

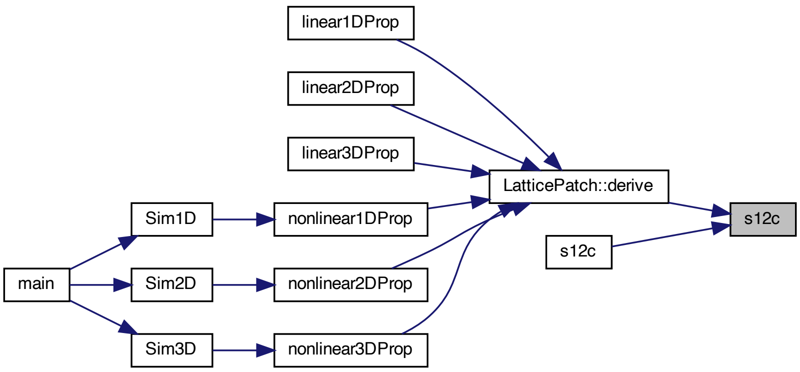
```
sunrealtype s12c (
            const sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 179 of file DerivationStencils.h.

```
00179                                                      {
00180   return 1.0 / 5544.0 * udata[-6 * nx] - 1.0 / 385.0 * udata[-5 * nx] +
00181          1.0 / 56.0 * udata[-4 * nx] - 5.0 / 63.0 * udata[-3 * nx] +
00182          15.0 / 56.0 * udata[-2 * nx] - 6.0 / 7.0 * udata[-1 * nx] + 0 +
00183          6.0 / 7.0 * udata[1 * nx] - 15.0 / 56.0 * udata[2 * nx] +
00184          5.0 / 63.0 * udata[3 * nx] - 1.0 / 56.0 * udata[4 * nx] +
00185          1.0 / 385.0 * udata[5 * nx] - 1.0 / 5544.0 * udata[6 * nx];
00186 }
```

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

Here is the caller graph for this function:



6.4.2.14 s12c() [2/2]

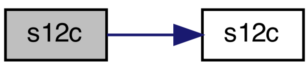
```
sunrealtype s12c (
            sunrealtype * udata ) [inline]
```

Definition at line 247 of file DerivationStencils.h.

```
00247 { return s12c(udata, 6); }
```

References s12c().

Here is the call graph for this function:



6.4.2.15 s12f() [1/2]

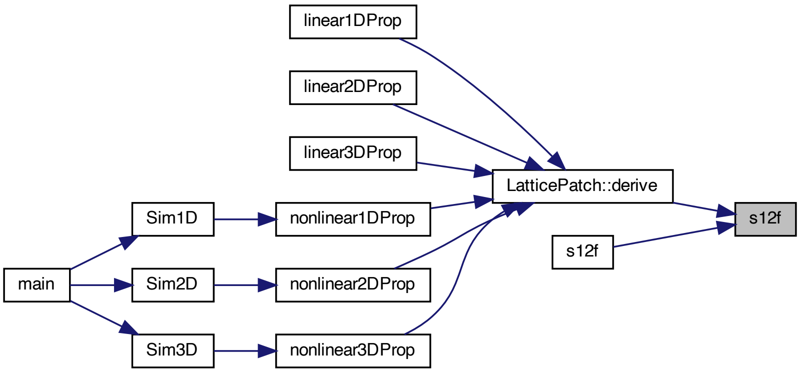
```
sunrealtype s12f (
            const sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 170 of file DerivationStencils.h.

```
00170                                                     {
00171   return -1.0 / 5544.0 * udata[-7 * nx] + 1.0 / 396.0 * udata[-6 * nx] -
00172          1.0 / 60.0 * udata[-5 * nx] + 5.0 / 72.0 * udata[-4 * nx] -
00173          5.0 / 24.0 * udata[-3 * nx] + 1.0 / 2.0 * udata[-2 * nx] -
00174          7.0 / 6.0 * udata[-1 * nx] + 13.0 / 42.0 * udata[0] +
00175          5.0 / 8.0 * udata[1 * nx] - 5.0 / 36.0 * udata[2 * nx] +
00176          1.0 / 36.0 * udata[3 * nx] - 1.0 / 264.0 * udata[4 * nx] +
00177          1.0 / 3960.0 * udata[5 * nx];
00178 }
```

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

Here is the caller graph for this function:



6.4.2.16 s12f() [2/2]

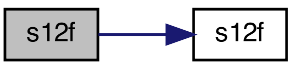
```
sunrealtype s12f (
            sunrealtype * udata ) [inline]
```

Definition at line 246 of file DerivationStencils.h.

```
00246 { return s12f(udata, 6); }
```

References s12f().

Here is the call graph for this function:



6.4.2.17 s13b() [1/2]

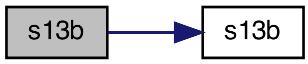
```
sunrealtype s13b (
            sunrealtype * udata )  [inline]
```

Definition at line 250 of file DerivationStencils.h.

```
00250 { return s13b(udata, 6); }
```

References s13b().

Here is the call graph for this function:



6.4.2.18 s13b() [2/2]

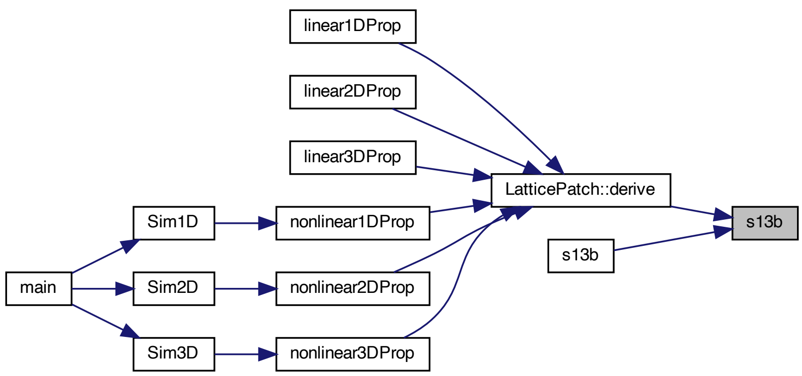
```
sunrealtype s13b (
            sunrealtype * udata,
            int nx )  [inline]
```

Definition at line 205 of file DerivationStencils.h.

```
00205                                                  {
00206   return 1.0 / 10296.0 * udata[-6 * nx] - 1.0 / 660.0 * udata[-5 * nx] +
00207          1.0 / 88.0 * udata[-4 * nx] - 1.0 / 18.0 * udata[-3 * nx] +
00208          5.0 / 24.0 * udata[-2 * nx] - 3.0 / 4.0 * udata[-1 * nx] -
00209          1.0 / 7.0 * udata[0] + udata[1 * nx] - 3.0 / 8.0 * udata[2 * nx] +
00210          5.0 / 36.0 * udata[3 * nx] - 1.0 / 24.0 * udata[4 * nx] +
00211          1.0 / 110.0 * udata[5 * nx] - 1.0 / 792.0 * udata[6 * nx] +
00212          1.0 / 12012.0 * udata[7 * nx];
00213 }
```

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

Here is the caller graph for this function:



6.4.2.19 s13f() [1/2]

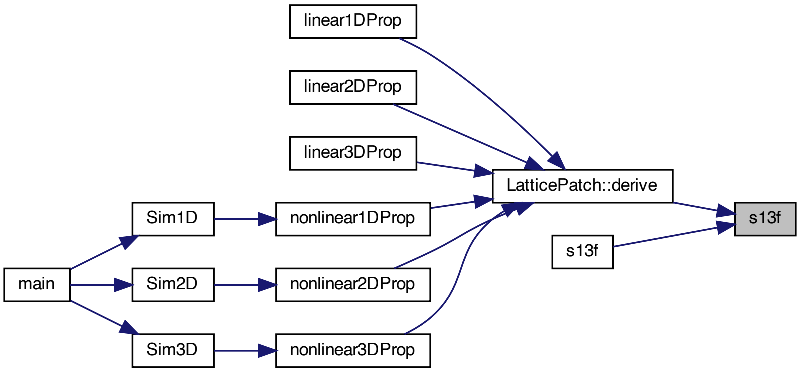
```
sunrealtype s13f (
            const sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 196 of file DerivationStencils.h.

```
                                                                    {
   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] -
          5.0 / 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 / 660.0 * udata[5 * nx] - 1.0 / 10296.0 * udata[6 * nx];
}
```

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

Here is the caller graph for this function:



6.4.2.20 s13f() [2/2]

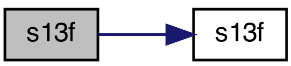
```
sunrealtype s13f (
            sunrealtype * udata ) [inline]
```

Definition at line 249 of file DerivationStencils.h.

```
{ return s13f(udata, 6); }
```

References s13f().

Here is the call graph for this function:



6.4.2.21 s1b() [1/2]

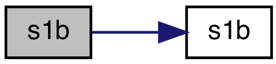
```
sunrealtype s1b (
            sunrealtype * udata )  [inline]
```

Definition at line 220 of file DerivationStencils.h.

```
00220 { return s1b(udata, 6); }
```

References s1b().

Here is the call graph for this function:



6.4.2.22 s1b() [2/2]

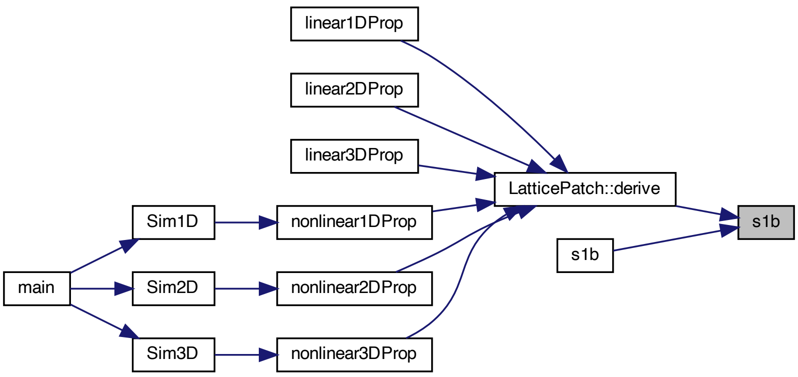
```
sunrealtype s1b (
            sunrealtype * udata,
            int nx )  [inline]
```

Definition at line 21 of file DerivationStencils.h.

```
00021                                                    {
00022   return -1.0 / 1.0 * udata[0] + udata[1 * nx];
00023 }
```

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

Here is the caller graph for this function:



6.4.2.23 s1f() [1/2]

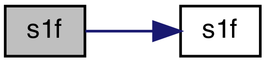
```
sunrealtype s1f (
            sunrealtype * udata )  [inline]
```

Definition at line 219 of file DerivationStencils.h.

```
00219 { return s1f(udata, 6); }
```

References s1f().

Here is the call graph for this function:



6.4.2.24 s1f() [2/2]

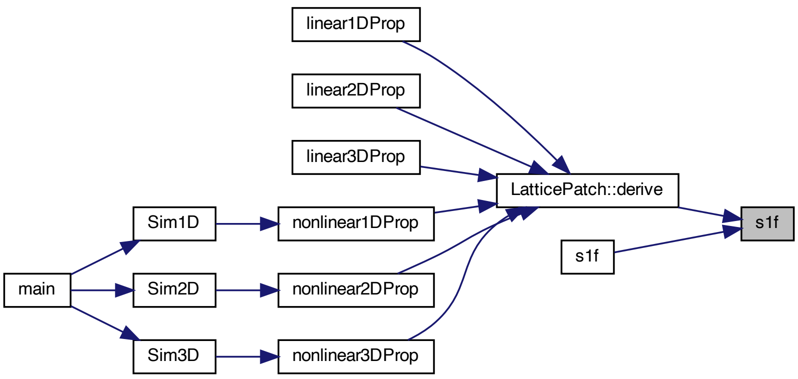
```
sunrealtype s1f (
            sunrealtype * udata,
            int nx )  [inline]
```

Definition at line 17 of file DerivationStencils.h.

```
00017                                             {
00018   return -1.0 / 1.0 * udata[-1 * nx] + udata[0];
00019 }
```

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

Here is the caller graph for this function:



6.4.2.25 s2b() [1/2]

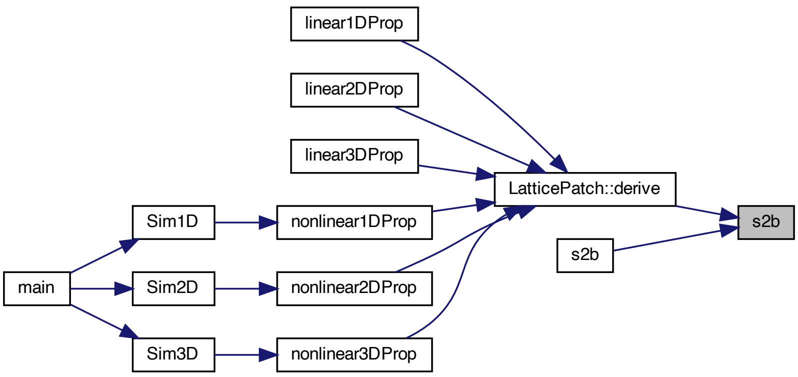
```
sunrealtype s2b (
            const sunrealtype * udata,
            int nx )  [inline]
```

Definition at line 32 of file DerivationStencils.h.

```
00032                                                  {
00033   return -3.0 / 2.0 * udata[0] + 2.0 / 1.0 * udata[1 * nx] -
00034          1.0 / 2.0 * udata[2 * nx];
00035 }
```

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

Here is the caller graph for this function:



6.4.2.26 s2b() [2/2]

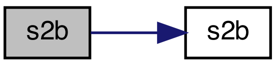
```
sunrealtype s2b (
            sunrealtype * udata )  [inline]
```

Definition at line 223 of file DerivationStencils.h.

```
00223 { return s2b(udata, 6); }
```

References s2b().

Here is the call graph for this function:



6.4.2.27 s2c() [1/2]

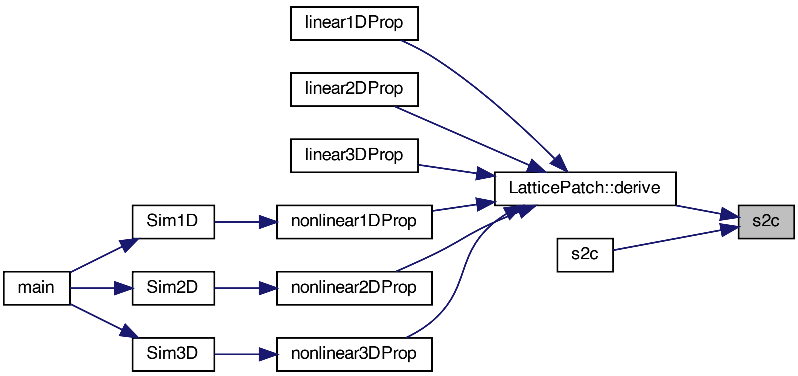
```
sunrealtype s2c (
            const sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 29 of file DerivationStencils.h.

```
00029                                                {
00030   return -1.0 / 2.0 * udata[-1 * nx] + 0 + 1.0 / 2.0 * udata[1 * nx];
00031 }
```

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

Here is the caller graph for this function:



6.4.2.28 s2c() [2/2]

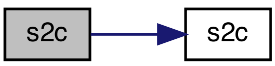
```
sunrealtype s2c (
            sunrealtype * udata ) [inline]
```

Definition at line 222 of file DerivationStencils.h.

```
00222 { return s2c(udata, 6); }
```

References s2c().

Here is the call graph for this function:



6.4.2.29 s2f() [1/2]

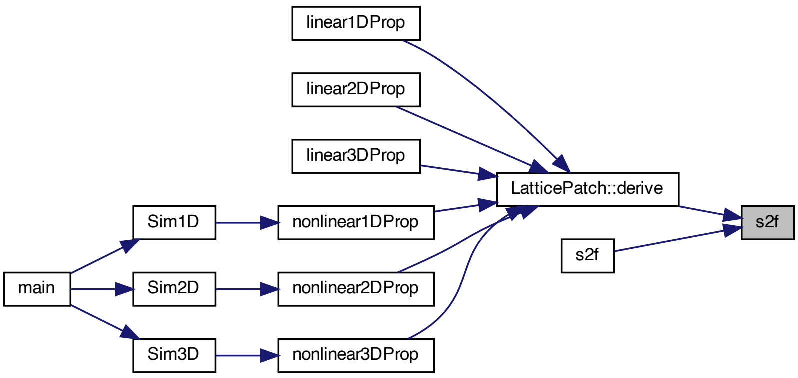
```
sunrealtype s2f (
            const sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 25 of file DerivationStencils.h.

```
00025                                                  {
00026   return 1.0 / 2.0 * udata[-2 * nx] - 2.0 / 1.0 * udata[-1 * nx] +
00027          3.0 / 2.0 * udata[0];
00028 }
```

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

Here is the caller graph for this function:



6.4.2.30 s2f() [2/2]

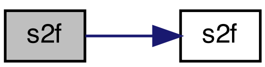
```
sunrealtype s2f (
            sunrealtype * udata ) [inline]
```

Definition at line 221 of file DerivationStencils.h.

```
00221 { return s2f(udata, 6); }
```

References s2f().

Here is the call graph for this function:



6.4.2.31 s3b() [1/2]

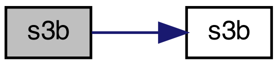
```
sunrealtype s3b (
            sunrealtype * udata )  [inline]
```

Definition at line 225 of file DerivationStencils.h.

```
00225 { return s3b(udata, 6); }
```

References s3b().

Here is the call graph for this function:



6.4.2.32 s3b() [2/2]

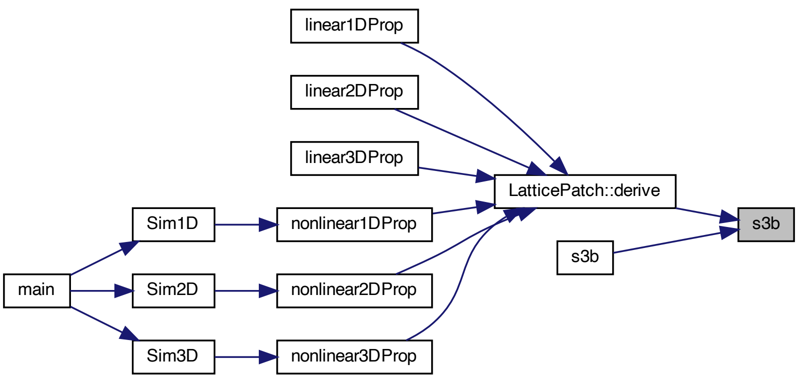
```
sunrealtype s3b (
            sunrealtype * udata,
            int nx )  [inline]
```

Definition at line 40 of file DerivationStencils.h.

```
00040                                              {
00041   return -1.0 / 3.0 * udata[-1 * nx] - 1.0 / 2.0 * udata[0] + udata[1 * nx] -
00042          1.0 / 6.0 * udata[2 * nx];
00043 }
```

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

Here is the caller graph for this function:



6.4.2.33 s3f() [1/2]

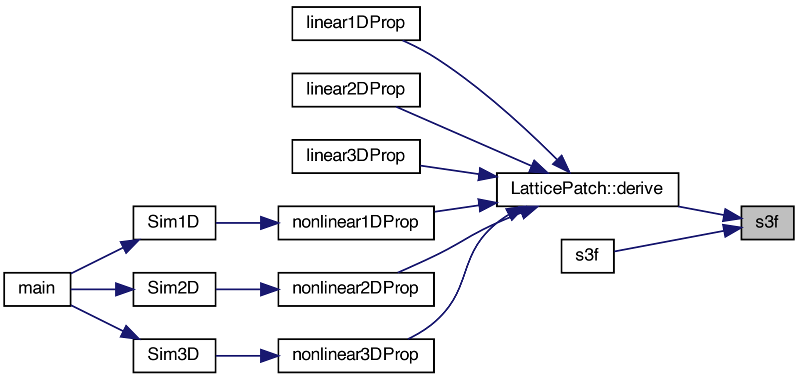
```
sunrealtype s3f (
            const sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 36 of file DerivationStencils.h.

```
00036                                                    {
00037   return 1.0 / 6.0 * udata[-2 * nx] - 1.0 / 1.0 * udata[-1 * nx] +
00038          1.0 / 2.0 * udata[0] + 1.0 / 3.0 * udata[1 * nx];
00039 }
```

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

Here is the caller graph for this function:



6.4.2.34 s3f() [2/2]

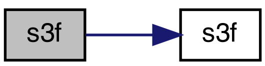
```
sunrealtype s3f (
            sunrealtype * udata ) [inline]
```

Definition at line 224 of file DerivationStencils.h.

```
00224 { return s3f(udata, 6); }
```

References s3f().

Here is the call graph for this function:



6.4.2.35 s4b() [1/2]

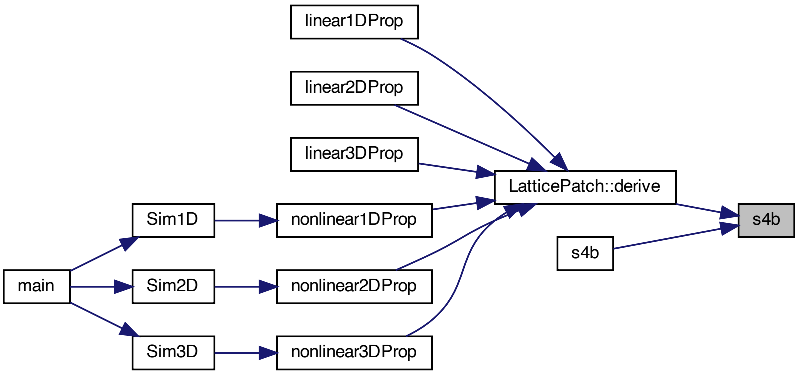
```
sunrealtype s4b (
              const sunrealtype * udata,
              int nx )  [inline]
```

Definition at line 53 of file DerivationStencils.h.

```
00053                                                          {
00054   return -1.0 / 4.0 * udata[-1 * nx] - 5.0 / 6.0 * udata[0] +
00055          3.0 / 2.0 * udata[1 * nx] - 1.0 / 2.0 * udata[2 * nx] +
00056          1.0 / 12.0 * udata[3 * nx];
00057 }
```

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

Here is the caller graph for this function:



6.4.2.36 s4b() [2/2]

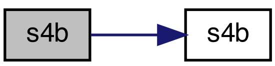
```
sunrealtype s4b (
              sunrealtype * udata )  [inline]
```

Definition at line 228 of file DerivationStencils.h.

```
00228 { return s4b(udata, 6); }
```

References s4b().

Here is the call graph for this function:



6.4.2.37 s4c() [1/2]

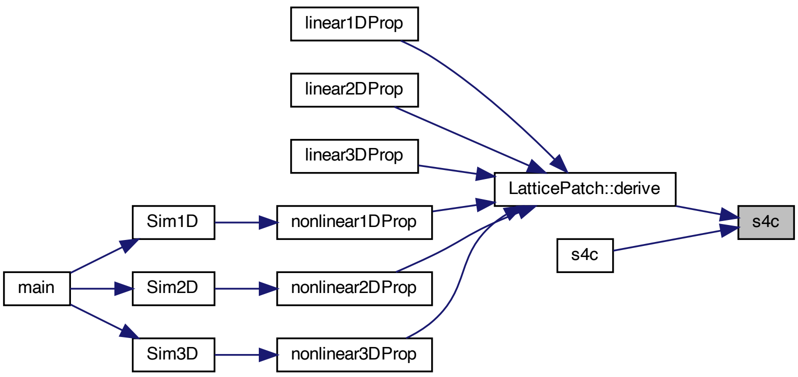
```
sunrealtype s4c (
            const sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 49 of file DerivationStencils.h.

```
00049                                                           {
00050   return 1.0 / 12.0 * udata[-2 * nx] - 2.0 / 3.0 * udata[-1 * nx] + 0 +
00051          2.0 / 3.0 * udata[1 * nx] - 1.0 / 12.0 * udata[2 * nx];
00052 }
```

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

Here is the caller graph for this function:



6.4.2.38 s4c() [2/2]

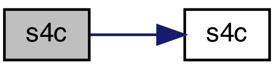
```
sunrealtype s4c (
            sunrealtype * udata ) [inline]
```

Definition at line 227 of file DerivationStencils.h.

```
00227 { return s4c(udata, 6); }
```

References s4c().

Here is the call graph for this function:



6.4.2.39 s4f() [1/2]

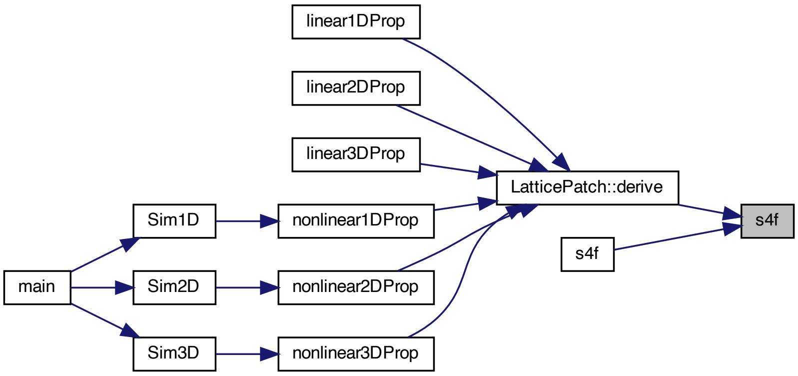
```
sunrealtype s4f (
            const sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 44 of file DerivationStencils.h.

```
00044                                                          {
00045   return -1.0 / 12.0 * udata[-3 * nx] + 1.0 / 2.0 * udata[-2 * nx] -
00046          3.0 / 2.0 * udata[-1 * nx] + 5.0 / 6.0 * udata[0] +
00047          1.0 / 4.0 * udata[1 * nx];
00048 }
```

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

Here is the caller graph for this function:



6.4.2.40 s4f() [2/2]

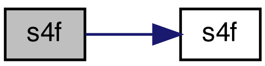
```
sunrealtype s4f (
            sunrealtype * udata ) [inline]
```

Definition at line 226 of file DerivationStencils.h.

```
00226 { return s4f(udata, 6); }
```

References s4f().

Here is the call graph for this function:



6.4.2.41 s5b() [1/2]

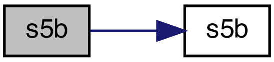
```
sunrealtype s5b (
            sunrealtype * udata ) [inline]
```

Definition at line 230 of file DerivationStencils.h.

```
00230 { return s5b(udata, 6); }
```

References s5b().

Here is the call graph for this function:



6.4.2.42 s5b() [2/2]

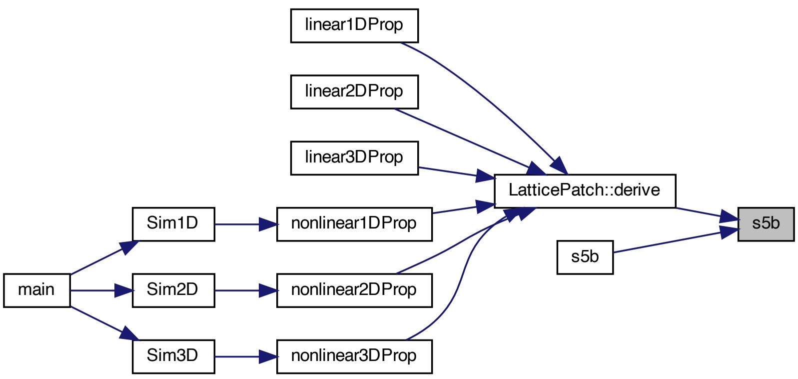
```
sunrealtype s5b (
            sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 63 of file DerivationStencils.h.

```
00063                                            {
00064   return 1.0 / 20.0 * udata[-2 * nx] - 1.0 / 2.0 * udata[-1 * nx] -
00065          1.0 / 3.0 * udata[0] + udata[1 * nx] - 1.0 / 4.0 * udata[2 * nx] +
00066          1.0 / 30.0 * udata[3 * nx];
00067 }
```

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

Here is the caller graph for this function:



6.4.2.43 s5f() [1/2]

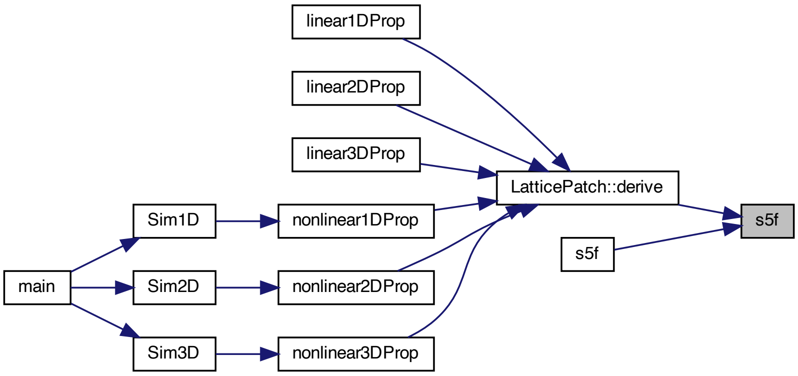
```
sunrealtype s5f (
            const sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 58 of file DerivationStencils.h.

```
00058                                                       {
00059   return -1.0 / 30.0 * udata[-3 * nx] + 1.0 / 4.0 * udata[-2 * nx] -
00060          1.0 / 1.0 * udata[-1 * nx] + 1.0 / 3.0 * udata[0] +
00061          1.0 / 2.0 * udata[1 * nx] - 1.0 / 20.0 * udata[2 * nx];
00062 }
```

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

Here is the caller graph for this function:



6.4.2.44 s5f() [2/2]

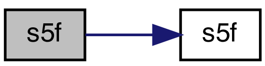
```
sunrealtype s5f (
            sunrealtype * udata ) [inline]
```

Definition at line 229 of file DerivationStencils.h.

```
00229 { return s5f(udata, 6); }
```

References s5f().

Here is the call graph for this function:



6.4.2.45 s6b() [1/2]

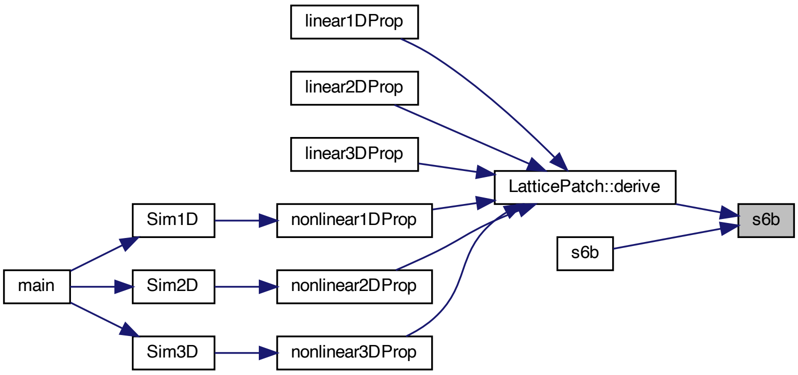
```
sunrealtype s6b (
            const sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 79 of file DerivationStencils.h.

```
00079                                                          {
00080   return 1.0 / 30.0 * udata[-2 * nx] - 2.0 / 5.0 * udata[-1 * nx] -
00081          7.0 / 12.0 * udata[0] + 4.0 / 3.0 * udata[1 * nx] -
00082          1.0 / 2.0 * udata[2 * nx] + 2.0 / 15.0 * udata[3 * nx] -
00083          1.0 / 60.0 * udata[4 * nx];
00084 }
```

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

Here is the caller graph for this function:



6.4.2.46 s6b() [2/2]

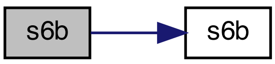
```
sunrealtype s6b (
            sunrealtype * udata ) [inline]
```

Definition at line 233 of file DerivationStencils.h.

```
00233 { return s6b(udata, 6); }
```

References s6b().

Here is the call graph for this function:



6.4.2.47 s6c() [1/2]

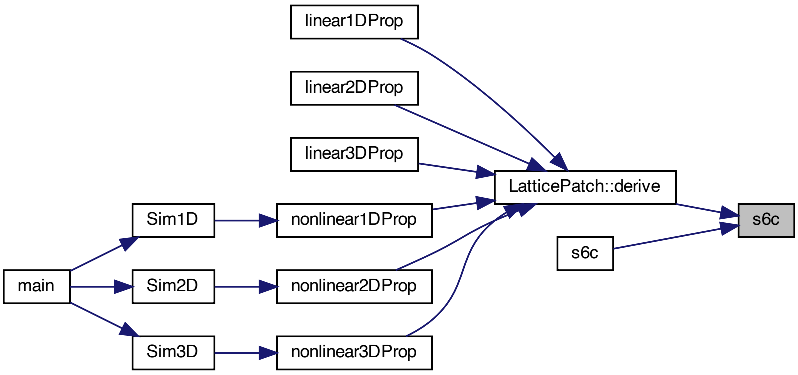
```
sunrealtype s6c (
            const sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 74 of file DerivationStencils.h.

```
00074                                                            {
00075   return -1.0 / 60.0 * udata[-3 * nx] + 3.0 / 20.0 * udata[-2 * nx] -
00076          3.0 / 4.0 * udata[-1 * nx] + 0 + 3.0 / 4.0 * udata[1 * nx] -
00077          3.0 / 20.0 * udata[2 * nx] + 1.0 / 60.0 * udata[3 * nx];
00078 }
```

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

Here is the caller graph for this function:



6.4.2.48 s6c() [2/2]

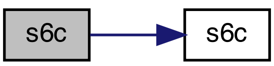
```
sunrealtype s6c (
            sunrealtype * udata ) [inline]
```

Definition at line 232 of file DerivationStencils.h.

```
00232 { return s6c(udata, 6); }
```

References s6c().

Here is the call graph for this function:



6.4.2.49 s6f() [1/2]

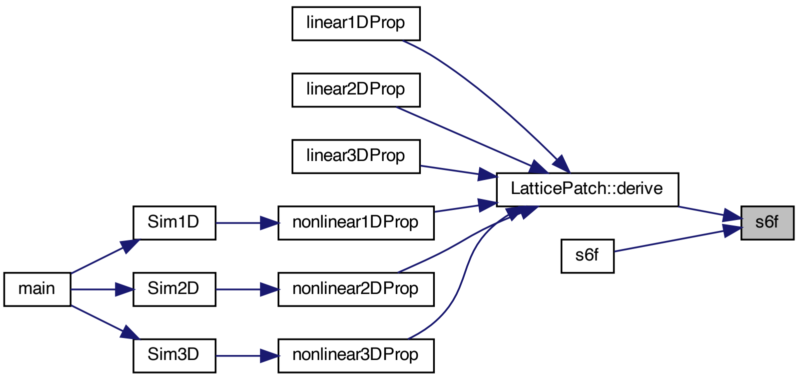
```
sunrealtype s6f (
            const sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 68 of file DerivationStencils.h.

```
00068                                                      {
00069   return 1.0 / 60.0 * udata[-4 * nx] - 2.0 / 15.0 * udata[-3 * nx] +
00070          1.0 / 2.0 * udata[-2 * nx] - 4.0 / 3.0 * udata[-1 * nx] +
00071          7.0 / 12.0 * udata[0] + 2.0 / 5.0 * udata[1 * nx] -
00072          1.0 / 30.0 * udata[2 * nx];
00073 }
```

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

Here is the caller graph for this function:



6.4.2.50 s6f() [2/2]

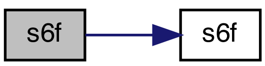
```
sunrealtype s6f (
            sunrealtype * udata ) [inline]
```

Definition at line 231 of file DerivationStencils.h.

```
00231 { return s6f(udata, 6); }
```

References s6f().

Here is the call graph for this function:



6.4.2.51 s7b() [1/2]

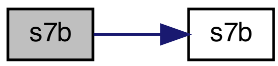
```
sunrealtype s7b (
            sunrealtype * udata )  [inline]
```

Definition at line 235 of file DerivationStencils.h.

```
00235 { return s7b(udata, 6); }
```

References s7b().

Here is the call graph for this function:



6.4.2.52 s7b() [2/2]

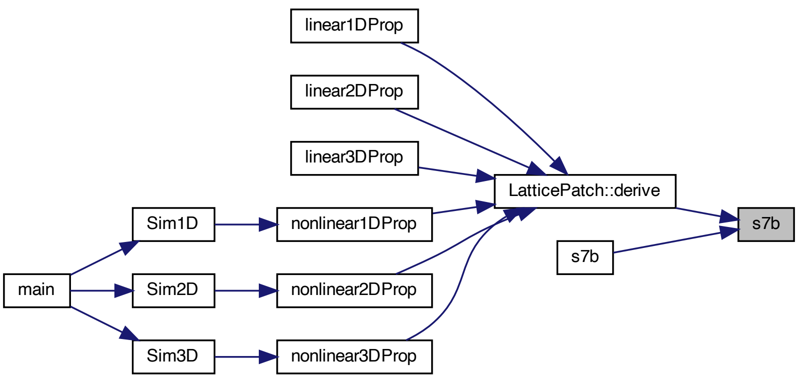
```
sunrealtype s7b (
            sunrealtype * udata,
            int nx )  [inline]
```

Definition at line 91 of file DerivationStencils.h.

```
00091                                            {
00092   return -1.0 / 105.0 * udata[-3 * nx] + 1.0 / 10.0 * udata[-2 * nx] -
00093          3.0 / 5.0 * udata[-1 * nx] - 1.0 / 4.0 * udata[0] + udata[1 * nx] -
00094          3.0 / 10.0 * udata[2 * nx] + 1.0 / 15.0 * udata[3 * nx] -
00095          1.0 / 140.0 * udata[4 * nx];
00096 }
```

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

Here is the caller graph for this function:



6.4.2.53 s7f() [1/2]

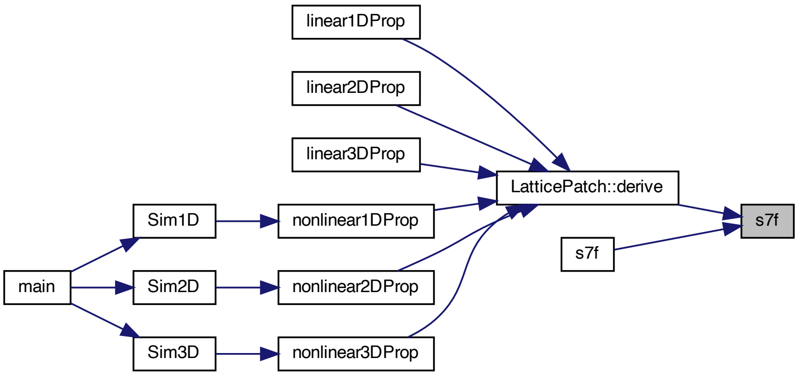
```
sunrealtype s7f (
            const sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 85 of file DerivationStencils.h.

```
                                                        {
  return 1.0 / 140.0 * udata[-4 * nx] - 1.0 / 15.0 * udata[-3 * nx] +
         3.0 / 10.0 * udata[-2 * nx] - 1.0 / 1.0 * udata[-1 * nx] +
         1.0 / 4.0 * udata[0] + 3.0 / 5.0 * udata[1 * nx] -
         1.0 / 10.0 * udata[2 * nx] + 1.0 / 105.0 * udata[3 * nx];
}
```

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

Here is the caller graph for this function:



6.4.2.54 s7f() [2/2]

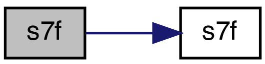
```
sunrealtype s7f (
            sunrealtype * udata ) [inline]
```

Definition at line 234 of file DerivationStencils.h.

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

References s7f().

Here is the call graph for this function:



6.4.2.55 s8b() [1/2]

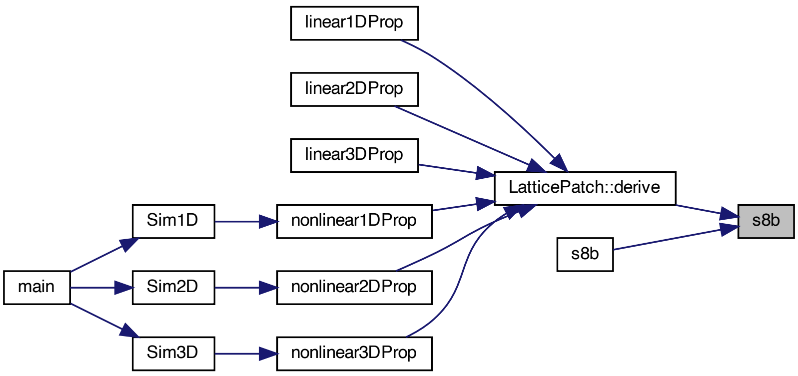
```
sunrealtype s8b (
            const sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 110 of file DerivationStencils.h.

```
00110                                                    {
00111   return -1.0 / 168.0 * udata[-3 * nx] + 1.0 / 14.0 * udata[-2 * nx] -
00112          1.0 / 2.0 * udata[-1 * nx] - 9.0 / 20.0 * udata[0] +
00113          5.0 / 4.0 * udata[1 * nx] - 1.0 / 2.0 * udata[2 * nx] +
00114          1.0 / 6.0 * udata[3 * nx] - 1.0 / 28.0 * udata[4 * nx] +
00115          1.0 / 280.0 * udata[5 * nx];
00116 }
```

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

Here is the caller graph for this function:



6.4.2.56 s8b() [2/2]

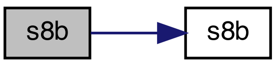
```
sunrealtype s8b (
            sunrealtype * udata ) [inline]
```

Definition at line 238 of file DerivationStencils.h.

```
00238 { return s8b(udata, 6); }
```

References s8b().

Here is the call graph for this function:



6.4.2.57 s8c() [1/2]

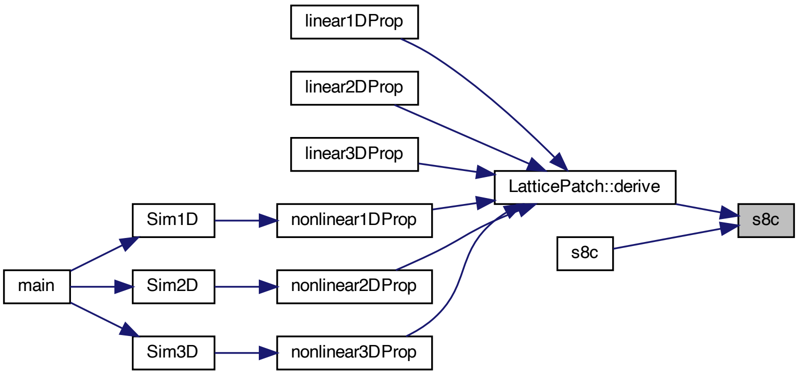
```
sunrealtype s8c (
            const sunrealtype * udata,
            int nx ) [inline]
```

Definition at line 104 of file DerivationStencils.h.

```
00104                                                          {
00105   return 1.0 / 280.0 * udata[-4 * nx] - 4.0 / 105.0 * udata[-3 * nx] +
00106          1.0 / 5.0 * udata[-2 * nx] - 4.0 / 5.0 * udata[-1 * nx] + 0 +
00107          4.0 / 5.0 * udata[1 * nx] - 1.0 / 5.0 * udata[2 * nx] +
00108          4.0 / 105.0 * udata[3 * nx] - 1.0 / 280.0 * udata[4 * nx];
00109 }
```

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

Here is the caller graph for this function:



6.4.2.58 s8c() [2/2]

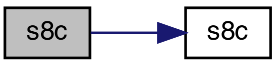
```
sunrealtype s8c (
            sunrealtype * udata ) [inline]
```

Definition at line 237 of file DerivationStencils.h.

```
00237 { return s8c(udata, 6); }
```

References s8c().

Here is the call graph for this function:



6.4.2.59 s8f() [1/2]

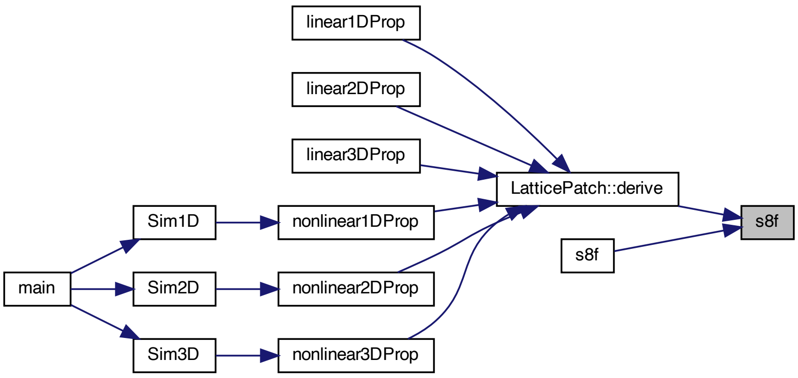
```
sunrealtype s8f (
            const sunrealtype * udata,
            int nx )  [inline]
```

Definition at line 97 of file DerivationStencils.h.

```
00097                                                     {
00098   return -1.0 / 280.0 * udata[-5 * nx] + 1.0 / 28.0 * udata[-4 * nx] -
00099          1.0 / 6.0 * udata[-3 * nx] + 1.0 / 2.0 * udata[-2 * nx] -
00100          5.0 / 4.0 * udata[-1 * nx] + 9.0 / 20.0 * udata[0] +
00101          1.0 / 2.0 * udata[1 * nx] - 1.0 / 14.0 * udata[2 * nx] +
00102          1.0 / 168.0 * udata[3 * nx];
00103 }
```

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

Here is the caller graph for this function:



6.4.2.60 s8f() [2/2]

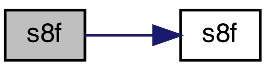
```
sunrealtype s8f (
            sunrealtype * udata )  [inline]
```

Definition at line 236 of file DerivationStencils.h.

```
00236 { return s8f(udata, 6); }
```

References s8f().

Here is the call graph for this function:



6.4.2.61 s9b() [1/2]

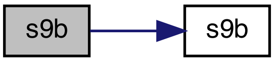
```
sunrealtype s9b (
            sunrealtype * udata )  [inline]
```

Definition at line 240 of file DerivationStencils.h.

```
00240 { return s9b(udata, 6); }
```

References s9b().

Here is the call graph for this function:



6.4.2.62 s9b() [2/2]

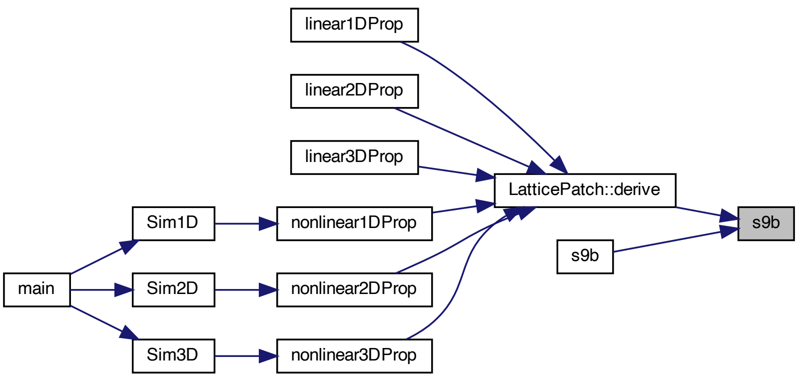
```
sunrealtype s9b (
            sunrealtype * udata,
            int nx )  [inline]
```

Definition at line 124 of file DerivationStencils.h.

```
00124                                                       {
00125   return 1.0 / 504.0 * udata[-4 * nx] - 1.0 / 42.0 * udata[-3 * nx] +
00126          1.0 / 7.0 * udata[-2 * nx] - 2.0 / 3.0 * udata[-1 * nx] -
00127          1.0 / 5.0 * udata[0] + udata[1 * nx] - 1.0 / 3.0 * udata[2 * nx] +
00128          2.0 / 21.0 * udata[3 * nx] - 1.0 / 56.0 * udata[4 * nx] +
00129          1.0 / 630.0 * udata[5 * nx];
00130 }
```

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

Here is the caller graph for this function:



6.4.2.63 s9f() [1/2]

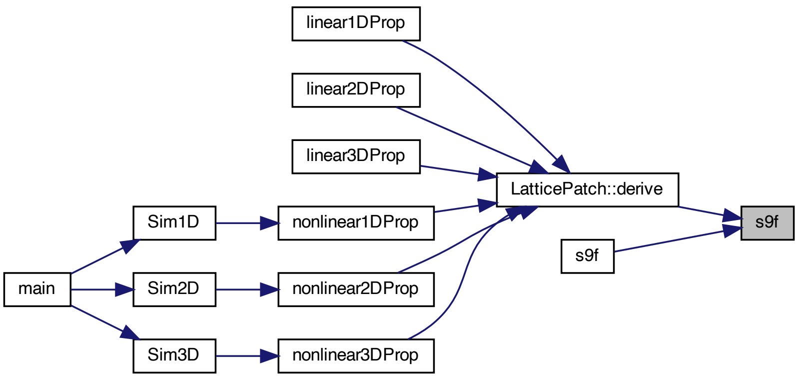
```
sunrealtype s9f (
            const sunrealtype * udata,
            int nx )  [inline]
```

Definition at line 117 of file DerivationStencils.h.

```
00117                                                     {
00118   return -1.0 / 630.0 * udata[-5 * nx] + 1.0 / 56.0 * udata[-4 * nx] -
00119          2.0 / 21.0 * udata[-3 * nx] + 1.0 / 3.0 * udata[-2 * nx] -
00120          1.0 / 1.0 * udata[-1 * nx] + 1.0 / 5.0 * udata[0] +
00121          2.0 / 3.0 * udata[1 * nx] - 1.0 / 7.0 * udata[2 * nx] +
00122          1.0 / 42.0 * udata[3 * nx] - 1.0 / 504.0 * udata[4 * nx];
00123 }
```

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

Here is the caller graph for this function:



6.4.2.64 s9f() [2/2]

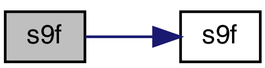
```
sunrealtype s9f (
            sunrealtype * udata )  [inline]
```

Definition at line 239 of file DerivationStencils.h.

```
00239 { return s9f(udata, 6); }
```

References s9f().

Here is the call graph for this function:



6.5 DerivationStencils.h

Go to the documentation of this file.

```
////////////////////////////////////////////////////////////////////
/// @file DerivationStencils.h
/// @brief Definition of derivation stencils from order 1 to 13
////////////////////////////////////////////////////////////////////

// Include Guard
#ifndef DERIVATIONSTENCILS
#define DERIVATIONSTENCILS

#include <sundials/sundials_types.h> /* definition of type sunrealtype */

//////////////////////////////////////////////////////////
// Stencils with variable nx -> data point dimension //
//////////////////////////////////////////////////////////

// Downwind (forward) dfferentiating
inline sunrealtype s1f(sunrealtype *udata, int nx) {
  return -1.0 / 1.0 * udata[-1 * nx] + udata[0];
}
// Upwind (backward) differentiating
inline sunrealtype s1b(sunrealtype *udata, int nx) {
  return -1.0 / 1.0 * udata[0] + udata[1 * nx];
}

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];
}
inline sunrealtype s2c(const sunrealtype *udata, int nx) {
  return -1.0 / 2.0 * udata[-1 * nx] + 0 + 1.0 / 2.0 * udata[1 * nx];
}
inline sunrealtype s2b(const sunrealtype *udata, int nx) {
  return -3.0 / 2.0 * udata[0] + 2.0 / 1.0 * udata[1 * nx] -
         1.0 / 2.0 * udata[2 * nx];
}
inline sunrealtype s3f(const sunrealtype *udata, int nx) {
  return 1.0 / 6.0 * udata[-2 * nx] - 1.0 / 1.0 * udata[-1 * nx] +
         1.0 / 2.0 * udata[0] + 1.0 / 3.0 * udata[1 * nx];
}
inline sunrealtype s3b(sunrealtype *udata, int nx) {
  return -1.0 / 3.0 * udata[-1 * nx] - 1.0 / 2.0 * udata[0] + udata[1 * nx] -
         1.0 / 6.0 * udata[2 * nx];
}
inline sunrealtype s4f(const sunrealtype *udata, int nx) {
  return -1.0 / 12.0 * udata[-3 * nx] + 1.0 / 2.0 * udata[-2 * nx] -
         3.0 / 2.0 * udata[-1 * nx] + 5.0 / 6.0 * udata[0] +
         1.0 / 4.0 * udata[1 * nx];
}
inline sunrealtype s4c(const sunrealtype *udata, int nx) {
  return 1.0 / 12.0 * udata[-2 * nx] - 2.0 / 3.0 * udata[-1 * nx] + 0 +
         2.0 / 3.0 * udata[1 * nx] - 1.0 / 12.0 * udata[2 * nx];
}
inline sunrealtype s4b(const sunrealtype *udata, int nx) {
  return -1.0 / 4.0 * udata[-1 * nx] - 5.0 / 6.0 * udata[0] +
         3.0 / 2.0 * udata[1 * nx] - 1.0 / 2.0 * udata[2 * nx] +
         1.0 / 12.0 * udata[3 * nx];
}
inline sunrealtype s5f(const sunrealtype *udata, int nx) {
  return -1.0 / 30.0 * udata[-3 * nx] + 1.0 / 4.0 * udata[-2 * nx] -
         1.0 / 1.0 * udata[-1 * nx] + 1.0 / 3.0 * udata[0] +
         1.0 / 2.0 * udata[1 * nx] - 1.0 / 20.0 * udata[2 * nx];
}
inline sunrealtype s5b(sunrealtype *udata, int nx) {
  return 1.0 / 20.0 * udata[-2 * nx] - 1.0 / 2.0 * udata[-1 * nx] -
         1.0 / 3.0 * udata[0] + udata[1 * nx] - 1.0 / 4.0 * udata[2 * nx] +
         1.0 / 30.0 * udata[3 * nx];
}
inline sunrealtype s6f(const sunrealtype *udata, int nx) {
  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];
}
inline sunrealtype s6c(const sunrealtype *udata, int nx) {
  return -1.0 / 60.0 * udata[-3 * nx] + 3.0 / 20.0 * udata[-2 * nx] -
         3.0 / 4.0 * udata[-1 * nx] + 0 + 3.0 / 4.0 * udata[1 * nx] -
         3.0 / 20.0 * udata[2 * nx] + 1.0 / 60.0 * udata[3 * nx];
}
inline sunrealtype s6b(const sunrealtype *udata, int nx) {
  return 1.0 / 30.0 * udata[-2 * nx] - 2.0 / 5.0 * udata[-1 * nx] -
         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] -
```

```
        1.0 / 60.0 * udata[4 * nx];
}
inline sunrealtype s7f(const sunrealtype *udata, int nx) {
  return 1.0 / 140.0 * udata[-4 * nx] - 1.0 / 15.0 * udata[-3 * nx] +
         3.0 / 10.0 * udata[-2 * nx] - 1.0 / 1.0 * udata[-1 * nx] +
         1.0 / 4.0 * udata[0] + 3.0 / 5.0 * udata[1 * nx] -
         1.0 / 10.0 * udata[2 * nx] + 1.0 / 105.0 * udata[3 * nx];
}
inline sunrealtype s7b(sunrealtype *udata, int nx) {
  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];
}
inline sunrealtype s8f(const sunrealtype *udata, int nx) {
  return -1.0 / 280.0 * udata[-5 * nx] + 1.0 / 28.0 * udata[-4 * nx] -
         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] +
         1.0 / 168.0 * udata[3 * nx];
}
inline sunrealtype s8c(const sunrealtype *udata, int nx) {
  return 1.0 / 280.0 * udata[-4 * nx] - 4.0 / 105.0 * udata[-3 * nx] +
         1.0 / 5.0 * udata[-2 * nx] - 4.0 / 5.0 * udata[-1 * nx] + 0 +
         4.0 / 5.0 * udata[1 * nx] - 1.0 / 5.0 * udata[2 * nx] +
         4.0 / 105.0 * udata[3 * nx] - 1.0 / 280.0 * udata[4 * nx];
}
inline sunrealtype s8b(const sunrealtype *udata, int nx) {
  return -1.0 / 168.0 * udata[-3 * nx] + 1.0 / 14.0 * udata[-2 * nx] -
         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] +
         1.0 / 280.0 * udata[5 * nx];
}
inline sunrealtype s9f(const sunrealtype *udata, int nx) {
  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] +
         1.0 / 42.0 * udata[3 * nx] - 1.0 / 504.0 * udata[4 * nx];
}
inline sunrealtype s9b(sunrealtype *udata, int nx) {
  return 1.0 / 504.0 * udata[-4 * nx] - 1.0 / 42.0 * udata[-3 * nx] +
         1.0 / 7.0 * udata[-2 * nx] - 2.0 / 3.0 * udata[-1 * nx] -
         1.0 / 5.0 * udata[0] + udata[1 * nx] - 1.0 / 3.0 * udata[2 * nx] +
         2.0 / 21.0 * udata[3 * nx] - 1.0 / 56.0 * udata[4 * nx] +
         1.0 / 630.0 * udata[5 * nx];
}
inline sunrealtype s10f(const sunrealtype *udata, int nx) {
  return 1.0 / 1260.0 * udata[-6 * nx] - 1.0 / 105.0 * udata[-5 * nx] +
         3.0 / 56.0 * udata[-4 * nx] - 4.0 / 21.0 * udata[-3 * nx] +
         1.0 / 2.0 * udata[-2 * nx] - 6.0 / 5.0 * udata[-1 * nx] +
         11.0 / 30.0 * udata[0] + 4.0 / 7.0 * udata[1 * nx] -
         3.0 / 28.0 * udata[2 * nx] + 1.0 / 63.0 * udata[3 * nx] -
         1.0 / 840.0 * udata[4 * nx];
}
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] -
         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];
}
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] -
         11.0 / 30.0 * udata[0] + 6.0 / 5.0 * udata[1 * nx] -
         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] -
         1.0 / 1260.0 * udata[6 * nx];
}
inline sunrealtype s11f(const sunrealtype *udata, int nx) {
  return 1.0 / 2772.0 * udata[-6 * nx] - 1.0 / 210.0 * udata[-5 * nx] +
         5.0 / 168.0 * udata[-4 * nx] - 5.0 / 42.0 * udata[-3 * nx] +
         5.0 / 14.0 * udata[-2 * nx] - 1.0 / 1.0 * udata[-1 * nx] +
         1.0 / 6.0 * udata[0] + 5.0 / 7.0 * udata[1 * nx] -
         5.0 / 28.0 * udata[2 * nx] + 5.0 / 126.0 * udata[3 * nx] -
         1.0 / 168.0 * udata[4 * nx] + 1.0 / 2310.0 * udata[5 * nx];
}
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] -
         5.0 / 168.0 * udata[4 * nx] + 1.0 / 210.0 * udata[5 * nx] -
         1.0 / 2772.0 * udata[6 * nx];
}
```

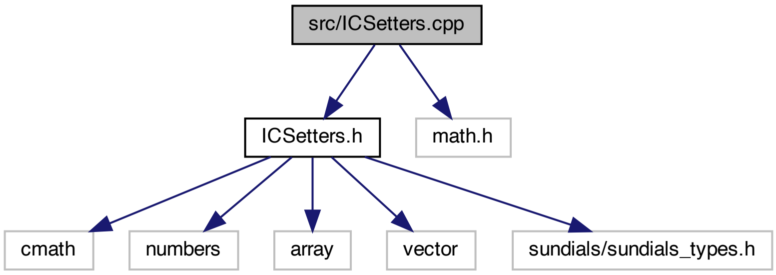
```
inline sunrealtype s12f(const sunrealtype *udata, int nx) {
  return -1.0 / 5544.0 * udata[-7 * nx] + 1.0 / 396.0 * udata[-6 * nx] -
         1.0 / 60.0 * udata[-5 * nx] + 5.0 / 72.0 * udata[-4 * nx] -
         5.0 / 24.0 * udata[-3 * nx] + 1.0 / 2.0 * udata[-2 * nx] -
         7.0 / 6.0 * udata[-1 * 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] +
         1.0 / 3960.0 * udata[5 * nx];
}
inline sunrealtype s12c(const sunrealtype *udata, int nx) {
  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];
}
inline sunrealtype s12b(const sunrealtype *udata, int nx) {
  return -1.0 / 3960.0 * udata[-5 * nx] + 1.0 / 264.0 * udata[-4 * nx] -
         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] +
         7.0 / 6.0 * udata[1 * nx] - 1.0 / 2.0 * udata[2 * nx] +
         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] +
         1.0 / 5544.0 * udata[7 * nx];
}
inline sunrealtype s13f(const sunrealtype *udata, int nx) {
  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] -
         5.0 / 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 / 660.0 * udata[5 * nx] - 1.0 / 10296.0 * udata[6 * nx];
}
inline sunrealtype s13b(sunrealtype *udata, int nx) {
  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] -
         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];
}

///////////////////////////////
// Stencils with nx fixed to 6//
///////////////////////////////

inline sunrealtype s1f(sunrealtype *udata) { return s1f(udata, 6); }
inline sunrealtype s1b(sunrealtype *udata) { return s1b(udata, 6); }
inline sunrealtype s2f(sunrealtype *udata) { return s2f(udata, 6); }
inline sunrealtype s2c(sunrealtype *udata) { return s2c(udata, 6); }
inline sunrealtype s2b(sunrealtype *udata) { return s2b(udata, 6); }
inline sunrealtype s3f(sunrealtype *udata) { return s3f(udata, 6); }
inline sunrealtype s3b(sunrealtype *udata) { return s3b(udata, 6); }
inline sunrealtype s4f(sunrealtype *udata) { return s4f(udata, 6); }
inline sunrealtype s4c(sunrealtype *udata) { return s4c(udata, 6); }
inline sunrealtype s4b(sunrealtype *udata) { return s4b(udata, 6); }
inline sunrealtype s5f(sunrealtype *udata) { return s5f(udata, 6); }
inline sunrealtype s5b(sunrealtype *udata) { return s5b(udata, 6); }
inline sunrealtype s6f(sunrealtype *udata) { return s6f(udata, 6); }
inline sunrealtype s6c(sunrealtype *udata) { return s6c(udata, 6); }
inline sunrealtype s6b(sunrealtype *udata) { return s6b(udata, 6); }
inline sunrealtype s7f(sunrealtype *udata) { return s7f(udata, 6); }
inline sunrealtype s7b(sunrealtype *udata) { return s7b(udata, 6); }
inline sunrealtype s8f(sunrealtype *udata) { return s8f(udata, 6); }
inline sunrealtype s8c(sunrealtype *udata) { return s8c(udata, 6); }
inline sunrealtype s8b(sunrealtype *udata) { return s8b(udata, 6); }
inline sunrealtype s9f(sunrealtype *udata) { return s9f(udata, 6); }
inline sunrealtype s9b(sunrealtype *udata) { return s9b(udata, 6); }
inline sunrealtype s10f(sunrealtype *udata) { return s10f(udata, 6); }
inline sunrealtype s10c(sunrealtype *udata) { return s10c(udata, 6); }
inline sunrealtype s10b(sunrealtype *udata) { return s10b(udata, 6); }
inline sunrealtype s11f(sunrealtype *udata) { return s11f(udata, 6); }
inline sunrealtype s11b(sunrealtype *udata) { return s11b(udata, 6); }
inline sunrealtype s12f(sunrealtype *udata) { return s12f(udata, 6); }
inline sunrealtype s12c(sunrealtype *udata) { return s12c(udata, 6); }
inline sunrealtype s12b(sunrealtype *udata) { return s12b(udata, 6); }
inline sunrealtype s13f(sunrealtype *udata) { return s13f(udata, 6); }
inline sunrealtype s13b(sunrealtype *udata) { return s13b(udata, 6); }

// End of Includeguard
#endif
```

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.

```
////////////////////////////////////////////////////////////////////////////////////////
/// @file ICSetters.cpp
/// @brief Implementation of the plane wave and Gaussian wave packets in 1D, 2D,
/// 3D
////////////////////////////////////////////////////////////////////////////////////////

#include "ICSetters.h"

#include <math.h>

/** PlaneWave1D construction with */
PlaneWave1D::PlaneWave1D(vector<sunrealtype> k, vector<sunrealtype> p,
                         vector<sunrealtype> phi) {
  kx = k[0]; /** - wavevectors \f$ k_x \f$ */
  ky = k[1]; /** - \f$ k_y \f$ */
  kz = k[2]; /** - \f$ k_z \f$ normalized to \f$ 1/\lambda \f$ */
  // 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$ */
  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$ */
}

/** PlaneWave1D implementation in space */
void PlaneWave1D::addToSpace(const sunrealtype x, const sunrealtype y, const sunrealtype z,
                             sunrealtype *pTo6Space) const {
  const sunrealtype wavelength =
      sqrt(kx * kx + ky * ky + kz * kz); /* \f$ 1/\lambda \f$ */
  const sunrealtype kScalarX = (kx * x + ky * y + kz * z) * 2 *
```

```
                              numbers::pi; /* \f$ 2\pi \ \vec{k} \cdot \vec{x} \f$ */
  // Plane wave definition
  const array<sunrealtype, 3> E{{                                   /* E-field vector */
                                px * cos(kScalarX - phix),    /* \f$ E_x \f$ */
                                py * cos(kScalarX - phiy),    /* \f$ E_y \f$ */
                                pz * cos(kScalarX - phiz)}}; /* \f$ E_z \f$ */
  // Put E-field into space
  pTo6Space[0] += E[0];
  pTo6Space[1] += E[1];
  pTo6Space[2] += E[2];
  // 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;
}

/** PlaneWave2D construction with */
PlaneWave2D::PlaneWave2D(vector<sunrealtype> k, vector<sunrealtype> p,
                              vector<sunrealtype> phi) {
  kx = k[0]; /** - wavevectors \f$ k_x \f$ */
  ky = k[1]; /** - \f$ k_y \f$ */
  kz = k[2]; /** - \f$ k_z \f$ normalized to \f$ 1/\lambda \f$*/
  // Amplitude bug: lower by factor 9
  px = p[0] / 9; /** - amplitude (polarization) in x-direction \f$ p_x \f$ */
  py = p[1] / 9; /** - amplitude (polarization) in y-direction \f$ p_y \f$ */
  pz = p[2] / 9; /** - 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$ */
}

/** PlaneWave2D implementation in space */
void PlaneWave2D::addToSpace(const sunrealtype x, const sunrealtype y, const sunrealtype z,
                                  sunrealtype *pTo6Space) const {
  const sunrealtype wavelength =
      sqrt(kx * kx + ky * ky + kz * kz); /* \f$ 1/\lambda \f$ */
  const sunrealtype kScalarX = (kx * x + ky * y + kz * z) * 2 *
                              numbers::pi; /* \f$ 2\pi \ \vec{k} \cdot \vec{x} \f$ */
  // Plane wave definition
  const array<sunrealtype, 3> E{{                                   /* E-field vector */
                                px * cos(kScalarX - phix),    /* \f$ E_x \f$ */
                                py * cos(kScalarX - phiy),    /* \f$ E_y \f$ */
                                pz * cos(kScalarX - phiz)}}; /* \f$ E_z \f$ */
  // Put E-field into space
  pTo6Space[0] += E[0];
  pTo6Space[1] += E[1];
  pTo6Space[2] += E[2];
  // 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;
}

/** PlaneWave3D construction with */
PlaneWave3D::PlaneWave3D(vector<sunrealtype> k, vector<sunrealtype> p,
                              vector<sunrealtype> phi) {
  kx = k[0];     /** - wavevectors \f$ k_x \f$ */
  ky = k[1];     /** - \f$ k_y \f$ */
  kz = k[2];     /** - \f$ k_z \f$ normalized to \f$ 1/\lambda \f$ */
  px = p[0];     /** - amplitude (polarization) in x-direction \f$ p_x \f$ */
  py = p[1];     /** - amplitude (polarization) in y-direction \f$ p_y \f$ */
  pz = p[2];     /** - 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$ */
}

/** PlaneWave3D implementation in space */
void PlaneWave3D::addToSpace(sunrealtype x, sunrealtype y, sunrealtype z,
                                  sunrealtype *pTo6Space) const {
  const sunrealtype wavelength =
      sqrt(kx * kx + ky * ky + kz * kz); /* \f$ 1/\lambda \f$ */
  const sunrealtype kScalarX = (kx * x + ky * y + kz * z) * 2 *
                              numbers::pi; /* \f$ 2\pi \ \vec{k} \cdot \vec{x} \f$ */
  // Plane wave definition
  const array<sunrealtype, 3> E{{/* E-field vector \f$ \vec{E}\f$*/
                                px * cos(kScalarX - phix),    /* \f$ E_x \f$ */
                                py * cos(kScalarX - phiy),    /* \f$ E_y \f$ */
                                pz * cos(kScalarX - phiz)}}; /* \f$ E_z \f$ */
  // Put E-field into space
  pTo6Space[0] += E[0];
  pTo6Space[1] += E[1];
  pTo6Space[2] += E[2];
  // 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;
```

```
}

/** Gauss1D construction with */
Gauss1D::Gauss1D(vector<sunrealtype> k, vector<sunrealtype> p,
                 vector<sunrealtype> xo, sunrealtype phig_,
                 vector<sunrealtype> phi) {
  kx = k[0];     /** - wavevectors \f$ k_x \f$ */
  ky = k[1];     /** - \f$ k_y \f$ */
  kz = k[2];     /** - \f$ k_z \f$ normalized to \f$ 1/\lambda \f$*/
  px = p[0];     /** - amplitude (polarization) in x-direction */
  py = p[1];     /** - amplitude (polarization) in y-direction */
  pz = p[2];     /** - amplitude (polarization) in z-direction */
  phix = phi[0]; /** - phase shift in x-direction */
  phiy = phi[1]; /** - phase shift in y-direction */
  phiz = phi[2]; /** - phase shift in z-direction */
  phig = phig_;  /** - width */
  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*/
}

/** Gauss1D implementation in space */
void Gauss1D::addToSpace(sunrealtype x, sunrealtype y, sunrealtype z,
                         sunrealtype *pTo6Space) const {
  const sunrealtype wavelength =
      sqrt(kx * kx + ky * ky + kz * kz); /* \f$ 1/\lambda \f$ */
  x = x - x0x; /* x-coordinate minus shift from origin */
  y = y - x0y; /* y-coordinate minus shift from origin */
  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$ */
  const sunrealtype envelopeAmp =
      exp(-(x * x + y * y + z * z) / phig / phig); /* enveloping Gauss shape */
  // Gaussian wave definition
  const array<sunrealtype, 3> E{
      {                                           /* E-field vector */
       px * cos(kScalarX - phix) * envelopeAmp,   /* \f$ E_x \f$ */
       py * cos(kScalarX - phiy) * envelopeAmp,   /* \f$ E_y \f$ */
       pz * cos(kScalarX - phiz) * envelopeAmp}}; /* \f$ E_z \f$ */
  // Put E-field into space
  pTo6Space[0] += E[0];
  pTo6Space[1] += E[1];
  pTo6Space[2] += E[2];
  // 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;
}

/** Gauss2D construction with */
Gauss2D::Gauss2D(vector<sunrealtype> dis_, vector<sunrealtype> axis_,
                 sunrealtype Amp_, sunrealtype phip_, sunrealtype w0_,
                 sunrealtype zr_, sunrealtype Ph0_, sunrealtype PhA_) {
  dis = dis_;           /** - center it approaches */
  axis = axis_;         /** - direction form where it comes */
  Amp = Amp_;           /** - amplitude */
  phip = phip_;         /** - polarization rotation from TE-mode */
  w0 = w0_;             /** - taille */
  zr = zr_;             /** - Rayleigh length */
  Ph0 = Ph0_;           /** - beam center */
  PhA = PhA_;           /** - 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
}

void Gauss2D::addToSpace(sunrealtype x, sunrealtype y, sunrealtype z,
                         sunrealtype *pTo6Space) const {
  //\f$ \vec{x} = \vec{x}_0-\vec{dis} \f$ // coordinates minus distance to
  //origin
  x -= dis[0];
  y -= dis[1];
  // z-=dis[2];
  z = NAN;
  //  \f$ z_g = \vec{x}\cdot\vec{e}_g \f$ projection on propagation axis
  const sunrealtype zg =
      x * axis[0] + y * axis[1]; //+z*axis[2];  // =z-z0 -> propagation
                                 //direction, minus origin
  // \f$ r = \sqrt{\vec{x}^2 -z_g^2} \f$ -> pythagoras of radius minus
  // 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$
  const sunrealtype wz = w0 * sqrt(1 + (zg * zg / zr / zr)); // waist at position z
  // \f$ g(z) = atan(z_g/z_r) \f$
  const sunrealtype gz = atan(zg / zr); // Gouy phase
  // \f$ R(z) = z_g*(1+(z_r/z_g)^2) \f$
```

```
  sunrealtype Rz = NAN; // beam curvature
  if (zg != 0)
    Rz = zg * (1 + (zr * zr / zg / zg));
  else
    Rz = 1e308;
  // wavenumber \f$ k = 2\pi/\lambda \f$
  const sunrealtype k = 2 * numbers::pi / lambda;
  // \f$ \Phi_F = kr^2/(2*R(z))+g(z)-kz_g \f$
  const sunrealtype PhF =
      -k * r * r / (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$ -
  // CVode is a diva, no chance to remove the square in the second exponential
  // -> h too small
  const sunrealtype G2D = sqrt(w0 / wz) * exp(-r * r / wz / wz) *
                          exp(-(zg - Ph0) * (zg - Ph0) / PhA / PhA) *
                          cos(PhF); // gauss shape
  // \f$ c_\alpha =\vec{e}_x\cdot\vec{axis} \f$
  // projection components; do like this for CVode convergence -> otherwise
  // results in machine error values for non-existant field components if
  // axis[0] and axis[1] are given
  const sunrealtype ca =
      axis[0]; // x-component of propagation axis which is given as parameter
  const sunrealtype sa = sqrt(1 - ca * ca); // no z-component for 2D propagation
  // E-field to space: polarization in xy-plane (A2) is projection of
  // z-polarization (A1) on x- and y-directions
  pTo6Space[0] += sa * (G2D * A2);
  pTo6Space[1] += -ca * (G2D * A2);
  pTo6Space[2] += G2D * A1;
  // B-field -> negative derivative wrt polarization shift of E-field
  pTo6Space[3] += -sa * (G2D * A1);
  pTo6Space[4] += ca * (G2D * A1);
  pTo6Space[5] += G2D * A2;
}

/** Gauss3D construction with */
Gauss3D::Gauss3D(vector<sunrealtype> dis_, vector<sunrealtype> axis_,
                 sunrealtype Amp_,
                 // vector<sunrealtype> pol_,
                 sunrealtype phip_, sunrealtype w0_, sunrealtype zr_,
                 sunrealtype Ph0_, sunrealtype PhA_) {
  dis = dis_;   /** - center it approaches */
  axis = axis_; /** - direction from where it comes */
  Amp = Amp_;   /** - amplitude */
  // pol=pol_;
  phip = phip_; /** - polarization rotation form TE-mode */
  w0 = w0_;     /** - taille */
  zr = zr_;     /** - Rayleigh length */
  Ph0 = Ph0_;   /** - beam center */
  PhA = PhA_;   /** - beam length */
  lambda = numbers::pi * w0 * w0 / zr;
  A1 = Amp * cos(phip);
  A2 = Amp * sin(phip);
}

/** Gauss3D implementation in space */
void Gauss3D::addToSpace(sunrealtype x, sunrealtype y, sunrealtype z,
                         sunrealtype *pTo6Space) const {
  x -= dis[0];
  y -= dis[1];
  z -= dis[2];
  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));
  const sunrealtype gz = atan(zg / zr);
  sunrealtype Rz = NAN;
  if (zg != 0)
    Rz = zg * (1 + (zr * zr / zg / zg));
  else
    Rz = 1e308;
  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);
  const sunrealtype ca = axis[0];
  const sunrealtype sa = sqrt(1 - ca * ca);
  pTo6Space[0] += sa * (G3D * A2);
  pTo6Space[1] += -ca * (G3D * A2);
  pTo6Space[2] += G3D * A1;
  pTo6Space[3] += -sa * (G3D * A1);
  pTo6Space[4] += ca * (G3D * A1);
  pTo6Space[5] += G3D * A2;
}

/** Evaluate lattice point values to zero and add field values */
void ICSetter::eval(sunrealtype x, sunrealtype y, sunrealtype z,
                    sunrealtype *pTo6Space) {
  pTo6Space[0] = 0;
```

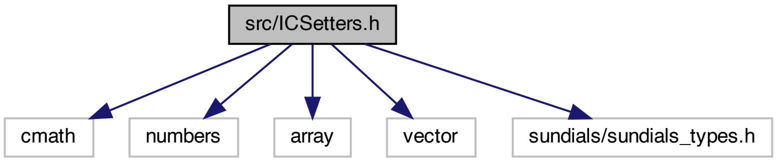
```
  pTo6Space[1] = 0;
  pTo6Space[2] = 0;
  pTo6Space[3] = 0;
  pTo6Space[4] = 0;
  pTo6Space[5] = 0;
  add(x, y, z, pTo6Space);
}

/** Add all initial field values to the lattice space */
void ICSetter::add(sunrealtype x, sunrealtype y, sunrealtype z,
                   sunrealtype *pTo6Space) {
  for (const auto wave : planeWaves1D)
    wave.addToSpace(x, y, z, pTo6Space);
  for (const auto wave : planeWaves2D)
    wave.addToSpace(x, y, z, pTo6Space);
  for (const auto wave : planeWaves3D)
    wave.addToSpace(x, y, z, pTo6Space);
  for (const auto wave : gauss1Ds)
    wave.addToSpace(x, y, z, pTo6Space);
  for (const auto wave : gauss2Ds)
    wave.addToSpace(x, y, z, pTo6Space);
  for (const auto wave : gauss3Ds)
    wave.addToSpace(x, y, z, pTo6Space);
}

/** Add plane waves in 1D to their container vector */
void ICSetter::addPlaneWave1D(vector<sunrealtype> k, vector<sunrealtype> p,
                              vector<sunrealtype> phi) {
  planeWaves1D.emplace_back(PlaneWave1D(k, p, phi));
}

/** Add plane waves in 2D to their container vector */
void ICSetter::addPlaneWave2D(vector<sunrealtype> k, vector<sunrealtype> p,
                              vector<sunrealtype> phi) {
  planeWaves2D.emplace_back(PlaneWave2D(k, p, phi));
}

/** Add plane waves in 3D to their container vector */
void ICSetter::addPlaneWave3D(vector<sunrealtype> k, vector<sunrealtype> p,
                              vector<sunrealtype> phi) {
  planeWaves3D.emplace_back(PlaneWave3D(k, p, phi));
}

/** Add Gaussian waves in 1D to their container vector */
void ICSetter::addGauss1D(vector<sunrealtype> k, vector<sunrealtype> p,
                          vector<sunrealtype> xo, sunrealtype phig_,
                          vector<sunrealtype> phi) {
  gauss1Ds.emplace_back(Gauss1D(k, p, xo, phig_, phi));
}

/** Add Gaussian waves in 2D to their container vector */
void ICSetter::addGauss2D(vector<sunrealtype> dis_, vector<sunrealtype> axis_,
                          sunrealtype Amp_, sunrealtype phip_, sunrealtype w0_,
                          sunrealtype zr_, sunrealtype Ph0_, sunrealtype PhA_) {
  gauss2Ds.emplace_back(
      Gauss2D(dis_, axis_, Amp_, phip_, w0_, zr_, Ph0_, PhA_));
}

/** Add Gaussian waves in 3D to their container vector */
void ICSetter::addGauss3D(vector<sunrealtype> dis_, vector<sunrealtype> axis_,
                          sunrealtype Amp_, sunrealtype phip_, sunrealtype w0_,
                          sunrealtype zr_, sunrealtype Ph0_, sunrealtype PhA_) {
  gauss3Ds.emplace_back(
      Gauss3D(dis_, axis_, Amp_, phip_, w0_, zr_, Ph0_, PhA_));
}
```

6.8 src/ICSetters.h File Reference

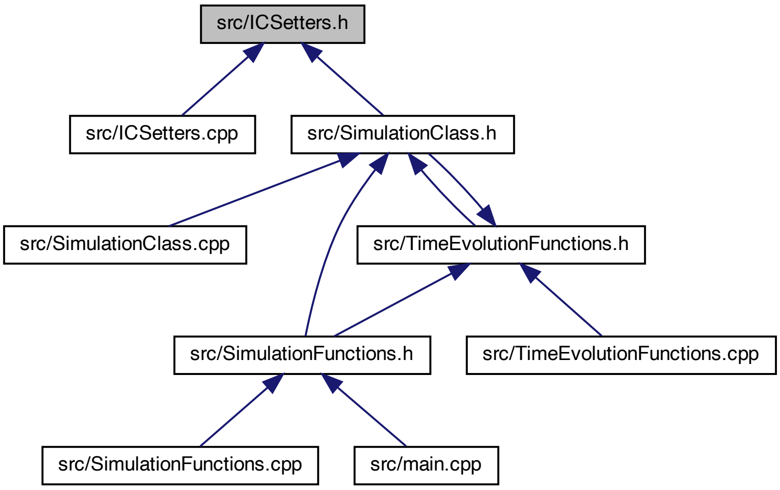
Declaration of the plane wave and Gaussian wave packets in 1D, 2D, 3D.

```
#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.

```
////////////////////////////////////////////////////////////////////////////////////////
/// @file ICSetters.h
/// @brief Declaration of the plane wave and Gaussian wave packets in 1D, 2D, 3D
////////////////////////////////////////////////////////////////////////////////////////

// Include Guard
#ifndef ICSETTERS
#define ICSETTERS

// math, constants, vector, and array
#include <cmath>
//#include <mathimf.h>
#include <numbers>
#include <array>
#include <vector>

#include <sundials/sundials_types.h> /* definition of type sunrealtype */

using namespace std;

/** @brief super-class for plane waves
 *
 * They are given in the form \f$ \vec{E} = \vec{E}_0 \ \cos \left( \vec{k}
 * \cdot \vec{x} - \vec{\phi} \right) \f$ */
class PlaneWave {
protected:
  /// wavenumber \f$ k_x \f$
  sunrealtype kx;
  /// wavenumber \f$ k_y \f$
  sunrealtype ky;
  /// wavenumber \f$ k_z \f$
  sunrealtype kz;
  /// polarization & amplitude in x-direction, \f$ p_x \f$
  sunrealtype px;
  /// polarization & amplitude in y-direction, \f$ p_y \f$
  sunrealtype py;
  /// polarization & amplitude in z-direction, \f$ p_z \f$
  sunrealtype pz;
  /// phase shift in x-direction, \f$ \phi_x \f$
  sunrealtype phix;
  /// phase shift in y-direction, \f$ \phi_y \f$
  sunrealtype phiy;
  /// phase shift in z-direction, \f$ \phi_z \f$
  sunrealtype phiz;
};

/** @brief class for plane waves in 1D */
class PlaneWave1D : public PlaneWave {
public:
  /// construction with default parameters
  PlaneWave1D(vector<sunrealtype> k = {1, 0, 0},
              vector<sunrealtype> p = {0, 0, 1},
              vector<sunrealtype> phi = {0, 0, 0});
  /// function for the actual implementation in the lattice
  void addToSpace(sunrealtype x, sunrealtype y, sunrealtype z,
                  sunrealtype *pTo6Space) const;
};

/** @brief class for plane waves in 2D */
class PlaneWave2D : public PlaneWave {
public:
  /// construction with default parameters
  PlaneWave2D(vector<sunrealtype> k = {1, 0, 0},
              vector<sunrealtype> p = {0, 0, 1},
              vector<sunrealtype> phi = {0, 0, 0});
  /// function for the actual implementation in the lattice
  void addToSpace(sunrealtype x, sunrealtype y, sunrealtype z,
                  sunrealtype *pTo6Space) const;
};
```

```
/** @brief class for plane waves in 3D */
class PlaneWave3D : public PlaneWave {
public:
  /// construction with default parameters
  PlaneWave3D(vector<sunrealtype> k = {1, 0, 0},
              vector<sunrealtype> p = {0, 0, 1},
              vector<sunrealtype> phi = {0, 0, 0});
  /// function for the actual implementation in space
  void addToSpace(sunrealtype x, sunrealtype y, sunrealtype z,
                  sunrealtype *pTo6Space) const;
};

/** @brief class for Gaussian waves in 1D
 *
 * They are given in the form \f$ \vec{E}=\vec{p} \, \exp \left(
 * -(\vec{x}-\vec{x}_0)^2 / \Phi_g^2 \right) \, \cos(\vec{k} \cdot \vec{x}) \f$
 */
class Gauss1D {
private:
  /// wavenumber \f$ k_x \f$
  sunrealtype kx;
  /// wavenumber \f$ k_y \f$
  sunrealtype ky;
  /// wavenumber \f$ k_z \f$
  sunrealtype kz;
  /// polarization & amplitude in x-direction, \f$ p_x \f$
  sunrealtype px;
  /// polarization & amplitude in y-direction, \f$ p_y \f$
  sunrealtype py;
  /// polarization & amplitude in z-direction, \f$ p_z \f$
  sunrealtype pz;
  /// phase shift in x-direction, \f$ \phi_x \f$
  sunrealtype phix;
  /// phase shift in y-direction, \f$ \phi_y \f$
  sunrealtype phiy;
  /// phase shift in z-direction, \f$ \phi_z \f$
  sunrealtype phiz;
  /// center of pulse in x-direction, \f$ x_0 \f$
  sunrealtype x0x;
  /// center of pulse in y-direction, \f$ y_0 \f$
  sunrealtype x0y;
  /// center of pulse in z-direction, \f$ z_0 \f$
  sunrealtype x0z;
  /// pulse width \f$ \Phi_g \f$
  sunrealtype phig;

public:
  /// construction with default parameters
  Gauss1D(vector<sunrealtype> k = {1, 0, 0}, vector<sunrealtype> p = {0, 0, 1},
          vector<sunrealtype> xo = {0, 0, 0}, sunrealtype phig_ = 1.01,
          vector<sunrealtype> phi = {0, 0, 0});
  /// function for the actual implementation in space
  void addToSpace(sunrealtype x, sunrealtype y, sunrealtype z,
                  sunrealtype *pTo6Space) const;

public:
};

/** @brief class for Gaussian waves in 2D
 *
 * They are given in the form
 * \f$ \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)  \f$ with
 * - propagation direction (subtracted distance to origin) \f$ z_g \f$
 * - radial distance to propagation axis \f$ r = \sqrt{\vec{x}^2 -z_g^2} \f$
 * - \f$ k = 2\pi / \lambda \f$
 * - waist at position z, \f$ \omega(z) = w_0 \, \sqrt{1+(z_g/z_R)^2} \f$
 * - Gouy phase \f$ g(z) = \tan^{-1}(z_g/z_r) \f$
 * - beam curvature \f$ R(z) = z_g \, (1+(z_r/z_g)^2) \f$
 * obtained via the chosen parameters */
class Gauss2D {
private:
  /// distance maximum to origin
  vector<sunrealtype> dis;
  /// normalized propagation axis
  vector<sunrealtype> axis;
  /// amplitude \f$ A\f$
  sunrealtype Amp;
  /// polarization rotation from TE-mode around propagation direction
  // that determines \f$ \vec{\epsilon}\f$ above
  sunrealtype phip;
  /// taille \f$ \omega_0 \f$
  sunrealtype w0;
  /// Rayleigh length \f$ z_R = \pi \omega_0^2 / \lambda \f$
  sunrealtype zr;
```

```
  /// center of beam \f$ \Phi_0 \f$
  sunrealtype Ph0;
  /// length of beam \f$ \Phi_A \f$
  sunrealtype PhA;
  /// amplitude projection on TE-mode
  sunrealtype A1;
  /// amplitude projection on xy-plane
  sunrealtype A2;
  /// wavelength \f$ \lambda \f$
  sunrealtype lambda;

public:
  /// construction with default parameters
  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);
  /// function for the actual implementation in space
  void addToSpace(sunrealtype x, sunrealtype y, sunrealtype z,
                  sunrealtype *pTo6Space) const;

public:
};

/** @brief class for Gaussian waves in 3D
 *
 * They are given in the form
 * \f$ \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)  \f$ with
 * - propagation direction (subtracted distance to origin) \f$ z_g \f$
 * - radial distance to propagation axis \f$ r = \sqrt{\vec{x}^2 -z_g^2} \f$
 * - \f$ k = 2\pi / \lambda \f$
 * - waist at position z, \f$ \omega(z) = w_0 \, \sqrt{1+(z_g/z_R)^2} \f$
 * - Gouy phase \f$ g(z) = \tan^{-1}(z_g/z_r) \f$
 * - beam curvature \f$ R(z) = z_g \, (1+(z_r/z_g)^2) \f$
 * obtained via the chosen parameters */
class Gauss3D {
private:
  /// distance maximum to origin
  vector<sunrealtype> dis;
  /// normalized propagation axis
  vector<sunrealtype> axis;
  /// amplitude \f$ A\f$
  sunrealtype Amp;
  /// polarization rotation from TE-mode around propagation direction
  // that determines \f$ \vec{\epsilon}\f$ above
  sunrealtype phip;
  // polarization
  // vector<sunrealtype> pol;
  /// taille \f$ \omega_0 \f$
  sunrealtype w0;
  /// Rayleigh length \f$ z_R = \pi \omega_0^2 / \lambda \f$
  sunrealtype zr;
  /// center of beam \f$ \Phi_0 \f$
  sunrealtype Ph0;
  /// length of beam \f$ \Phi_A \f$
  sunrealtype PhA;
  /// amplitude projection on TE-mode (z-axis)
  sunrealtype A1;
  /// amplitude projection on xy-plane
  sunrealtype A2;
  /// wavelength \f$ \lambda \f$
  sunrealtype lambda;

public:
  /// construction with default parameters
  Gauss3D(vector<sunrealtype> dis_ = {0, 0, 0},
          vector<sunrealtype> axis_ = {1, 0, 0}, sunrealtype Amp_ = 1.0l,
          sunrealtype phip_ = 0,
          // sunrealtype pol_={0,0,1},
          sunrealtype w0_ = 1e-5, sunrealtype zr_ = 4e-5,
          sunrealtype Ph0_ = 2e-5, sunrealtype PhA_ = 0.45e-5);
  /// function for the actual implementation in space
  void addToSpace(sunrealtype x, sunrealtype y, sunrealtype z,
                  sunrealtype *pTo6Space) const;

public:
};

/** @brief ICSetter class to initialize wave types with default parameters */
class ICSetter {
private:
  /// container vector for plane waves in 1D
  vector<PlaneWave1D> planeWaves1D;
  /// container vector for plane waves in 2D
  vector<PlaneWave2D> planeWaves2D;
```

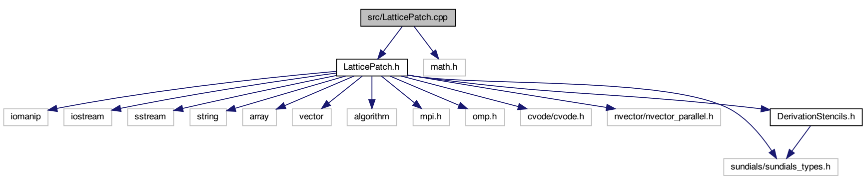
```
  /// container vector for plane waves in 3D
  vector<PlaneWave3D> planeWaves3D;
  /// container vector for Gaussian waves in 1D
  vector<Gauss1D> gauss1Ds;
  /// container vector for Gaussian waves in 2D
  vector<Gauss2D> gauss2Ds;
  /// container vector for Gaussian waves in 3D
  vector<Gauss3D> gauss3Ds;

public:
  /// function to set all coordinates to zero and then `add` the field values
  void eval(sunrealtype x, sunrealtype y, sunrealtype z,
            sunrealtype *pTo6Space);
  /// function to fill the lattice space with initial field values
  // of all field vector containers
  void add(sunrealtype x, sunrealtype y, sunrealtype z, sunrealtype *pTo6Space);
  /// function to add plane waves in 1D to their container vector
  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 2D 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 3D 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 Gaussian waves in 1D 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_ = 1.01,
                  vector<sunrealtype> phi = {0, 0, 0});
  /// function to add Gaussian waves in 2D to their container vector
  void 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 3D to their container vector
  void 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);
};

// End of Includeguard
#endif
```

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()

```
int check_retval (
            void * returnvalue,
            const char * funcname,
            int opt,
            int id )
```

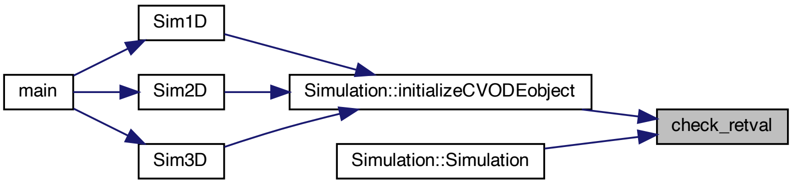
Check function return value. From CVode examples. opt == 0 means SUNDIALS function allocates memory so check if returned NULL pointer opt == 1 means SUNDIALS function returns an integer value so check if retval $<$ 0 opt == 2 means function allocates memory so check if returned NULL pointer

Definition at line 841 of file LatticePatch.cpp.

```
00841                                                                                 {
00842   int *retval = nullptr;
00843
00844   /* Check if SUNDIALS function returned NULL pointer - no memory allocated */
00845   if (opt == 0 && returnvalue == nullptr) {
00846     fprintf(stderr,
00847             "\nSUNDIALS_ERROR(%d): %s() failed - returned NULL pointer\n\n", id,
00848             funcname);
00849     return (1);
00850   }
00851
00852   /* Check if retval < 0 */
00853   else if (opt == 1) {
00854     retval = (int *)returnvalue;
00855     if (*retval < 0) {
00856       fprintf(stderr, "\nSUNDIALS_ERROR(%d): %s() failed with retval = %d\n\n",
00857               id, funcname, *retval);
00858       return (1);
00859     }
00860   }
00861
00862   /* Check if function returned NULL pointer - no memory allocated */
00863   else if (opt == 2 && returnvalue == nullptr) {
00864     fprintf(stderr,
00865             "\nMEMORY_ERROR(%d): %s() failed - returned NULL pointer\n\n", id,
00866             funcname);
00867     return (1);
00868   }
00869
00870   return (0);
00871 }
```

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

Here is the caller graph for this function:



6.10.2.2 errorKill()

```
void errorKill (
            const string & errorMessage )
```

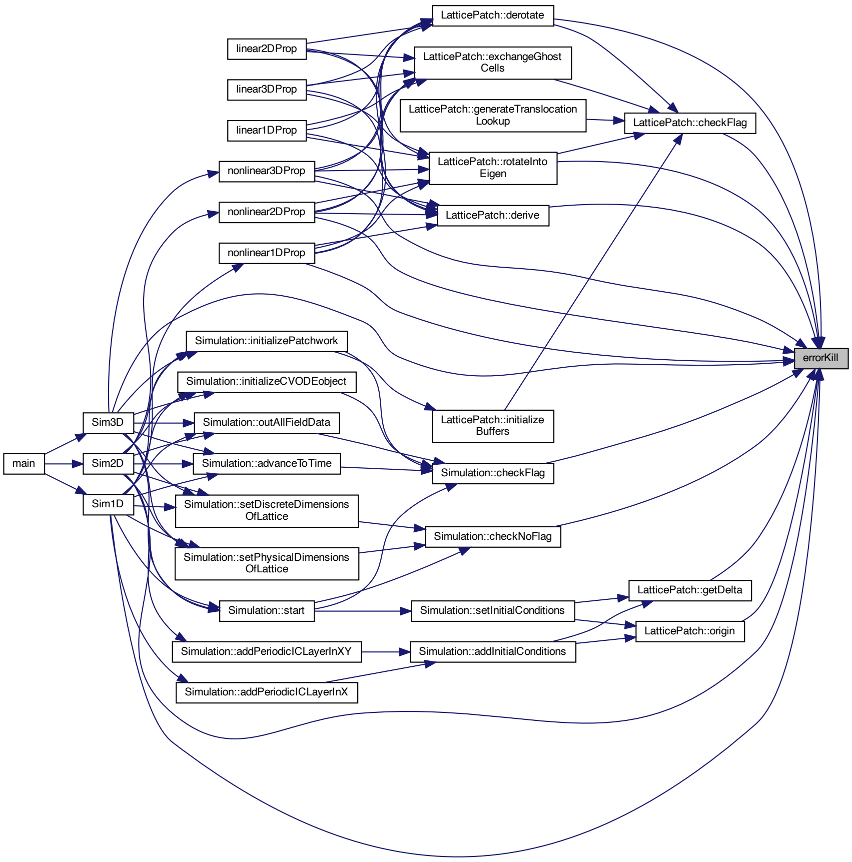
Print a specific error message to stdout.

Definition at line 828 of file LatticePatch.cpp.

```
00828                                      {
00829   cerr « endl « "Error: " « errorMessage « " Aborting..." « endl;
00830   MPI_Abort(MPI_COMM_WORLD, 1);
00831   return;
00832 }
```

Referenced by LatticePatch::checkFlag(), Simulation::checkFlag(), Simulation::checkNoFlag(), LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::getDelta(), nonlinear1DProp(), nonlinear2DProp(), nonlinear3DProp(), LatticePatch::origin(), LatticePatch::rotateIntoEigen(), Sim1D(), Sim2D(), and Sim3D().

Here is the caller graph for this function:



6.10.2.3 generatePatchwork()

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

Set up the patchwork.

friend function for creating the patchwork slicing of the overall lattice

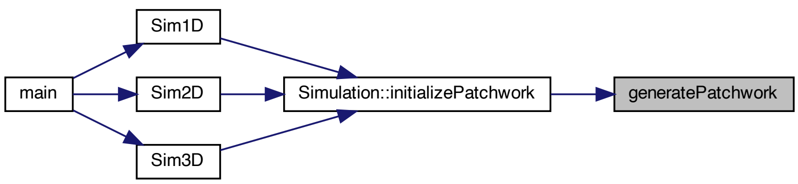
Definition at line 109 of file LatticePatch.cpp.

```
00110                                                                      {
00111   // Retrieve the ghost layer 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
00116   const int my_prc = envelopeLattice.my_prc;
00117   // Determine thicknes of the slice
00118   const sunindextype tot_NOXP = envelopeLattice.get_tot_nx(); // total points of lattice
00119   const sunindextype tot_NOYP = envelopeLattice.get_tot_ny();
```

```
    const sunindextype tot_NOZP = envelopeLattice.get_tot_nz();
    // position of the patch in the lattice of patches - process associated to
    // position
    const sunindextype LIx = my_prc % DLx;
    const sunindextype LIy = (my_prc / DLx) % DLy;
    const sunindextype LIz = (my_prc / DLx) / DLy;
    // Determine the number of points in the patch and first absolute points in
    // each dimension
    const sunindextype local_NOXP = tot_NOXP / DLx;
    const sunindextype local_NOYP = tot_NOYP / DLy;
    const sunindextype local_NOZP = tot_NOZP / DLz;
    // absolute positions of the first point in each dimension
    const sunindextype firstXPoint = local_NOXP * LIx;
    const sunindextype firstYPoint = local_NOYP * LIy;
    const sunindextype firstZPoint = local_NOZP * LIz;
    // total number of points in the patch
    const sunindextype local_NODP = dPD * local_NOXP * local_NOYP * local_NOZP;

    // Set patch up with above derived quantities
    patchToMold.dx = envelopeLattice.get_dx();
    patchToMold.dy = envelopeLattice.get_dy();
    patchToMold.dz = envelopeLattice.get_dz();
    patchToMold.x0 = firstXPoint * patchToMold.dx;
    patchToMold.y0 = firstYPoint * patchToMold.dy;
    patchToMold.z0 = firstZPoint * patchToMold.dz;
    patchToMold.LIx = LIx;
    patchToMold.LIy = LIy;
    patchToMold.LIz = LIz;
    patchToMold.nx = local_NOXP;
    patchToMold.ny = local_NOYP;
    patchToMold.nz = local_NOZP;
    patchToMold.lx = patchToMold.nx * patchToMold.dx;
    patchToMold.ly = patchToMold.ny * patchToMold.dy;
    patchToMold.lz = patchToMold.nz * patchToMold.dz;
    /* Create and allocate memory for parallel vectors with defined local and
     * global lenghts *
     * (-> CVode problem sizes Nlocal and N)
     * for field data and temporal derivatives and set extra pointers to them */
    patchToMold.u =
        N_VNew_Parallel(envelopeLattice.comm, local_NODP,
                        envelopeLattice.get_tot_noDP(), envelopeLattice.sunctx);
    patchToMold.uData = NV_DATA_P(patchToMold.u);
    patchToMold.du =
        N_VNew_Parallel(envelopeLattice.comm, local_NODP,
                        envelopeLattice.get_tot_noDP(), envelopeLattice.sunctx);
    patchToMold.duData = NV_DATA_P(patchToMold.du);
    // 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;
    const int s_min = min(s1, min(s2, s3));
    patchToMold.uAux.resize(s1 * s2 * s3 / s_min * (s_min + 2 * gLW) * dPD);
    patchToMold.uAuxData = &patchToMold.uAux[0];
    patchToMold.envelopeLattice = &envelopeLattice;
    // Set patch "name" to process number -> only for debugging
    // patchToMold.ID=my_prc;
    // set flag
    patchToMold.statusFlags = FLatticePatchSetUp;
    patchToMold.generateTranslocationLookup();
    return 0;
}
```

Referenced by Simulation::initializePatchwork().

Here is the caller graph for this function:



6.11 LatticePatch.cpp

Go to the documentation of this file.

```
////////////////////////////////////////////////////////////////////////////////
/// @file LatticePatch.cpp
/// @brief Costruction of the overall envelope lattice and the lattice patches
////////////////////////////////////////////////////////////////////////////////

#include "LatticePatch.h"

#include <math.h>

////////////////////////////////////////////////////////
//// Implementation of Lattice component functions ////
////////////////////////////////////////////////////////

/// Initialize the cartesian communicator
void Lattice::initializeCommunicator(const int nx, const int ny,
        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),
                    static_cast<int>(per)};
  // Create the cartesian communicator for MPI_COMM_WORLD
  MPI_Cart_create(MPI_COMM_WORLD, 3, dims, periods, 1, &comm);
  // Set MPI variables of the lattice
  MPI_Comm_size(comm, &(n_prc));
  MPI_Comm_rank(comm, &(my_prc));
  // Associate name to the communicator to identify it -> for debugging and
  // nicer error messages
  constexpr char lattice_comm_name[] = "Lattice";
  MPI_Comm_set_name(comm, lattice_comm_name);

  // Test if process naming is the same for both communicators
  /*
  int MYPRC;
  MPI_Comm_rank(MPI_COMM_WORLD,&MYPRC);
  cout«"\r"«my_prc«"\t"«MYPRC«endl;
  */
}

/// Construct the lattice and set the stencil order
Lattice::Lattice(const int StO) : stencilOrder(StO),
    ghostLayerWidth(StO/2+1) {
  statusFlags = 0;
}

/// Set the number of points in each dimension of the lattice
void Lattice::setDiscreteDimensions(const sunindextype _nx,
        const sunindextype _ny, const sunindextype _nz) {
  // copy the given data for number of points
  tot_nx = _nx;
  tot_ny = _ny;
  tot_nz = _nz;
  // compute the resulting number of points and datapoints
  tot_noP = tot_nx * tot_ny * tot_nz;
  tot_noDP = dataPointDimension * tot_noP;
  // compute the new Delta, the physical resolution
  dx = tot_lx / tot_nx;
  dy = tot_ly / tot_ny;
  dz = tot_lz / tot_nz;
}

/// Set the physical size of the lattice
void Lattice::setPhysicalDimensions(const sunrealtype _lx,
        const sunrealtype _ly, const sunrealtype _lz) {
  tot_lx = _lx;
  tot_ly = _ly;
  tot_lz = _lz;
  // calculate physical distance between points
  dx = tot_lx / tot_nx;
  dy = tot_ly / tot_ny;
  dz = tot_lz / tot_nz;
  statusFlags |= FLatticeDimensionSet;
}

/////////////////////////////////////////////////////////////
//// Implementation of LatticePatch component functions ////
/////////////////////////////////////////////////////////////

/// Construct the lattice patch
LatticePatch::LatticePatch() {
  // set default origin coordinates to (0,0,0)
  x0 = y0 = z0 = 0;
  // set default position in Lattice-Patchwork to (0,0,0)
  LIx = LIy = LIz = 0;
```

```
  // set default physical lentgth for lattice patch to (0,0,0)
  lx = ly = lz = 0;
  // set default discrete length for lattice patch to (0,1,1)
  /* This is done in this manner as even in 1D simulations require a 1 point
   * width */
  nx = 0;
  ny = nz = 1;

  // u is not initialized as it wouldn't make any sense before the dimensions
  // are set idem for the enveloping lattice

  // set default statusFlags to non set
  statusFlags = 0;
}

/// Destruct the patch and thereby destroy the NVectors
LatticePatch::~LatticePatch() {
  // Deallocate memory for solution vector
  if (statusFlags & FLatticePatchSetUp) {
    // Destroy data vectors
    N_VDestroy_Parallel(u);
    N_VDestroy_Parallel(du);
  }
}

/// Set up the patchwork
int generatePatchwork(const Lattice &envelopeLattice, LatticePatch &patchToMold,
                      const int DLx, const int DLy, const int DLz) {
  // Retrieve the ghost layer depth
  const int gLW = envelopeLattice.get_ghostLayerWidth();
  // Retrieve the data point dimension
  const int dPD = envelopeLattice.get_dataPointDimension();
  // MPI process/patch
  const int my_prc = envelopeLattice.my_prc;
  // Determine thicknes of the slice
  const sunindextype tot_NOXP = envelopeLattice.get_tot_nx(); // total points of lattice
  const sunindextype tot_NOYP = envelopeLattice.get_tot_ny();
  const sunindextype tot_NOZP = envelopeLattice.get_tot_nz();
  // position of the patch in the lattice of patches - process associated to
  // position
  const sunindextype LIx = my_prc % DLx;
  const sunindextype LIy = (my_prc / DLx) % DLy;
  const sunindextype LIz = (my_prc / DLx) / DLy;
  // Determine the number of points in the patch and first absolute points in
  // each dimension
  const sunindextype local_NOXP = tot_NOXP / DLx;
  const sunindextype local_NOYP = tot_NOYP / DLy;
  const sunindextype local_NOZP = tot_NOZP / DLz;
  // absolute positions of the first point in each dimension
  const sunindextype firstXPoint = local_NOXP * LIx;
  const sunindextype firstYPoint = local_NOYP * LIy;
  const sunindextype firstZPoint = local_NOZP * LIz;
  // total number of points in the patch
  const sunindextype local_NODP = dPD * local_NOXP * local_NOYP * local_NOZP;

  // Set patch up with above derived quantities
  patchToMold.dx = envelopeLattice.get_dx();
  patchToMold.dy = envelopeLattice.get_dy();
  patchToMold.dz = envelopeLattice.get_dz();
  patchToMold.x0 = firstXPoint * patchToMold.dx;
  patchToMold.y0 = firstYPoint * patchToMold.dy;
  patchToMold.z0 = firstZPoint * patchToMold.dz;
  patchToMold.LIx = LIx;
  patchToMold.LIy = LIy;
  patchToMold.LIz = LIz;
  patchToMold.nx = local_NOXP;
  patchToMold.ny = local_NOYP;
  patchToMold.nz = local_NOZP;
  patchToMold.lx = patchToMold.nx * patchToMold.dx;
  patchToMold.ly = patchToMold.ny * patchToMold.dy;
  patchToMold.lz = patchToMold.nz * patchToMold.dz;
  /* Create and allocate memory for parallel vectors with defined local and
   * global lenghts *
   * (-> CVode problem sizes Nlocal and N)
   * for field data and temporal derivatives and set extra pointers to them */
  patchToMold.u =
      N_VNew_Parallel(envelopeLattice.comm, local_NODP,
                      envelopeLattice.get_tot_noDP(), envelopeLattice.sunctx);
  patchToMold.uData = NV_DATA_P(patchToMold.u);
  patchToMold.du =
      N_VNew_Parallel(envelopeLattice.comm, local_NODP,
                      envelopeLattice.get_tot_noDP(), envelopeLattice.sunctx);
  patchToMold.duData = NV_DATA_P(patchToMold.du);
  // 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;
  const int s_min = min(s1, min(s2, s3));
```

```
  patchToMold.uAux.resize(s1 * s2 * s3 / s_min * (s_min + 2 * gLW) * dPD);
  patchToMold.uAuxData = &patchToMold.uAux[0];
  patchToMold.envelopeLattice = &envelopeLattice;
  // Set patch "name" to process number -> only for debugging
  // patchToMold.ID=my_prc;
  // set flag
  patchToMold.statusFlags = FLatticePatchSetUp;
  patchToMold.generateTranslocationLookup();
  return 0;
}

/// Return the discrete size of the patch: number of lattice patch points in
/// specified dimension
int LatticePatch::discreteSize(int dir) const {
  switch (dir) {
  case 0:
    return nx * ny * nz;
  case 1:
    return nx;
  case 2:
    return ny;
  case 3:
    return nz;
  // case 4: return uAux.size(); // for debugging
  default:
    return -1;
  }
}

/// Return the physical origin of the patch in a dimension
sunrealtype LatticePatch::origin(const int dir) const {
  switch (dir) {
  case 1:
    return x0;
  case 2:
    return y0;
  case 3:
    return z0;
  default:
    errorKill("LatticePatch::origin function called with wrong dir parameter");
    return -1;
  }
}

/// Return the distance between points in the patch in a dimension
sunrealtype LatticePatch::getDelta(const int dir) const {
  switch (dir) {
  case 1:
    return dx;
  case 2:
    return dy;
  case 3:
    return dz;
  default:
    errorKill(
        "LatticePatch::getDelta function called with wrong dir parameter");
    return -1;
  }
}

/** 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 */
void LatticePatch::generateTranslocationLookup() {
  // Check that the lattice has been set up
  checkFlag(FLatticeDimensionSet);
  // lenghts for auxilliary layers, including ghost layers
  const int gLW = envelopeLattice->get_ghostLayerWidth();
  const int mx = nx + 2 * gLW;
  const int my = ny + 2 * gLW;
  const int mz = nz + 2 * gLW;
  // sizes for lookup vectors
  // generate u->uAux
  uTox.resize(nx * ny * nz);
  uToy.resize(nx * ny * nz);
  uToz.resize(nx * ny * nz);
  // generate uAux->u with length including halo
  xTou.resize(mx * ny * nz);
  yTou.resize(nx * my * nz);
  zTou.resize(nx * ny * mz);
  // variables for cartesian position in the 3D discrete lattice
  int px = 0, py = 0, pz = 0;
  for (int i = 0; i < uToy.size(); i++) { // loop over all points in the patch
    // 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)
    uTox[i] = (px + gLW) + py * mx +
              pz * mx * ny; // unroll (de-flatten) cartesian dimension
    xTou[px + py * mx + pz * mx * ny] =
        i; // match cartesian point to u location
    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;
  }
  // same for ghost layer lookup tables
  lgcTox.resize(gLW * ny * nz);
  rgcTox.resize(gLW * ny * nz);
  for (int i = 0; i < lgcTox.size(); i++) {
    px = i % gLW;
    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;
  }
  lgcToy.resize(gLW * nx * nz);
  rgcToy.resize(gLW * nx * nz);
  for (int i = 0; i < lgcToy.size(); i++) {
    px = i % nx;
    py = (i / nx) % gLW;
    pz = (i / nx) / gLW;
    lgcToy[i] = py + pz * my + px * my * nz;
    rgcToy[i] = py + ny + gLW + pz * my + px * my * nz;
  }
  lgcToz.resize(gLW * nx * ny);
  rgcToz.resize(gLW * nx * ny);
  for (int i = 0; i < lgcToz.size(); i++) {
    px = i % nx;
    py = (i / nx) % ny;
    pz = (i / nx) / ny;
    lgcToz[i] = pz + px * mz + py * mz * nx;
    rgcToz[i] = pz + nz + gLW + px * mz + py * mz * nx;
  }
  statusFlags |= TranslocationLookupSetUp;
}

/** Rotate into eigenraum along R matrices of paper using below rotation
 * functions
 * -> uAuxData gets the rotated left-halo-, inner-patch-, right-halo-data */
void LatticePatch::rotateIntoEigen(const int dir) {
  // Check that the lattice, ghost layers as well as the translocation lookups
  // have been set up;
  checkFlag(FLatticePatchSetUp);
  checkFlag(TranslocationLookupSetUp);
  checkFlag(GhostLayersInitialized); // this check is only after call to
                                     // exchange ghost cells
  switch (dir) {
  case 1:
    rotateToX(uAuxData, gCLData, lgcTox);
    rotateToX(uAuxData, uData, uTox);
    rotateToX(uAuxData, gCRData, rgcTox);
    break;
  case 2:
    rotateToY(uAuxData, gCLData, lgcToy);
    rotateToY(uAuxData, uData, uToy);
    rotateToY(uAuxData, gCRData, rgcToy);
    break;
  case 3:
    rotateToZ(uAuxData, gCLData, lgcToz);
    rotateToZ(uAuxData, uData, uToz);
    rotateToZ(uAuxData, gCRData, rgcToz);
    break;
  default:
    errorKill("Tried to rotate into the wrong direction");
    break;
  }
}

/// Rotate halo and inner-patch data vectors with rotation matrix Rx into
/// eigenspace of Z matrix and write to auxiliary vector
inline void LatticePatch::rotateToX(sunrealtype *outArray,
                                    const sunrealtype *inArray,
                                    const vector<int> &lookup) {
  int ii = 0, target = 0;
#pragma ivdep
#pragma omp simd // safelen(6)
  for (int i = 0; i < lookup.size(); i++) {
    // get correct u-vector and spatial indices along previously defined lookup
    // tables
    target = envelopeLattice->get_dataPointDimension() * lookup[i];
    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];
    outArray[target + 3] = -inArray[2 + ii] + inArray[4 + ii];
    outArray[target + 4] = inArray[3 + ii];
    outArray[target + 5] = inArray[ii];
  }
}

/// Rotate halo and inner-patch data vectors with rotation matrix Ry into
/// eigenspace of Z matrix and write to auxiliary vector
inline void LatticePatch::rotateToY(sunrealtype *outArray,
                                    const sunrealtype *inArray,
                                    const vector<int> &lookup) {
  int ii = 0, target = 0;
#pragma ivdep
#pragma omp simd
  for (int i = 0; i < lookup.size(); i++) {
    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];
    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];
  }
}

/// Rotate halo and inner-patch data vectors with rotation matrix Rz into
/// eigenspace of Z matrix and write to auxiliary vector
inline void LatticePatch::rotateToZ(sunrealtype *outArray,
                                    const sunrealtype *inArray,
                                    const vector<int> &lookup) {
  int ii = 0, target = 0;
#pragma ivdep
#pragma omp simd
  for (int i = 0; i < lookup.size(); i++) {
    target = envelopeLattice->get_dataPointDimension() * lookup[i];
    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];
    outArray[target + 5] = inArray[2 + ii];
  }
}

/// Derotate uAux with transposed rotation matrices and write to derivative
/// buffer - normalization is done here by the factor 1/2
void LatticePatch::derotate(int dir, sunrealtype *buffOut) {
  // Check that the lattice as well as the translocation lookups have been set
  // up;
  checkFlag(FLatticePatchSetUp);
  checkFlag(TranslocationLookupSetUp);
  const int dPD = envelopeLattice->get_dataPointDimension();
  const int gLW = envelopeLattice->get_ghostLayerWidth();
  const int uSize = discreteSize();
  int ii = 0, target = 0;
  switch (dir) {
  case 1:
#pragma ivdep
#pragma omp simd
    for (int i = 0; i < uSize; i++) {
      // get correct indices in u and rotation space
      target = dPD * i;
      ii = dPD * (uTox[i] - 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.;
      buffOut[target + 5] = (uAux[ii] + uAux[2 + ii]) / 2.;
    }
    break;
  case 2:
#pragma omp simd
    for (int i = 0; i < uSize; i++) {
      target = dPD * i;
      ii = dPD * (uToy[i] - gLW);
      buffOut[target + 0] = (uAux[ii] - uAux[2 + ii]) / 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];
      buffOut[target + 5] = (uAux[ii] + uAux[2 + ii]) / 2.;
    }
```

```
    break;
  case 3:
#pragma omp simd
    for (int i = 0; i < uSize; i++) {
      target = dPD * i;
      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];
      buffOut[target + 3] = (uAux[1 + ii] + uAux[3 + ii]) / 2.;
      buffOut[target + 4] = (uAux[ii] + uAux[2 + ii]) / 2.;
      buffOut[target + 5] = uAux[4 + ii];
    }
    break;
  default:
    errorKill("Tried to derotate from the wrong direction");
    break;
  }
}

/// Create buffers to save derivative values, optimizing computational load
void LatticePatch::initializeBuffers() {
  // Check that the lattice has been set up
  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);
  // Set pointers used for propagation functions
  buffData[0] = &buffX[0];
  buffData[1] = &buffY[0];
  buffData[2] = &buffZ[0];
  statusFlags |= BuffersInitialized;
}

/// Perform the ghost cell exchange in a specified direction
void LatticePatch::exchangeGhostCells(const int dir) {
  // Check that the lattice has been set up
  checkFlag(FLatticeDimensionSet);
  checkFlag(FLatticePatchSetUp);
  // 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();
  // In the chosen direction m is set to ghost layer width while the others
  // remain to form the plane
  switch (dir) {
  case 1:
    mx = gLW;
    my = ny;
    mz = nz;
    distToRight = (nx - gLW);
    break;
  case 2:
    mx = nx;
    my = gLW;
    mz = nz;
    distToRight = nx * (ny - gLW);
    break;
  case 3:
    mx = nx;
    my = ny;
    mz = gLW;
    distToRight = nx * ny * (nz - gLW);
    break;
  }
  // total number of exchanged points
  const int dPD = envelopeLattice->get_dataPointDimension();
  const int exchangeSize = mx * my * mz * dPD;
  // provide size of the halos for ghost cells
  ghostCellLeft.resize(exchangeSize);
  ghostCellRight.resize(ghostCellLeft.size());
  ghostCellLeftToSend.resize(ghostCellLeft.size());
  ghostCellRightToSend.resize(ghostCellLeft.size());
  gCLData = &ghostCellLeft[0];
  gCRData = &ghostCellRight[0];
  statusFlags |= GhostLayersInitialized;

  // Initialize running index li for the halo buffers, and index ui of uData for
  // data transfer
  int li = 0, ui = 0;

  for (int iz = 0; iz < mz; iz++) {
    for (int iy = 0; iy < my; iy++) {
      // uData vector start index of halo data to be transferred
      // 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) * dPD;
      // copy left halo data from uData to buffer, transfer size is given by
      // x-length (not x-range) perhaps faster but more fragile C lib copy
      // operation (contained in cstring header)
      /*
      memcpy(&ghostCellLeftToSend[li],
             &uData[ui],
             sizeof(sunrealtype)*mx*dPD);
      // increase ui by the distance to vis-a-vis boundary and copy right halo
      data to buffer ui+=distToRight*dPD; memcpy(&ghostCellRightToSend[li],
             &uData[ui],
             sizeof(sunrealtype)*mx*dPD);
      */
      // 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;
      copy(&uData[ui], &uData[ui + mx * dPD], &ghostCellRightToSend[li]);

      // increase halo index by transferred items per y-iteration step
      // (x-length)
      li += mx * dPD;
    }
  }

  /* Send and receive the data to and from neighboring latticePatches */
  // Adjust direction to cartesian communicator
  int dim = 2; // default for dir==1
  if (dir == 2) {
    dim = 1;
  } else if (dir == 3) {
    dim = 0;
  }
  MPI_Request requests[2];
  int rank_source = 0, rank_dest = 0;
  MPI_Cart_shift(envelopeLattice->comm, dim, -1, &rank_source,
                 &rank_dest); // s.t. rank_dest is left & v.v.

  // nonblocking Isend/Irecv
  /*
  MPI_Isend(&ghostCellLeftToSend[0], exchangeSize, MPI_SUNREALTYPE, rank_dest,
  1, envelopeLattice->comm, &requests[0]); MPI_Irecv(&ghostCellRight[0],
  exchangeSize, MPI_SUNREALTYPE, rank_source, 1, envelopeLattice->comm,
  &requests[0]); MPI_Isend(&ghostCellRightToSend[0], exchangeSize,
  MPI_SUNREALTYPE, rank_source, 2, envelopeLattice->comm, &requests[1]);
  MPI_Irecv(&ghostCellLeft[0], exchangeSize, MPI_SUNREALTYPE, rank_dest, 2,
  envelopeLattice->comm, &requests[1]);

  MPI_Waitall(2, requests, MPI_STATUS_IGNORE);
  */

  // blocking Sendrecv:

  MPI_Sendrecv(&ghostCellLeftToSend[0], exchangeSize, MPI_SUNREALTYPE,
               rank_dest, 1, &ghostCellRight[0], exchangeSize, MPI_SUNREALTYPE,
               rank_source, 1, envelopeLattice->comm, MPI_STATUS_IGNORE);
  MPI_Sendrecv(&ghostCellRightToSend[0], exchangeSize, MPI_SUNREALTYPE,
               rank_source, 2, &ghostCellLeft[0], exchangeSize, MPI_SUNREALTYPE,
               rank_dest, 2, envelopeLattice->comm, MPI_STATUS_IGNORE);
}

/// Check if all flags are set
void LatticePatch::checkFlag(unsigned int flag) const {
  if (!(statusFlags & flag)) {
    string errorMessage;
    switch (flag) {
    case FLatticePatchSetUp:
      errorMessage = "The Lattice patch was not set up please make sure to "
                     "initilize a Lattice topology";
      break;
    case TranslocationLookupSetUp:
      errorMessage = "The translocation lookup tables have not been generated, "
                     "please be sure to run generateTranslocationLookup()";
      break;
    case GhostLayersInitialized:
      errorMessage = "The space for the ghost layers has not been allocated, "
                     "please be sure to run initializeGhostLayer()";
      break;
    case BuffersInitialized:
      errorMessage = "The space for the buffers has not been allocated, please "
                     "be sure to run initializeBuffers()";
      break;
    default:
      errorMessage = "Uppss, you've made a non-standard error, sadly I can't "
                     "help you there";
      break;
    }
```

```
    errorKill(errorMessage);
  }
  return;
}

/// Calculate derivatives in the patch (uAux) in the specified direction
void LatticePatch::derive(const int dir) {
  // ghost layer width
  const int gLW = envelopeLattice->get_ghostLayerWidth();
  // dimensionality of data points -> 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;
  // width of patch only in given direction
  const int dirWidthO = discreteSize(dir);
  // size of plane perpendicular to given dimension
  const int perpPlainSize = discreteSize() / discreteSize(dir);
  // physical distance between points in that direction
  sunrealtype dxi = NAN;
  switch (dir) {
  case 1:
    dxi = dx;
    break;
  case 2:
    dxi = dy;
    break;
  case 3:
    dxi = dz;
    break;
  default:
    dxi = 1;
    errorKill("Tried to derive in the wrong direction");
    break;
  }
  // Derive according to chosen stencil accuracy order (which determines also
  // gLW)
  const int order = envelopeLattice->get_stencilOrder();
  switch (order) {
  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] = s1b(&uAux[j + 0]) / dxi;
        uAux[j + 1 - gLW * dPD] = s1b(&uAux[j + 1]) / dxi;
        uAux[j + 2 - gLW * dPD] = s1f(&uAux[j + 2]) / dxi;
        uAux[j + 3 - gLW * dPD] = s1f(&uAux[j + 3]) / dxi;
        uAux[j + 4 - gLW * dPD] = s1f(&uAux[j + 4]) / dxi;
        uAux[j + 5 - gLW * dPD] = s1f(&uAux[j + 5]) / dxi;
      }
    }
    break;
  case 2:
    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] = s2b(&uAux[j + 0]) / dxi;
        uAux[j + 1 - gLW * dPD] = s2b(&uAux[j + 1]) / dxi;
        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;
        uAux[j + 5 - gLW * dPD] = s2c(&uAux[j + 5]) / dxi;
      }
    }
    break;
  case 3:
    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] = s3b(&uAux[j + 0]) / dxi;
        uAux[j + 1 - gLW * dPD] = s3b(&uAux[j + 1]) / dxi;
        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 + 5]) / dxi;
      }
    }
    break;
  case 4:
    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] = s4b(&uAux[j + 0]) / dxi;
        uAux[j + 1 - gLW * dPD] = s4b(&uAux[j + 1]) / dxi;
        uAux[j + 2 - gLW * dPD] = s4f(&uAux[j + 2]) / dxi;
        uAux[j + 3 - gLW * dPD] = s4f(&uAux[j + 3]) / dxi;
        uAux[j + 4 - gLW * dPD] = s4c(&uAux[j + 4]) / dxi;
        uAux[j + 5 - gLW * dPD] = s4c(&uAux[j + 5]) / dxi;
```

```
      }
    }
    break;
  case 5:
    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] = s5b(&uAux[j + 0]) / dxi;
        uAux[j + 1 - gLW * dPD] = s5b(&uAux[j + 1]) / dxi;
        uAux[j + 2 - gLW * dPD] = s5f(&uAux[j + 2]) / dxi;
        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;
      }
    }
    break;
  case 6:
    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] = s6b(&uAux[j + 0]) / dxi;
        uAux[j + 1 - gLW * dPD] = s6b(&uAux[j + 1]) / dxi;
        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;
        uAux[j + 5 - gLW * dPD] = s6c(&uAux[j + 5]) / dxi;
      }
    }
    break;
  case 7:
    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] = s7b(&uAux[j + 0]) / dxi;
        uAux[j + 1 - gLW * dPD] = s7b(&uAux[j + 1]) / dxi;
        uAux[j + 2 - gLW * dPD] = s7f(&uAux[j + 2]) / dxi;
        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;
      }
    }
    break;
  case 8:
    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] = 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;
        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 + 5]) / dxi;
      }
    }
    break;
  case 9:
    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] = s9b(&uAux[j + 0]) / dxi;
        uAux[j + 1 - gLW * dPD] = s9b(&uAux[j + 1]) / dxi;
        uAux[j + 2 - gLW * dPD] = s9f(&uAux[j + 2]) / dxi;
        uAux[j + 3 - gLW * dPD] = s9f(&uAux[j + 3]) / dxi;
        uAux[j + 4 - gLW * dPD] = s9f(&uAux[j + 4]) / dxi;
        uAux[j + 5 - gLW * dPD] = s9f(&uAux[j + 5]) / dxi;
      }
    }
    break;
  case 10:
    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] = s10b(&uAux[j + 0]) / dxi;
        uAux[j + 1 - gLW * dPD] = s10b(&uAux[j + 1]) / dxi;
        uAux[j + 2 - gLW * dPD] = s10f(&uAux[j + 2]) / dxi;
        uAux[j + 3 - gLW * dPD] = s10f(&uAux[j + 3]) / dxi;
        uAux[j + 4 - gLW * dPD] = s10c(&uAux[j + 4]) / dxi;
        uAux[j + 5 - gLW * dPD] = s10c(&uAux[j + 5]) / dxi;
      }
    }
    break;
  case 11:
    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] = s11b(&uAux[j + 0]) / dxi;
        uAux[j + 1 - gLW * dPD] = s11b(&uAux[j + 1]) / dxi;
```

```
        uAux[j + 2 - gLW * dPD] = s11f(&uAux[j + 2]) / dxi;
        uAux[j + 3 - gLW * dPD] = s11f(&uAux[j + 3]) / dxi;
        uAux[j + 4 - gLW * dPD] = s11f(&uAux[j + 4]) / dxi;
        uAux[j + 5 - gLW * dPD] = s11f(&uAux[j + 5]) / dxi;
      }
    }
    break;
  case 12:
    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] = s12b(&uAux[j + 0]) / dxi;
        uAux[j + 1 - gLW * dPD] = s12b(&uAux[j + 1]) / dxi;
        uAux[j + 2 - gLW * dPD] = s12f(&uAux[j + 2]) / dxi;
        uAux[j + 3 - gLW * dPD] = s12f(&uAux[j + 3]) / dxi;
        uAux[j + 4 - gLW * dPD] = s12c(&uAux[j + 4]) / dxi;
        uAux[j + 5 - gLW * dPD] = s12c(&uAux[j + 5]) / dxi;
      }
    }
    break;
  case 13:
    // Iterate through all points in the plane perpendicular to the given
    // direction
    for (int i = 0; i < perpPlainSize; i++) {
      // 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) {
        /* Compute the stencil derivative for any of the six field components
         * with a ghostlayer width adjusted to the order of the finite
         * difference scheme */
        uAux[j + 0 - gLW * dPD] = s13b(&uAux[j + 0]) / dxi;
        uAux[j + 1 - gLW * dPD] = s13b(&uAux[j + 1]) / dxi;
        uAux[j + 2 - gLW * dPD] = s13f(&uAux[j + 2]) / dxi;
        uAux[j + 3 - gLW * dPD] = s13f(&uAux[j + 3]) / dxi;
        uAux[j + 4 - gLW * dPD] = s13f(&uAux[j + 4]) / dxi;
        uAux[j + 5 - gLW * dPD] = s13f(&uAux[j + 5]) / dxi;
      }
    }
    break;

  default:
    errorKill("Please set an existing stencil order");
    break;
  }
}

///////// Helper functions /////////

/// Print a specific error message to stdout
void errorKill(const string & errorMessage) {
  cerr « endl « "Error: " « errorMessage « " Aborting..." « endl;
  MPI_Abort(MPI_COMM_WORLD, 1);
  return;
}

/** 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 */
int check_retval(void *returnvalue, const char *funcname, int opt, int id) {
  int *retval = nullptr;

  /* Check if SUNDIALS function returned NULL pointer - no memory allocated */
  if (opt == 0 && returnvalue == nullptr) {
    fprintf(stderr,
            "\nSUNDIALS_ERROR(%d): %s() failed - returned NULL pointer\n\n", id,
            funcname);
    return (1);
  }

  /* Check if retval < 0 */
  else if (opt == 1) {
    retval = (int *)returnvalue;
    if (*retval < 0) {
      fprintf(stderr, "\nSUNDIALS_ERROR(%d): %s() failed with retval = %d\n\n",
              id, funcname, *retval);
      return (1);
    }
  }

  /* Check if function returned NULL pointer - no memory allocated */
  else if (opt == 2 && returnvalue == nullptr) {
    fprintf(stderr,
            "\nMEMORY_ERROR(%d): %s() failed - returned NULL pointer\n\n", id,
```

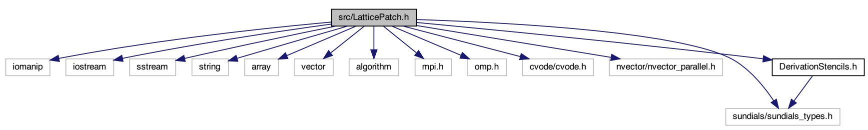
```
                funcname);
       return (1);
   }

   return (0);
}
```

6.12 src/LatticePatch.h File Reference

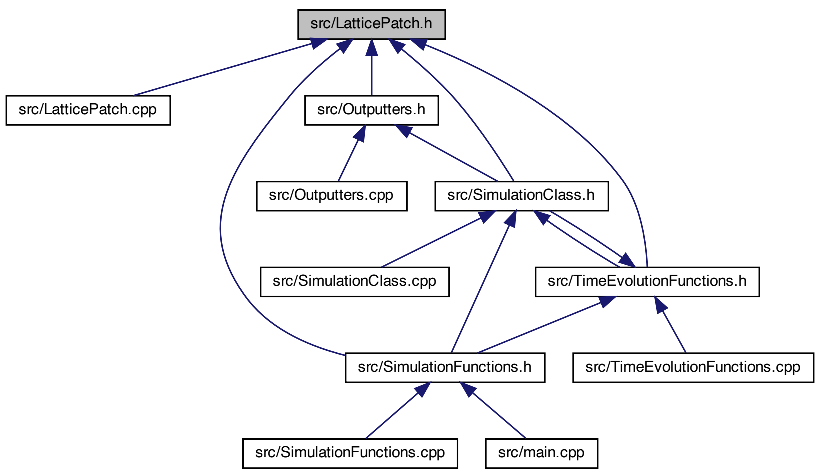
Declaration of the lattice and lattice patches.

```
#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 "DerivationStencils.h"
```

Include dependency graph for LatticePatch.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 37 of file LatticePatch.h.

```
00037                    {
00038     FLatticeDimensionSet = 0x01,  // 1
00039     /*OPT_B = 0x02,  // 2
00040     OPT_C = 0x04,  // 4
00041     OPT_D = 0x08,  // 8
00042     OPT_E = 0x10,  // 16
00043     OPT_F = 0x20,*/  // 32
00044 };
```

6.12.2.2 LatticePatchOptions

```
enum LatticePatchOptions
```

lattice patch construction checking flags

Enumerator

FLatticePatchSetUp	
TranslocationLookupSetUp	
GhostLayersInitialized	
BuffersInitialized	

Definition at line 127 of file LatticePatch.h.

```
00127                               {
00128   FLatticePatchSetUp = 0x01,
00129   TranslocationLookupSetUp = 0x02,
00130   GhostLayersInitialized = 0x04,
00131   BuffersInitialized = 0x08
00132   /*OPT_D = 0x08,
00133   OPT_E = 0x10,
00134   OPT_F = 0x20,*/
00135 };
```

6.12.3 Function Documentation

6.12.3.1 check_retval()

```
int check_retval (
            void * returnvalue,
            const char * funcname,
            int opt,
            int id )
```

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

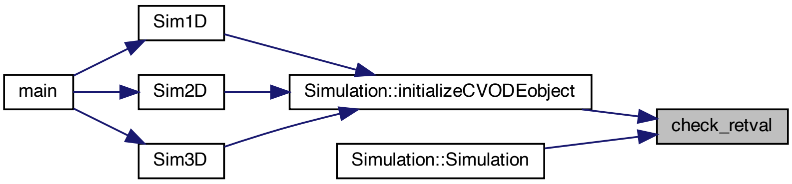
Definition at line 841 of file LatticePatch.cpp.

```
00841                                                                              {
00842   int *retval = nullptr;
00843 
00844   /* Check if SUNDIALS function returned NULL pointer - no memory allocated */
00845   if (opt == 0 && returnvalue == nullptr) {
00846     fprintf(stderr,
00847             "\nSUNDIALS_ERROR(%d): %s() failed - returned NULL pointer\n\n", id,
00848             funcname);
00849     return (1);
00850   }
00851 
00852   /* Check if retval < 0 */
00853   else if (opt == 1) {
00854     retval = (int *)returnvalue;
00855     if (*retval < 0) {
00856       fprintf(stderr, "\nSUNDIALS_ERROR(%d): %s() failed with retval = %d\n\n",
00857               id, funcname, *retval);
00858       return (1);
00859     }
00860   }
00861 
```

```
  /* Check if function returned NULL pointer - no memory allocated */
  else if (opt == 2 && returnvalue == nullptr) {
    fprintf(stderr,
            "\nMEMORY_ERROR(%d): %s() failed - returned NULL pointer\n\n", id,
            funcname);
    return (1);
  }

  return (0);
}
```

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

Here is the caller graph for this function:



6.12.3.2 errorKill()

```
void errorKill (
            const string & errorMessage )
```

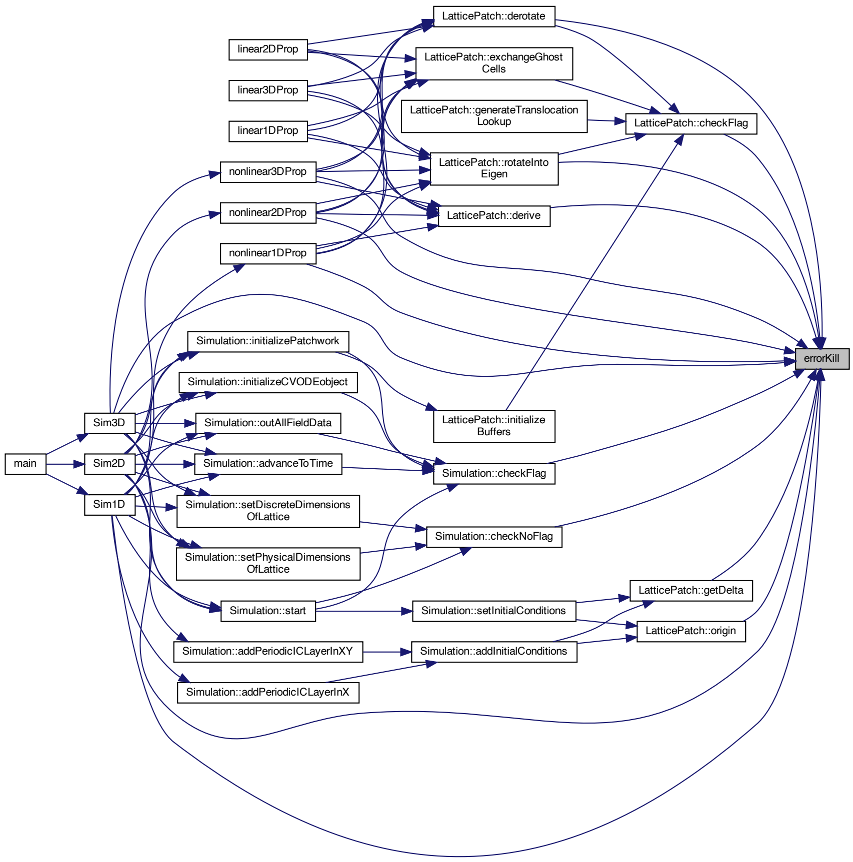
Print a specific error message to stdout.

Definition at line 828 of file LatticePatch.cpp.

```
00828                                   {
00829   cerr « endl « "Error: " « errorMessage « " Aborting..." « endl;
00830   MPI_Abort(MPI_COMM_WORLD, 1);
00831   return;
00832 }
```

Referenced by LatticePatch::checkFlag(), Simulation::checkFlag(), Simulation::checkNoFlag(), LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::getDelta(), nonlinear1DProp(), nonlinear2DProp(), nonlinear3DProp(), LatticePatch::origin(), 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.

```
///////////////////////////////////////////////////////////////////////////
/// @file LatticePatch.h
/// @brief Declaration of the lattice and lattice patches
///////////////////////////////////////////////////////////////////////////

// Include Guard
#ifndef LATTICEPATCH
#define LATTICEPATCH

// IO
#include <iomanip>
#include <iostream>
#include <sstream>

// string, container, algorithm
#include <string>
//#include <string_view>
#include <array>
#include <vector>
#include <algorithm>

// MPI & OpenMP
#include <mpi.h>
#include <omp.h>

// Sundials
#include <cvode/cvode.h>                    /* prototypes for CVODE fcts. */
#include <nvector/nvector_parallel.h> /* definition of N_Vector and macros */
#include <sundials/sundials_types.h>  /* definition of type sunrealtype */
```

```cpp

// stencils
#include "DerivationStencils.h"

using namespace std;

// lattice construction checking flags
enum LatticeOptions {
    FLatticeDimensionSet = 0x01,  // 1
    /*OPT_B = 0x02,  // 2
    OPT_C = 0x04,  // 4
    OPT_D = 0x08,  // 8
    OPT_E = 0x10,  // 16
    OPT_F = 0x20,*/  // 32
};

/** @brief Lattice class for the construction of the enveloping discrete
 * simulation space */
class Lattice {
private:
  /// physical size of the lattice in x-direction
  sunrealtype tot_lx;
  /// physical size of the lattice in y-direction
  sunrealtype tot_ly;
  /// physical size of the lattice in z-direction
  sunrealtype tot_lz;
  /// number of points in x-direction
  sunindextype tot_nx;
  /// number of points in y-direction
  sunindextype tot_ny;
  /// number of points in z-direction
  sunindextype tot_nz;
  /// total number of lattice points
  sunindextype tot_noP;
  /// dimension of each data point -> set once and for all
  static constexpr int dataPointDimension = 6;
  /// number of lattice points times data dimension of each point
  sunindextype tot_noDP;
  /// physical distance between lattice points in x-direction
  sunrealtype dx;
  /// physical distance between lattice points in y-direction
  sunrealtype dy;
  /// physical distance between lattice points in z-direction
  sunrealtype dz;
  /// stencil order
  const int stencilOrder;
  /// required width of ghost layers (depends on the stencil order)
  const int ghostLayerWidth;
  /// char for checking if lattice flags are set
  unsigned char statusFlags;

public:
  /// number of MPI processes
  int n_prc;
  /// number of MPI process
  int my_prc;
  /// personal communicator of the lattice
  MPI_Comm comm;
  /// function to create and deploy the cartesian communicator
  void initializeCommunicator(const int nx, const int ny,
          const int nz, const bool per);
  /// default construction
  Lattice(const int StO);
  /// SUNContext object
  SUNContext sunctx;
  /// SUNProfiler object
  SUNProfiler profobj;
  /// component function for resizing the discrete dimensions of the lattice
  void setDiscreteDimensions(const sunindextype _nx,
          const sunindextype _ny, const sunindextype _nz);
  /// component function for resizing the physical size of the lattice
  void setPhysicalDimensions(const sunrealtype _lx,
          const sunrealtype _ly, const sunrealtype _lz);
  ///@{
  /** getter function */
  [[nodiscard]] const sunrealtype &get_tot_lx() const { return tot_lx; }
  [[nodiscard]] const sunrealtype &get_tot_ly() const { return tot_ly; }
  [[nodiscard]] const sunrealtype &get_tot_lz() const { return tot_lz; }
  [[nodiscard]] const sunindextype &get_tot_nx() const { return tot_nx; }
  [[nodiscard]] const sunindextype &get_tot_ny() const { return tot_ny; }
  [[nodiscard]] const sunindextype &get_tot_nz() const { return tot_nz; }
  [[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; }
  [[nodiscard]] const sunrealtype &get_dy() const { return dy; }
  [[nodiscard]] const sunrealtype &get_dz() const { return dz; }
  [[nodiscard]] constexpr int get_dataPointDimension() const {
```

```
    return dataPointDimension;
  }
  [[nodiscard]] const int &get_stencilOrder() const { return stencilOrder; }
  [[nodiscard]] const int &get_ghostLayerWidth() const {
    return ghostLayerWidth;
  }
  ///@}
};

/// lattice patch construction checking flags
enum LatticePatchOptions {
  FLatticePatchSetUp = 0x01,
  TranslocationLookupSetUp = 0x02,
  GhostLayersInitialized = 0x04,
  BuffersInitialized = 0x08
  /*OPT_D = 0x08,
  OPT_E = 0x10,
  OPT_F = 0x20,*/
};

/** @brief LatticePatch class for the construction of the patches in the
 * enveloping lattice */
class LatticePatch {
private:
  /// origin of the patch in physical space; x-coordinate
  sunrealtype x0;
  /// origin of the patch in physical space; y-coordinate
  sunrealtype y0;
  /// origin of the patch in physical space; z-coordinate
  sunrealtype z0;
  /// inner position of lattice-patch in the lattice patchwork; x-points
  sunindextype LIx;
  /// inner position of lattice-patch in the lattice patchwork; y-points
  sunindextype LIy;
  /// inner position of lattice-patch in the lattice patchwork; z-points
  sunindextype LIz;
  /// physical size of the lattice-patch in the x-dimension
  sunrealtype lx;
  /// physical size of the lattice-patch in the y-dimension
  sunrealtype ly;
  /// physical size of the lattice-patch in the z-dimension
  sunrealtype lz;
  /// number of points in the lattice patch in the x-dimension
  sunindextype nx;
  /// number of points in the lattice patch in the y-dimension
  sunindextype ny;
  /// number of points in the lattice patch in the z-dimension
  sunindextype nz;
  /// physical distance between lattice points in x-direction
  sunrealtype dx;
  /// physical distance between lattice points in y-direction
  sunrealtype dy;
  /// physical distance between lattice points in z-direction
  sunrealtype dz;
  /// pointer to the enveloping lattice
  const Lattice *envelopeLattice;
  ///@{
  /** translocation lookup table */
  vector<int> uTox, uToy, uToz, xTou, yTou, zTou;
  ///@}
  /// aid (auxilliarly) vector including ghost cells to compute the derivatives
  vector<sunrealtype> uAux;
  ///@{
  /** buffer to save spatial derivative values */
  vector<sunrealtype> buffX, buffY, buffZ;
  ///@}
  ///@{
  /** buffer for passing ghost cell data */
  vector<sunrealtype> ghostCellLeft, ghostCellRight, ghostCellLeftToSend,
      ghostCellRightToSend, ghostCellsToSend, ghostCells;
  ///@}
  ///@{
  /** ghost cell translocation lookup table */
  vector<int> lgcTox, rgcTox, lgcToy, rgcToy, lgcToz, rgcToz;
  ///@}
  /** char for checking flags */
  unsigned char statusFlags;
  ///@{
  /** rotate and translocate an input array according to a lookup into an output
   * array */
  inline void rotateToX(sunrealtype *outArray, const sunrealtype *inArray,
                        const vector<int> &lookup);
  inline void rotateToY(sunrealtype *outArray, const sunrealtype *inArray,
                        const vector<int> &lookup);
  inline void rotateToZ(sunrealtype *outArray, const sunrealtype *inArray,
                        const vector<int> &lookup);
  ///@}
```

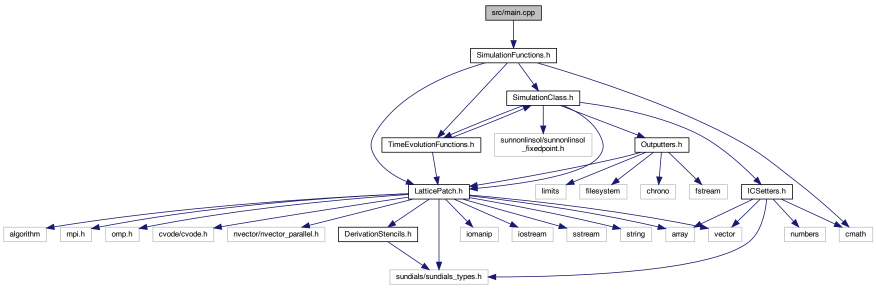
```
public:
  /// ID of the LatticePatch, corresponds to process number
  // (required solely for debugging)
  int ID;
  /// N_Vector for saving field components u=(E,B) in lattice points
  N_Vector u;
  /// N_Vector for saving temporal derivatives of the field data
  N_Vector du;
  /// pointer to field data
  sunrealtype *uData;
  /// pointer to auxiliary data vector
  sunrealtype *uAuxData;
  /// pointer to time-derivative data
  sunrealtype *duData;
  ///@{
  /** pointer to halo data */
  sunrealtype *gCLData, *gCRData;
  ///@}
  /// pointer to spatial derivative data buffers
  array<sunrealtype *, 3> buffData;
  /// constructor setting up a default first lattice patch
  LatticePatch();
  /// destructor freeing parallel vectors
  ~LatticePatch();
  /// friend function for creating the patchwork slicing of the overall lattice
  friend int generatePatchwork(const Lattice &envelopeLattice,
                               LatticePatch &patchToMold, const int DLx,
                               const int DLy, const int DLz);
  /// function to get the discrete size of the LatticePatch
  // (0 direction corresponds to total)
  int discreteSize(int dir=0) const;
  /// function to get the origin of the patch
  sunrealtype origin(const int dir) const;
  /// function to get distance between points
  sunrealtype getDelta(const int dir) const;
  /// function to fill out the lookup tables
  // for translocation and de-translocation of data point
  void generateTranslocationLookup();
  /// function to rotate u into Z-matrix eigenraum
  // and make it the primary lattice direction of dir
  void rotateIntoEigen(const int dir);
  /// function to derotate uAux into dudata lattice direction of x
  void derotate(int dir, sunrealtype *buffOut);
  /// initialize ghost cells for halo exchange
  void initializeGhostLayer();
  /// initialize buffers to save derivatives
  void initializeBuffers();
  /// function to exchange ghost cells in uAux for the derivative
  void exchangeGhostCells(const int dir);
  /// function to derive the centered values in uAux and save them noncentered
  void derive(const int dir);
  /// function to check if a flag has been set and if not abort
  void checkFlag(unsigned int flag) const;
};

// helper function for error messages
void errorKill(const string & errorMessage);

// helper function to check for CVode success
int check_retval(void *returnvalue, const char *funcname, int opt, int id);

// End of Includeguard
#endif
```

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

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

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

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
00011     MPI_Init (&argc, &argv);
00012     MPI_Comm comm = MPI_COMM_WORLD;
00013     // Prepare MPI for Master-only threading
00014     //int provided;
00015     //MPI_Init_thread(&argc, &argv, MPI_THREAD_FUNNELED, &provided);
00016 
00017     int rank = 0;
00018     MPI_Comm_rank(comm,&rank);
00019     double ti=MPI_Wtime(); // Overall start time
00020 
00021     /** Determine the output directory.
00022      * A "SimResults" folder will be created if non-existent
00023      * with a subdirectory named in the identifier format
00024      * "yy-mm-dd_hh-MM-ss" that contains the csv files     */
00025     constexpr auto outputDirectory = "/path/to/directory/";
00026 
00027 
00028     //------------ BEGIN OF CONFIGURATION ------------//
00029 
00030     //////////////////// - 1D - //////////////////////
00031     /** A 1D simulation with specified */
00032 
00033     //// Specify your settings here ////
00034     constexpr array <sunrealtype,2> CVodeTolerances={1.0e-16,1.0e-16}; /// - relative and absolute tolerances of the CVode solver
00035     constexpr int StencilOrder=13;                                     /// - accuracy order of the stencils in the range 1-13
00036     constexpr sunrealtype physical_sidelength=300e-6;                  /// - physical length of the lattice in meters
00037     constexpr sunindextype latticepoints=6e3;                          /// - number of lattice points
00038     constexpr bool periodic=true;                                      /// - periodic or vanishing boundary values
00039     int processOrder=3;                                                /// - included processes of the weak-field expansion, see README.md
00040     constexpr sunrealtype simulationTime=100.0e-6l;                    /// -  physical total simulation time
00041     constexpr int numberOfSteps=100;                                   /// -  discrete time steps
00042     constexpr int outputStep=100;                                      /// -  output step multiples
00043 
```

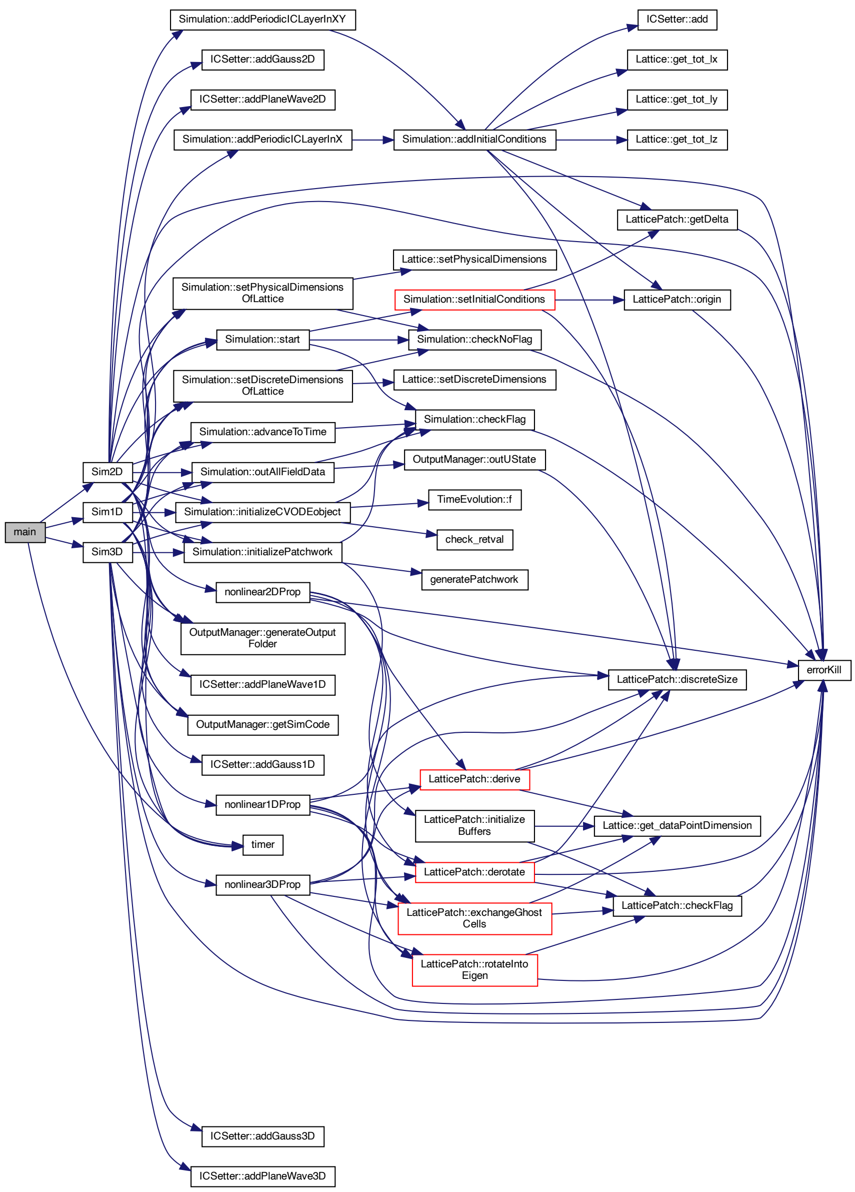
```
    /// Add electromagnetic waves.
    planewave plane1;                 /// A plane wave with
    plane1.k = {1e5,0,0};             /// - wavevector (normalized to \f$ 1/\lambda \f$)
    plane1.p = {0,0,0.1};             /// - amplitude/polarization
    plane1.phi = {0,0,0};             /// - phase shift
    planewave plane2;                 /// Another plane wave with
    plane2.k = {-1e6,0,0};            /// - wavevector (normalized to \f$ 1/\lambda \f$)
    plane2.p = {0,0,0.5};             /// - amplitude/polarization
    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 waves.
    vector<planewave> planewaves;
    //planewaves.emplace_back(plane1);
    //planewaves.emplace_back(plane2);

    gaussian1D gauss1;                /// A Gaussian wave with
    gauss1.k = {1.0e6,0,0};           /// - wavevector (normalized to \f$ 1/\lambda \f$)
    gauss1.p = {0,0,0.1};             /// - polarization/amplitude
    gauss1.x0 = {100e-6,0,0};         /// - shift from origin
    gauss1.phig = 5e-6;               /// - width
    gauss1.phi = {0,0,0};             /// - phase shift
    gaussian1D gauss2;                /// Another Gaussian with
    gauss2.k = {-0.2e6,0,0};          /// - wavevector (normalized to \f$ 1/\lambda \f$)
    gauss2.p = {0,0,0.5};             /// - polarization/amplitude
    gauss2.x0 = {200e-6,0,0};         /// - shift from origin
    gauss2.phig = 15e-6;              /// - width
    gauss2.phi = {0,0,0};             /// - phase shift
    // Do not comment out this vector, even if no Gaussian wave is used. But if, emplace used Gaussian waves.
    vector<gaussian1D> Gaussians1D;
    Gaussians1D.emplace_back(gauss1);
    Gaussians1D.emplace_back(gauss2);

    //// Do not change this below ////
    int *interactions = &processOrder;
    Sim1D(CVodeTolerances,StencilOrder,physical_sidelength,latticepoints,
            periodic,interactions,simulationTime,numberOfSteps,
            outputDirectory,outputStep,
            planewaves,Gaussians1D);

    ////////////////////////////////////////////////////


    //////////////////// - 2D - /////////////////////
    /** A 2D simulation with specified */

    //// Specify your settings here ////
    constexpr array<sunrealtype,2> CVodeTolerances={1.0e-12,1.0e-12};  /// - relative and absolute tolerances of the CVode solver
    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 lattice in the given dimensions in meters
    constexpr array<sunindextype,2> latticepoints_per_dim={800,800};   /// - number of lattice points per dimension
    constexpr array<int,2> patches_per_dim={2,2};                      /// - slicing of discrete dimensions into patches
    constexpr bool periodic=true;                                      /// - periodic or vanishing boundary values
    int processOrder=3;                                                /// - included processes of the weak-field expansion, see README.md
    constexpr sunrealtype simulationTime=40e-6l;                       /// - physical total simulation time
    constexpr int numberOfSteps=100;                                   /// - discrete time steps
    constexpr int outputStep=100;                                      /// - output step multiples

    /// Add electromagnetic waves.
    planewave plane1;                   /// A plane wave with
    plane1.k = {1e5,0,0};               /// - wavevector (normalized to \f$ 1/\lambda \f$)
    plane1.p = {0,0,0.1};               /// - amplitude/polarization
    plane1.phi = {0,0,0};               /// - phase shift
    planewave plane2;                   /// Another plane wave with
    plane2.k = {-1e6,0,0};              /// - wavevector
    plane2.p = {0,0,0.5};               /// - amplitude/polarization
    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 waves.
    vector<planewave> planewaves;
    //planewaves.emplace_back(plane1);
    //planewaves.emplace_back(plane2);

    gaussian2D gauss1;                  /// A Gaussian wave with
    gauss1.x0 = {40e-6,40e-6};          /// - center it approaches
    gauss1.axis = {1,0};                /// - normalized direction _from_ which the wave approaches the center
    gauss1.amp = 0.5;                   /// - amplitude
    gauss1.phip = 2*atan(0);            /// - polarization rotation from TE-mode (z-axis)
```

```
    gauss1.w0 = 2.3e-6;                 /// - taille
    gauss1.zr = 16.619e-6;              /// - Rayleigh length
    /// the wavelength is determined by the relation \f$ \lambda = \pi*w_0^2/z_R \f$
    gauss1.ph0 = 2e-5;                  /// - beam center
    gauss1.phA = 0.45e-5;               /// - beam length
    gaussian2D gauss2;                  /// Another Gaussian wave with
    gauss2.x0 = {40e-6,40e-6};          /// - center it approaches
    gauss2.axis = {-0.7071,0.7071};     /// - normalized direction from which the wave approaches the center
    gauss2.amp = 0.5;                   /// - amplitude
    gauss2.phip = 2*atan(0);            /// - polarization rotation fom TE-mode (z-axis)
    gauss2.w0 = 2.3e-6;                 /// - taille
    gauss2.zr = 16.619e-6;              /// - Rayleigh length
    gauss2.ph0 = 2e-5;                  /// - beam center
    gauss2.phA = 0.45e-5;               /// - beam length
    // Do not comment out this vector, even if no Gaussian wave is used. But if, emplace used Gaussian waves.
    vector<gaussian2D> Gaussians2D;
    Gaussians2D.emplace_back(gauss1);
    Gaussians2D.emplace_back(gauss2);

    //// 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 "
            "divisible by the number of patches in that direction.");
    int * interactions = &processOrder;
    Sim2D(CVodeTolerances,StencilOrder,physical_sidelengths,
            latticepoints_per_dim,patches_per_dim,periodic,interactions,
            simulationTime,numberOfSteps,outputDirectory,outputStep,
            planewaves,Gaussians2D);

    ////////////////////////////////////////////////////


    //////////////////// - 3D - //////////////////////
    /** A 3D simulation with specified */

    //// Specify your settings here ////
    constexpr array<sunrealtype,2> CVodeTolerances={1.0e-12,1.0e-12};        /// - relative and absolute tolerances of the CVode solver
    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 in meters
    constexpr array<sunindextype,3> latticepoints_per_dim={800,800,200};     /// - number of lattice points in any dimension
    constexpr array<int,3> patches_per_dim= {8,8,2};                         /// - slicing of discrete dimensions into patches
    constexpr bool periodic=false;                                           /// - perodic or non-periodic boundaries
    int processOrder=3;                                                      /// - processes of the weak-field expansion, see README.md
    constexpr sunrealtype simulationTime=20e-6;                              /// - physical total simulation time
    constexpr int numberOfSteps=50;                                          /// - discrete time steps
    constexpr int outputStep=50;                                             /// - output step multiples
    /// Add electromagnetic waves.
    planewave plane1;                    /// A plane wave with
    plane1.k = {1e5,0,0};                /// - wavevector (normalized to \f$ 1/\lambda \f$)
    plane1.p = {0,0,0.1};                /// - amplitude/polarization
    plane1.phi = {0,0,0};                /// - phase shift
    planewave plane2;                    /// Another plane wave with
    plane2.k = {-1e6,0,0};               /// - wavevector (normalized to \f$ 1/\lambda \f$)
    plane2.p = {0,0,0.5};                /// - amplitude/polarization
    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 waves.
    vector<planewave> planewaves;
    //planewaves.emplace_back(plane1);
    //planewaves.emplace_back(plane2);

    gaussian3D gauss1;                   /// A Gaussian wave with
    gauss1.x0 = {40e-6,40e-6,10e-6};     /// - center it approaches
    gauss1.axis = {1,0,0};               /// - normalized direction _from_ which the wave approaches the center
    gauss1.amp = 0.05;                   /// - amplitude
    gauss1.phip = 2*atan(0);             /// - polarization rotation from TE-mode (z-axis)
    gauss1.w0 = 3.5e-6;                  /// - taille
    gauss1.zr = 19.242e-6;               /// - Rayleigh length
    /// the wavelength is determined by the relation \f$ \lambda = \pi*w_0^2/z_R \f$
    gauss1.ph0 = 2e-5;                   /// - beam center
    gauss1.phA = 0.45e-5;                /// - beam length
    gaussian3D gauss2;                   /// Another Gaussian wave with
    gauss2.x0 = {40e-6,40e-6,10e-6};     /// - center it approaches
```

```
    gauss2.axis = {0,1,0};              /// - normalized direction from which the wave approaches the center
    gauss2.amp = 0.05;                  /// - amplitude
    gauss2.phip = 2*atan(0);            /// - polarization rotation from TE-mode (z-axis)
    gauss2.w0 = 3.5e-6;                 /// - taille
    gauss2.zr = 19.242e-6;              /// - Rayleigh length
    gauss2.ph0 = 2e-5;                  /// - beam center
    gauss2.phA = 0.45e-5;               /// - beam length
    // Do not comment out this vector, even if no Gaussian wave is used. But if, emplace used Gaussian waves.
    vector<gaussian3D> Gaussians3D;
    Gaussians3D.emplace_back(gauss1);
    Gaussians3D.emplace_back(gauss2);

    //// 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 &&
            latticepoints_per_dim[2]%patches_per_dim[2]==0,
            "The number of lattice points in each dimension must be "
            "divisible by the number of patches in that direction.");
    int *interactions = &processOrder;
    Sim3D(CVodeTolerances,StencilOrder,physical_sidelengths,
            latticepoints_per_dim,patches_per_dim,periodic,interactions,
            simulationTime,numberOfSteps,outputDirectory,outputStep,
            planewaves,Gaussians3D);

    ///////////////////////////////////////////////////

    //------------- END OF CONFIGURATION -------------//

    double tf=MPI_Wtime(); // Overall finish time
    if(rank==0) {cout«endl; timer(ti,tf);} // Print the elapsed time

    // Finalize MPI environment
    MPI_Finalize();

    return 0;
}
```

References planewave::k, gaussian1D::k, planewave::p, gaussian1D::p, planewave::phi, gaussian1D::phi, gaussian1D::phig, 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.

```
/// @file main.cpp
/// @brief Main function to configure the user's simulation settings


#include "SimulationFunctions.h"   /* complete simulation functions and all headers */


int main(int argc, char *argv[])
{
    // Initialize MPI environment
    MPI_Init (&argc, &argv);
    MPI_Comm comm = MPI_COMM_WORLD;
    // Prepare MPI for Master-only threading
    //int provided;
```

```
    //MPI_Init_thread(&argc, &argv, MPI_THREAD_FUNNELED, &provided);

    int rank = 0;
    MPI_Comm_rank(comm,&rank);
    double ti=MPI_Wtime(); // Overall start time

    /** 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     */
    constexpr auto outputDirectory = "/path/to/directory/";


    //------------ BEGIN OF CONFIGURATION ------------//

    //////////////////// - 1D - //////////////////////
    /** A 1D simulation with specified */

    //// Specify your settings here ////
    constexpr array <sunrealtype,2> CVodeTolerances={1.0e-16,1.0e-16}; /// - relative and absolute tolerances of the CVode solver
    constexpr int StencilOrder=13;                                      /// - accuracy order of the stencils in the range 1-13
    constexpr sunrealtype physical_sidelength=300e-6;                   /// - physical length of the lattice in meters
    constexpr sunindextype latticepoints=6e3;                           /// - number of lattice points
    constexpr bool periodic=true;                                       /// - periodic or vanishing boundary values
    int processOrder=3;                                                 /// - included processes of the weak-field expansion, see README.md
    constexpr sunrealtype simulationTime=100.0e-6l;                     /// -  physical total simulation time
    constexpr int numberOfSteps=100;                                    /// -  discrete time steps
    constexpr int outputStep=100;                                       /// -  output step multiples

    /// Add electromagnetic waves.
    planewave plane1;                /// A plane wave with
    plane1.k = {1e5,0,0};            /// - wavevector (normalized to \f$ 1/\lambda \f$)
    plane1.p = {0,0,0.1};            /// - amplitude/polarization
    plane1.phi = {0,0,0};            /// - phase shift
    planewave plane2;                /// Another plane wave with
    plane2.k = {-1e6,0,0};           /// - wavevector (normalized to \f$ 1/\lambda \f$)
    plane2.p = {0,0,0.5};            /// - amplitude/polarization
    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 waves.
    vector<planewave> planewaves;
    //planewaves.emplace_back(plane1);
    //planewaves.emplace_back(plane2);

    gaussian1D gauss1;               /// A Gaussian wave with
    gauss1.k = {1.0e6,0,0};          /// - wavevector (normalized to \f$ 1/\lambda \f$)
    gauss1.p = {0,0,0.1};            /// - polarization/amplitude
    gauss1.x0 = {100e-6,0,0};        /// - shift from origin
    gauss1.phig = 5e-6;              /// - width
    gauss1.phi = {0,0,0};            /// - phase shift
    gaussian1D gauss2;               /// Another Gaussian with
    gauss2.k = {-0.2e6,0,0};         /// - wavevector (normalized to \f$ 1/\lambda \f$)
    gauss2.p = {0,0,0.5};            /// - polarization/amplitude
    gauss2.x0 = {200e-6,0,0};        /// - shift from origin
    gauss2.phig = 15e-6;             /// - width
    gauss2.phi = {0,0,0};            /// - phase shift
    // Do not comment out this vector, even if no Gaussian wave is used. But if, emplace used Gaussian waves.
    vector<gaussian1D> Gaussians1D;
    Gaussians1D.emplace_back(gauss1);
    Gaussians1D.emplace_back(gauss2);

    //// Do not change this below ////
    int *interactions = &processOrder;
    Sim1D(CVodeTolerances,StencilOrder,physical_sidelength,latticepoints,
            periodic,interactions,simulationTime,numberOfSteps,
            outputDirectory,outputStep,
            planewaves,Gaussians1D);

    ////////////////////////////////////////////////////


    //////////////////// - 2D - //////////////////////
    /** A 2D simulation with specified */

    //// Specify your settings here ////
    constexpr array<sunrealtype,2> CVodeTolerances={1.0e-12,1.0e-12};  /// - relative and absolute tolerances of the CVode solver
    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
```

```
lattice in the given dimensions in meters
    constexpr array<sunindextype,2> latticepoints_per_dim={800,800};   /// - number of lattice points
per dimension
    constexpr array<int,2> patches_per_dim={2,2};                      /// - slicing of discrete
dimensions into patches
    constexpr bool periodic=true;                                      /// - periodic or vanishing
boundary values
    int processOrder=3;                                                /// - included processes of the
weak-field expansion, see README.md
    constexpr sunrealtype simulationTime=40e-6l;                       /// - physical total simulation
time
    constexpr int numberOfSteps=100;                                   /// - discrete time steps
    constexpr int outputStep=100;                                      /// - output step multiples

    /// Add electromagnetic waves.
    planewave plane1;                  /// A plane wave with
    plane1.k = {1e5,0,0};              /// - wavevector (normalized to \f$ 1/\lambda \f$)
    plane1.p = {0,0,0.1};              /// - amplitude/polarization
    plane1.phi = {0,0,0};              /// - phase shift
    planewave plane2;                  /// Another plane wave with
    plane2.k = {-1e6,0,0};             /// - wavevector
    plane2.p = {0,0,0.5};              /// - amplitude/polarization
    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
waves.
    vector<planewave> planewaves;
    //planewaves.emplace_back(plane1);
    //planewaves.emplace_back(plane2);

    gaussian2D gauss1;                 /// A Gaussian wave with
    gauss1.x0 = {40e-6,40e-6};         /// - center it approaches
    gauss1.axis = {1,0};               /// - normalized direction _from_ which the wave approaches the
center
    gauss1.amp = 0.5;                  /// - amplitude
    gauss1.phip = 2*atan(0);           /// - polarization rotation from TE-mode (z-axis)
    gauss1.w0 = 2.3e-6;                /// - taille
    gauss1.zr = 16.619e-6;             /// - Rayleigh length
    /// the wavelength is determined by the relation \f$ \lambda = \pi*w_0^2/z_R \f$
    gauss1.ph0 = 2e-5;                 /// - beam center
    gauss1.phA = 0.45e-5;              /// - beam length
    gaussian2D gauss2;                 /// Another Gaussian wave with
    gauss2.x0 = {40e-6,40e-6};         /// - center it approaches
    gauss2.axis = {-0.7071,0.7071};    /// - normalized direction from which the wave approaches the
center
    gauss2.amp = 0.5;                  /// - amplitude
    gauss2.phip = 2*atan(0);           /// - polarization rotation fom TE-mode (z-axis)
    gauss2.w0 = 2.3e-6;                /// - taille
    gauss2.zr = 16.619e-6;             /// - Rayleigh length
    gauss2.ph0 = 2e-5;                 /// - beam center
    gauss2.phA = 0.45e-5;              /// - beam length
    // Do not comment out this vector, even if no Gaussian wave is used. But if, emplace used Gaussian
waves.
    vector<gaussian2D> Gaussians2D;
    Gaussians2D.emplace_back(gauss1);
    Gaussians2D.emplace_back(gauss2);

    //// 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 "
            "divisible by the number of patches in that direction.");
    int * interactions = &processOrder;
    Sim2D(CVodeTolerances,StencilOrder,physical_sidelengths,
            latticepoints_per_dim,patches_per_dim,periodic,interactions,
            simulationTime,numberOfSteps,outputDirectory,outputStep,
            planewaves,Gaussians2D);

    ////////////////////////////////////////////////////


    //////////////////// - 3D - /////////////////////
    /** A 3D simulation with specified */

    //// Specify your settings here ////
    constexpr array<sunrealtype,2> CVodeTolerances={1.0e-12,1.0e-12};        /// - relative and
absolute tolerances of the CVode solver
    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
in meters
    constexpr array<sunindextype,3> latticepoints_per_dim={800,800,200};     /// - number of lattice
points in any dimension
    constexpr array<int,3> patches_per_dim= {8,8,2};                          /// - slicing of discrete
dimensions into patches
    constexpr bool periodic=false;                                            /// - perodic or
non-periodic boundaries
    int processOrder=3;                                                       /// - processes of the
```

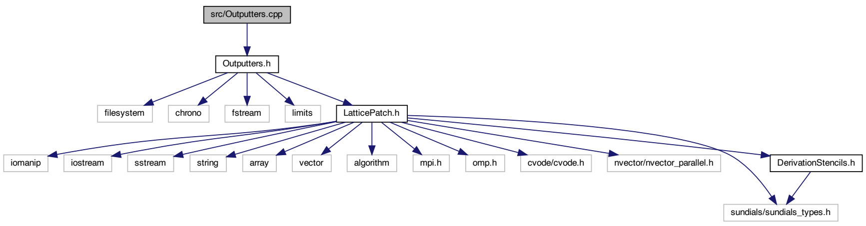
```
weak-field expansion, see README.md
    constexpr sunrealtype simulationTime=20e-6;                     /// - physical total simulation time
    constexpr int numberOfSteps=50;                                 /// - discrete time steps
    constexpr int outputStep=50;                                    /// - output step multiples
    /// Add electromagnetic waves.
    planewave plane1;                  /// A plane wave with
    plane1.k = {1e5,0,0};              /// - wavevector (normalized to \f$ 1/\lambda \f$)
    plane1.p = {0,0,0.1};              /// - amplitude/polarization
    plane1.phi = {0,0,0};              /// - phase shift
    planewave plane2;                  /// Another plane wave with
    plane2.k = {-1e6,0,0};             /// - wavevector (normalized to \f$ 1/\lambda \f$)
    plane2.p = {0,0,0.5};              /// - amplitude/polarization
    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 waves.
    vector<planewave> planewaves;
    //planewaves.emplace_back(plane1);
    //planewaves.emplace_back(plane2);

    gaussian3D gauss1;                 /// A Gaussian wave with
    gauss1.x0 = {40e-6,40e-6,10e-6};   /// - center it approaches
    gauss1.axis = {1,0,0};             /// - normalized direction _from_ which the wave approaches the center
    gauss1.amp = 0.05;                 /// - amplitude
    gauss1.phip = 2*atan(0);           /// - polarization rotation from TE-mode (z-axis)
    gauss1.w0 = 3.5e-6;                /// - taille
    gauss1.zr = 19.242e-6;             /// - Rayleigh length
    /// the wavelength is determined by the relation \f$ \lambda = \pi*w_0^2/z_R \f$
    gauss1.ph0 = 2e-5;                 /// - beam center
    gauss1.phA = 0.45e-5;              /// - beam length
    gaussian3D gauss2;                 /// Another Gaussian wave with
    gauss2.x0 = {40e-6,40e-6,10e-6};   /// - center it approaches
    gauss2.axis = {0,1,0};             /// - normalized direction from which the wave approaches the center
    gauss2.amp = 0.05;                 /// - amplitude
    gauss2.phip = 2*atan(0);           /// - polarization rotation from TE-mode (z-axis)
    gauss2.w0 = 3.5e-6;                /// - taille
    gauss2.zr = 19.242e-6;             /// - Rayleigh length
    gauss2.ph0 = 2e-5;                 /// - beam center
    gauss2.phA = 0.45e-5;              /// - beam length
    // Do not comment out this vector, even if no Gaussian wave is used. But if, emplace used Gaussian waves.
    vector<gaussian3D> Gaussians3D;
    Gaussians3D.emplace_back(gauss1);
    Gaussians3D.emplace_back(gauss2);

    //// 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 &&
            latticepoints_per_dim[2]%patches_per_dim[2]==0,
            "The number of lattice points in each dimension must be "
            "divisible by the number of patches in that direction.");
    int *interactions = &processOrder;
    Sim3D(CVodeTolerances,StencilOrder,physical_sidelengths,
            latticepoints_per_dim,patches_per_dim,periodic,interactions,
            simulationTime,numberOfSteps,outputDirectory,outputStep,
            planewaves,Gaussians3D);

    ////////////////////////////////////////////////////

    //------------ END OF CONFIGURATION ------------//

    double tf=MPI_Wtime(); // Overall finish time
    if(rank==0) {cout«endl; timer(ti,tf);} // Print the elapsed time

    // Finalize MPI environment
    MPI_Finalize();

    return 0;
}
```

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.

```
//////////////////////////////////////////////////////////////$
/// @file Outputters.cpp
/// @brief Generation of output writing to disk
//////////////////////////////////////////////////////////////$

#include "Outputters.h"

/// Directly generate the simCode at construction
OutputManager::OutputManager() {
  simCode = SimCodeGenerator();
  MPI_Comm_rank(MPI_COMM_WORLD, &myPrc);
}

/// Generate the identifier number reverse from year to minute in the format
/// yy-mm-dd_hh-MM-ss
string OutputManager::SimCodeGenerator() {
  const chrono::time_point<chrono::system_clock> now{
      chrono::system_clock::now()};
  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};

  stringstream temp;
  temp « setfill('0') « setw(2)
       « 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()) « "_"
       « setfill('0') « setw(2) « hms.hours().count() « "-" « setfill('0')
       « setw(2) « hms.minutes().count() « "-" « setfill('0') « setw(2)
       « hms.seconds().count();
  //« "_" « hms.subseconds().count(); // subseconds render the filename too
  //large
  return temp.str();
}

/** Generate the folder to save the data to by one process:
 * In the given directory it creates a direcory "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. */
void OutputManager::generateOutputFolder(const string &dir) {
  // Do this only once for the first process
  if (myPrc == 0) {
    if (!fs::is_directory(dir))
```

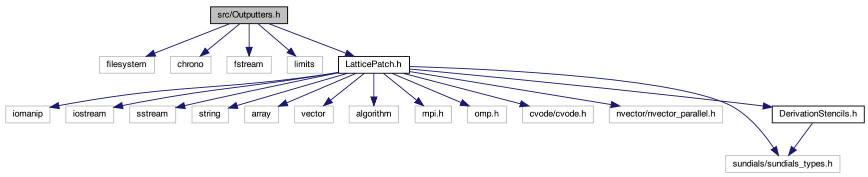
```
      fs::create_directory(dir);
    if (!fs::is_directory(dir + "/SimResults"))
      fs::create_directory(dir + "/SimResults");
    if (!fs::is_directory(dir + "/SimResults/" + simCode))
      fs::create_directory(dir + "/SimResults/" + simCode);
  }
  // path variable for the output generation
  Path = dir + "/SimResults/" + simCode + "/";

  ifstream fin("main.cpp");
  ofstream fout(Path + "config.txt");
  string line;
  int begin=1000;
  for (int i = 1; !fin.eof(); i++) {
    getline(fin, line);
    if (line.starts_with("    //------------ B")) {
        begin=i;
    }
    if (i < begin) {
      continue;
    }
    fout « line « endl;
    if (line.starts_with("    //------------- E")) {
        break;
    }
  }

  return;
}

/** Write the field data to a csv file from each process (patch) with the field
 * data into the simCode directory. The state (simulation step) denotes the
 * prefix and the suffix after an underscore is given by the process/patch
 * number */
void OutputManager::outUState(const int &state, const LatticePatch &latticePatch) {
  ofstream ofs;
  ofs.open(Path + to_string(state) + "_" + to_string(myPrc) + ".csv");
  // Set precision, number of digits for the values
  ofs « setprecision(numeric_limits<sunrealtype>::digits10);

  // Walk through each lattice point
  for (int i = 0; i < latticePatch.discreteSize() * 6; i += 6) {
    // Six columns to contain the field data: Ex,Ey,Ez,Bx,By,Bz
    ofs « latticePatch.uData[i + 0] « "," « latticePatch.uData[i + 1] « ","
        « latticePatch.uData[i + 2] « "," « latticePatch.uData[i + 3] « ","
        « latticePatch.uData[i + 4] « "," « latticePatch.uData[i + 5]
        « endl;
  }

  ofs.close();

  return;
}

/// Return the date+time simulation identifier for logging
string OutputManager::getSimCode() { return simCode; }
```

6.18 src/Outputters.h File Reference

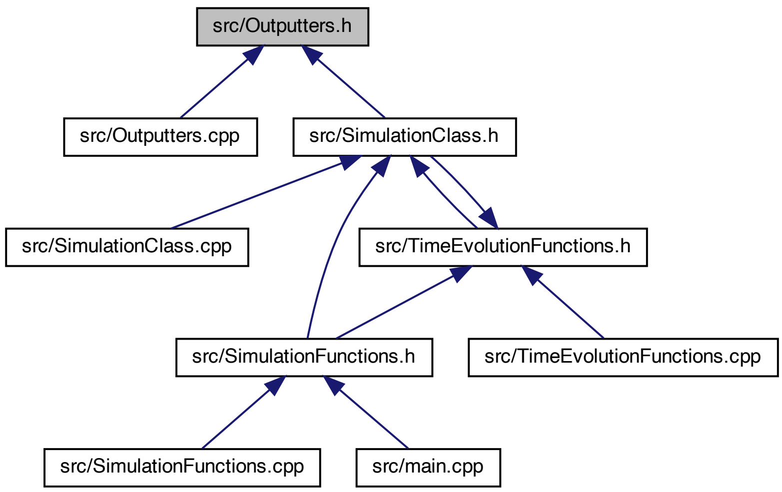
OutputManager class to outstream simulation data.

```
#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:



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.

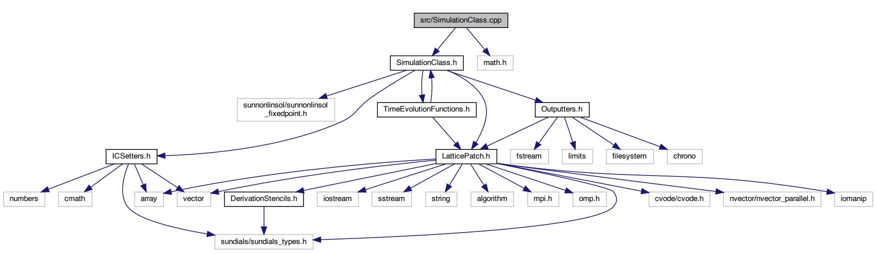
```
////////////////////////////////////////////////////////////
/// @file Outputters.h
/// @brief OutputManager class to outstream simulation data
////////////////////////////////////////////////////////////

// Include Guard
#ifndef OUTPUTTERS
#define OUTPUTTERS

// perform operations on the filesystem
#include <filesystem>

// output controlling with limits and timestep
#include <chrono>
#include <fstream>
#include <limits>

// project subfile header
#include "LatticePatch.h"

using namespace std;
namespace fs = std::filesystem;
namespace chrono = std::chrono;

/** @brief Output Manager class to generate and coordinate output writing to
 * disk */
class OutputManager {
private:
  /// function to create the Code of the Simulations
  static string SimCodeGenerator();
  /// varible to safe the SimCode generated at execution
  string simCode;
  /// variable for the path to the output folder
  string Path;
  /// process ID
  int myPrc;

public:
  /// default constructor
  OutputManager();
  /// function that creates folder to save simulation info
  void generateOutputFolder(const string &dir);
  /// output function for the whole lattice
  void outUState(const int &state, const LatticePatch &latticePatch);
  /// simCode getter function
  string getSimCode();
};

// End of Includeguard
#endif
```

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.

```
////////////////////////////////////////////////////////////////////////////////
/// @file SimulationClass.cpp
/// @brief 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>

/// Along with the simulation object, create the cartesian communicator and
/// SUNContext object
Simulation::Simulation(const int nx, const int ny, const int nz,
        const int StencilOrder, const bool periodicity) :
    lattice(StencilOrder){
  statusFlags = 0;
  t = 0;
  // Initialize the cartesian communicator
  lattice.initializeCommunicator(nx, ny, nz, periodicity);

  // Create the SUNContext object associated with the thread of execution
  int retval = 0;
  retval = SUNContext_Create(&lattice.comm, &lattice.sunctx);
  if (check_retval(&retval, "SUNContext_Create", 1, lattice.my_prc))
    MPI_Abort(lattice.comm, 1);
  // if (flag != CV_SUCCESS) { printf("SUNContext_Create failed, flag=%d.\n",
  // flag);
  //     MPI_Abort(lattice.comm, 1); }
}

/// Free the CVode solver memory and Sundials context object with the finish of
/// the simulation
Simulation::~Simulation() {
  // Free solver memory
  if (statusFlags & CvodeObjectSetUp) {
    // PrintFinalStats(cvode_mem); // TODO write this function as in cvodes
    // cvAdvDiff_bnd.c SUNDIALS_MARK_FUNCTION_END(lattice.profobj);
    CVodeFree(&cvode_mem);
    SUNContext_Free(&lattice.sunctx);
  }
}

/// Set the discrete dimensions, the number of points per dimension
void Simulation::setDiscreteDimensionsOfLattice(const sunindextype nx,
        const sunindextype ny, const sunindextype nz) {
  checkNoFlag(LatticePatchworkSetUp);
  lattice.setDiscreteDimensions(nx, ny, nz);
  statusFlags |= LatticeDiscreteSetUp;
}

/// Set the physical dimensions with lenghts in micro meters
void Simulation::setPhysicalDimensionsOfLattice(const sunrealtype lx,
        const sunrealtype ly, const sunrealtype lz) {
  checkNoFlag(LatticePatchworkSetUp);
  lattice.setPhysicalDimensions(lx, ly, lz);
  statusFlags |= LatticePhysicalSetUp;
}

/// Check that the lattice dimensions are set up and generate the patchwork
void Simulation::initializePatchwork(const int nx, const int ny,
        const int nz) {
  checkFlag(LatticeDiscreteSetUp);
  checkFlag(LatticePhysicalSetUp);

  // Generate the patchwork
  generatePatchwork(lattice, latticePatch, nx, ny, nz);
  latticePatch.initializeBuffers();
```

```

  statusFlags |= LatticePatchworkSetUp;
}

/// Configure CVODE
void Simulation::initializeCVODEobject(const sunrealtype reltol,
        const sunrealtype abstol) {
  checkFlag(SimulationStarted);

  // CVode settings return value
  int retval = 0;

  // Set the profiler
  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);
  //     MPI_Abort(lattice.comm, 1); }

  // SUNDIALS_MARK_FUNCTION_BEGIN(profobj);

  // Create CVODE object - returns a pointer to the cvode memory structure
  // with Adams method (Adams-Moulton formula) solver chosen for non-stiff ODE
  cvode_mem = CVodeCreate(CV_ADAMS, lattice.sunctx);

  // Specify user data and attach it to the main cvode memory block
  retval = CVodeSetUserData(
      cvode_mem,
      &latticePatch); // patch contains the user data as used in CVRhsFn
  if (check_retval(&retval, "CVodeSetUserData", 1, lattice.my_prc))
    MPI_Abort(lattice.comm, 1);
  // if (flag != CV_SUCCESS) { printf("CVodeSetUserData failed, flag=%d.\n",
  // flag);
  //     MPI_Abort(lattice.comm, 1); }

  // Initialize CVODE solver -> can only be called after start of simulation to
  // have data ready Provide required problem and solution specifications,
  // allocate internal memory, and initialize cvode
  retval = CVodeInit(cvode_mem, TimeEvolution::f, 0,
                     latticePatch.u); // allocate memory, CVRhsFn f, t_i=0, u
                                      // 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);
  //     MPI_Abort(lattice.comm, 1); }

  // Create fixed point nonlinear solver object (suitable for non-stiff ODE) and
  // attach it to CVode
  SUNNonlinearSolver NLS =
      SUNNonlinSol_FixedPoint(latticePatch.u, 0, lattice.sunctx);
  retval = CVodeSetNonlinearSolver(cvode_mem, NLS);
  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);
  //     MPI_Abort(lattice.comm, 1); }

  // Specify the maximum number of steps to be taken by the solver in its
  // attempt to reach the next output time
  retval = CVodeSetMaxNumSteps(cvode_mem, 10000);
  if (check_retval(&retval, "CVodeSetMaxNumSteps", 1, lattice.my_prc))
    MPI_Abort(lattice.comm, 1);
  // if (flag != CV_SUCCESS) { printf("CVodeSetMaxNumSteps failed, flag=%d.\n",
  // flag);
  //     MPI_Abort(lattice.comm, 1); }

  // Specify integration tolerances - a scalar relative tolerance and scalar
  // absolute tolerance
  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",
  // flag);
  //     MPI_Abort(lattice.comm, 1); }

  statusFlags |= CvodeObjectSetUp;
}

/// Check if the lattice patchwork is set up and set the initial conditions
void Simulation::start() {
  checkFlag(LatticeDiscreteSetUp);
  checkFlag(LatticePhysicalSetUp);
  checkFlag(LatticePatchworkSetUp);
  checkNoFlag(SimulationStarted);
  checkNoFlag(CvodeObjectSetUp);
  setInitialConditions();
```

```
  statusFlags |= SimulationStarted;
}

/// Set initial conditions: Fill the lattice points with the initial field
/// values
void Simulation::setInitialConditions() {
  const sunrealtype dx = latticePatch.getDelta(1);
  const sunrealtype dy = latticePatch.getDelta(2);
  const sunrealtype dz = latticePatch.getDelta(3);
  const int nx = latticePatch.discreteSize(1);
  const int ny = latticePatch.discreteSize(2);
  const sunrealtype x0 = latticePatch.origin(1);
  const sunrealtype y0 = latticePatch.origin(2);
  const sunrealtype z0 = latticePatch.origin(3);
  int px = 0, py = 0, pz = 0;
  // 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
    icsettings.eval(static_cast<sunrealtype>(px) * dx + x0,
            static_cast<sunrealtype>(py) * dy + y0,
            static_cast<sunrealtype>(pz) * dz + z0, &latticePatch.uData[i]);
  }
  return;
}

/// Use parameters to add periodic IC layers
void Simulation::addInitialConditions(const int xm, const int ym,
        const int zm /* zm=0 always */ ) {
  const sunrealtype dx = latticePatch.getDelta(1);
  const sunrealtype dy = latticePatch.getDelta(2);
  const sunrealtype dz = latticePatch.getDelta(3);
  const int nx = latticePatch.discreteSize(1);
  const int ny = latticePatch.discreteSize(2);
  // Correct for demanded displacement, rest as for setInitialConditions
  const sunrealtype x0 = latticePatch.origin(1) + xm*lattice.get_tot_lx();
  const sunrealtype y0 = latticePatch.origin(2) + ym*lattice.get_tot_ly();
  const sunrealtype z0 = latticePatch.origin(3) + zm*lattice.get_tot_lz();
  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;
    icsettings.add(static_cast<sunrealtype>(px) * dx + x0,
            static_cast<sunrealtype>(py) * dy + y0,
            static_cast<sunrealtype>(pz) * dz + z0, &latticePatch.uData[i]);
  }
  return;
}

/// Add initial conditions in one dimension
void Simulation::addPeriodicICLayerInX() {
  addInitialConditions(-1, 0, 0);
  addInitialConditions(1, 0, 0);
  return;
}

/// Add initial conditions in two dimensions
void Simulation::addPeriodicICLayerInXY() {
  addInitialConditions(-1, -1, 0);
  addInitialConditions(-1, 0, 0);
  addInitialConditions(-1, 1, 0);
  addInitialConditions(0, 1, 0);
  addInitialConditions(0, -1, 0);
  addInitialConditions(1, -1, 0);
  addInitialConditions(1, 0, 0);
  addInitialConditions(1, 1, 0);
  return;
}

/// Advance the solution in time - integrate the ODE over an interval t
void Simulation::advanceToTime(const sunrealtype &tEnd) {
  checkFlag(SimulationStarted);
  int flag = 0;
  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
                           // reached by the solver as t
  if (flag != CV_SUCCESS)
    printf("CVode failed, flag=%d.\n", flag);
}

/// Write specified simulations steps to disk
void Simulation::outAllFieldData(const int & state) {
  checkFlag(SimulationStarted);
```

```
  outputManager.outUState(state, latticePatch);
}

/// Check the presence configuration flags
void Simulation::checkFlag(unsigned int flag) const {
  if (!(statusFlags & flag)) {
    string errorMessage;
    switch (flag) {
    case LatticeDiscreteSetUp:
      errorMessage = "The discrete size of the Simulation has not been set up";
      break;
    case LatticePhysicalSetUp:
      errorMessage = "The physical size of the Simulation has not been set up";
      break;
    case LatticePatchworkSetUp:
      errorMessage = "The patchwork for the Simulation has not been set up";
      break;
    case CvodeObjectSetUp:
      errorMessage = "The CVODE object has not been initialized";
      break;
    case SimulationStarted:
      errorMessage = "The Simulation has not been started";
      break;
    default:
      errorMessage = "Uppss, you've made a non-standard error, sadly I can't "
                     "help you there";
      break;
    }
    errorKill(errorMessage);
  }
  return;
}

/// Check the absence of configuration flags
void Simulation::checkNoFlag(unsigned int flag) const {
  if ((statusFlags & flag)) {
    string errorMessage;
    switch (flag) {
    case LatticeDiscreteSetUp:
      errorMessage =
          "The discrete size of the Simulation has already been set up";
      break;
    case LatticePhysicalSetUp:
      errorMessage =
          "The physical size of the Simulation has already been set up";
      break;
    case LatticePatchworkSetUp:
      errorMessage = "The patchwork for the Simulation has already been set up";
      break;
    case CvodeObjectSetUp:
      errorMessage = "The CVODE object has already been initialized";
      break;
    case SimulationStarted:
      errorMessage = "The simulation has already started, some changes are no "
                     "longer possible";
      break;
    default:
      errorMessage = "Uppss, you've made a non-standard error, sadly I can't "
                     "help you there";
      break;
    }
    errorKill(errorMessage);
  }
  return;
}
```

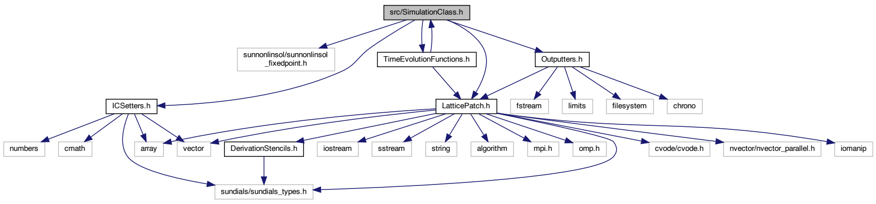
6.22 src/SimulationClass.h File Reference

Class for the Simulation object calling all functionality: from wave settings over lattice construction, time evolution and outputs initialization of the CVode object.

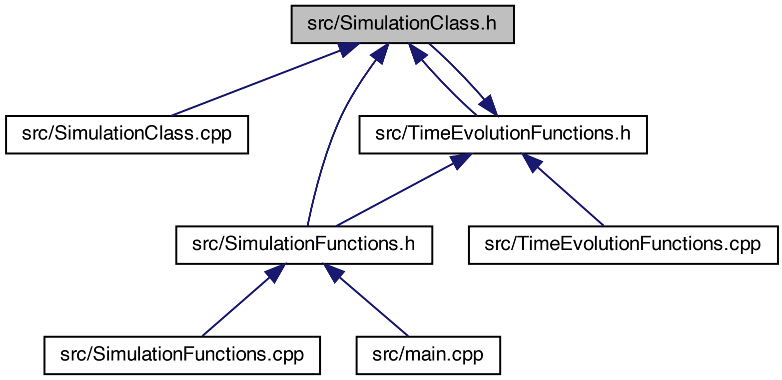
```
#include "sunnonlinsol/sunnonlinsol_fixedpoint.h"
#include "ICSetters.h"
#include "LatticePatch.h"
#include "Outputters.h"
```

```
#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.

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 24 of file SimulationClass.h.

```
00024                         {
00025   LatticeDiscreteSetUp = 0x01,
00026   LatticePhysicalSetUp = 0x02,
00027   LatticePatchworkSetUp = 0x04, // not used anymore
00028   CvodeObjectSetUp = 0x08,
00029   SimulationStarted = 0x10
00030   /*OPT_B = 0x02,
00031   OPT_C = 0x04,
00032   OPT_D = 0x08,
00033   OPT_E = 0x10,
00034   OPT_F = 0x20,*/
00035 };
```

6.23 SimulationClass.h

Go to the documentation of this file.

```
00001 ///////////////////////////////////////////////////////////////////////////////
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
00005 /// initialization of the CVode object
00006 ///////////////////////////////////////////////////////////////////////////////
00007
00008 // Include Guard
00009 #ifndef SIMULATIONCLASS
00010 #define SIMULATIONCLASS
00011
00012 /* access to the fixed point SUNNonlinearSolver */
00013 #include "sunnonlinsol/sunnonlinsol_fixedpoint.h"
00014
00015 // project subfile headers
00016 #include "ICSetters.h"
00017 #include "LatticePatch.h"
00018 #include "Outputters.h"
00019 #include "TimeEvolutionFunctions.h"
00020
00021 using namespace std;
00022
00023 /// simulation checking flags
00024 enum SimulationOptions {
00025   LatticeDiscreteSetUp = 0x01,
00026   LatticePhysicalSetUp = 0x02,
00027   LatticePatchworkSetUp = 0x04, // not used anymore
00028   CvodeObjectSetUp = 0x08,
00029   SimulationStarted = 0x10
00030   /*OPT_B = 0x02,
```

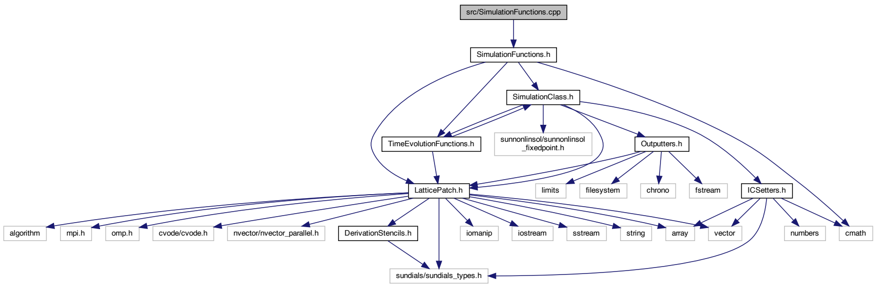
```
  OPT_C = 0x04,
  OPT_D = 0x08,
  OPT_E = 0x10,
  OPT_F = 0x20,*/
};

/** @brief Simulation class to instantiate the whole walkthrough of a Simulation
 */
class Simulation {
private:
  /// Lattice object
  Lattice lattice;
  /// LatticePatch object
  LatticePatch latticePatch;
  /// current time of the simulation
  sunrealtype t;
  /// char for checking simulation flags
  unsigned char statusFlags;

public:
  /// IC Setter object
  ICSetter icsettings;
  /// Output Manager object
  OutputManager outputManager;
  /// Pointer to CVode memory object - public to avoid cross library errors
  void *cvode_mem;
  /// constructor function for the creation of the cartesian communicator
  Simulation(const int nx, const int ny, const int nz, const int StencilOrder,
          const bool periodicity);
  /// destructor function freeing CVode memory and Sundials context
  ~Simulation();
  /// Reference to the cartesian communicator of the lattice -> for debugging
  MPI_Comm *get_cart_comm() { return &lattice.comm; };
  /// function to set discrete dimensions of the lattice
  void setDiscreteDimensionsOfLattice(const sunindextype _tot_nx,
          const sunindextype _tot_ny, const sunindextype _tot_nz);
  /// function to set physical dimensions of the lattice
  void setPhysicalDimensionsOfLattice(const sunrealtype lx, const sunrealtype ly,
                                      const sunrealtype lz);
  /// function to initialize the Patchwork
  void initializePatchwork(const int nx, const int ny, const int nz);
  /// function to initialize the CVODE object with all requirements
  void initializeCVODEobject(const sunrealtype reltol,
                             const sunrealtype abstol);
  /// function to start the simulation for time iteration
  void start();
  /// functions to set the initial field configuration onto the lattice
  void setInitialConditions();
  /// functions to add initial periodic field configurations
  void addInitialConditions(const int xm, const int ym, const int zm = 0);
  /// function to add a periodic IC Layer in one dimension
  void addPeriodicICLayerInX();
  /// function to add periodic IC Layers in two dimensions
  void addPeriodicICLayerInXY();
  /// function to advance solution in time with CVODE
  void advanceToTime(const sunrealtype &tEnd);
  /// function to generate Output of the whole field at a given time
  void outAllFieldData(const int & state);
  /// function to check that a flag has been set and if not print an error
  // message and cause an abort on all ranks
  void checkFlag(unsigned int flag) const;
  /// function to check that if flag has not been set and if print an error
  // message and cause an abort on all ranks
  void checkNoFlag(unsigned int flag) const;
};

// End of Includeguard
#endif
```

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 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 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 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()

```
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 vector< planewave > & planes,
            const vector< gaussian1D > & gaussians )
```

complete 1D Simulation function

Conduct the complete 1D simulation process

Definition at line 23 of file SimulationFunctions.cpp.

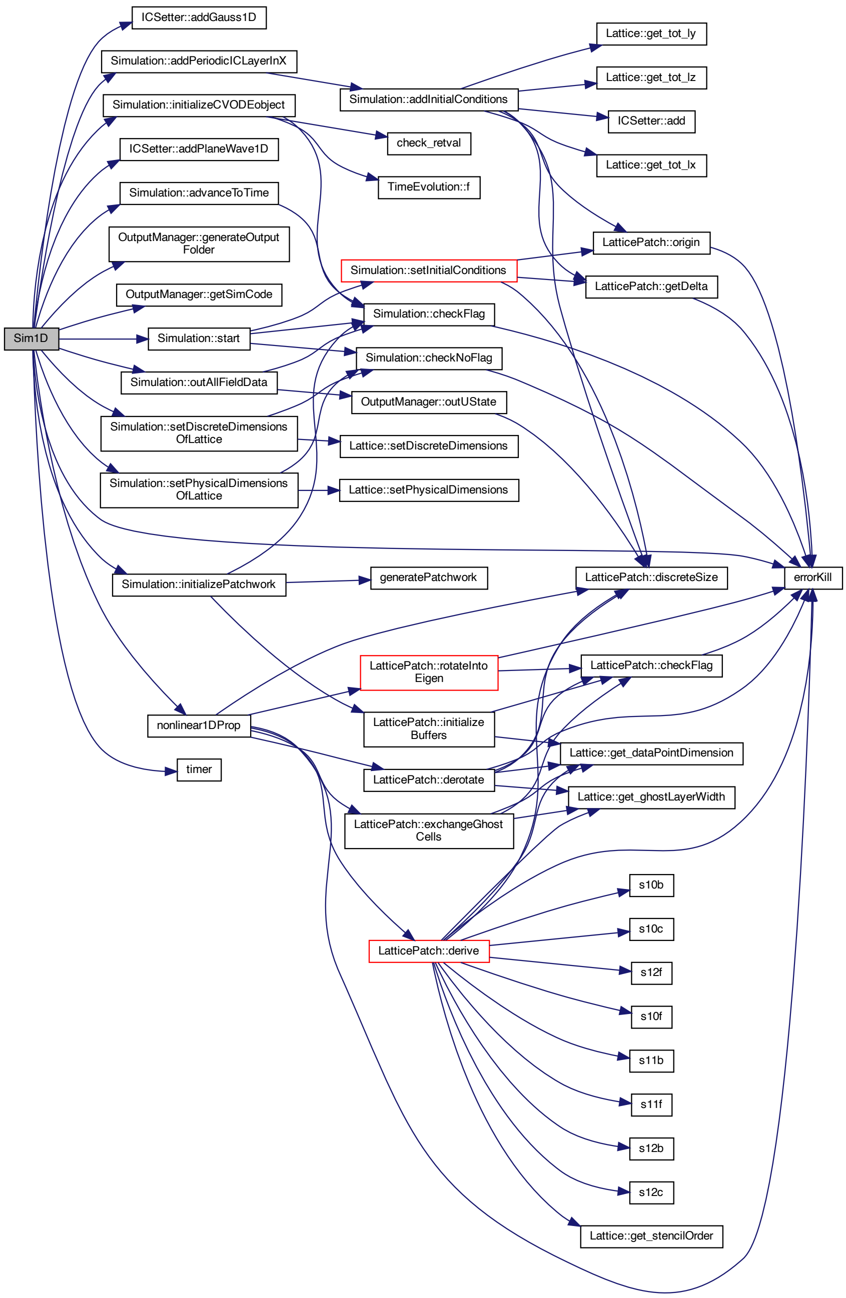
```
                                                    {

        // MPI data
        int myPrc = 0, nprc = 0;
        MPI_Comm_size(MPI_COMM_WORLD, &nprc);
        MPI_Comm_rank(MPI_COMM_WORLD, &myPrc);

        // Check feasibility of the patchwork decomposition
        if (myPrc == 0) {
            if (disc_dim % nprc != 0) {
              errorKill("The number of lattice points must be "
                        "divisible by the number of processes.");
            }
        }

        // Initialize the simulation, set up the cartesian communicator
        array<int, 3> patches = {nprc, 1, 1};
        Simulation sim(patches[0], patches[1], patches[2], StencilOrder, periodic);

        // Configure the patchwork
        sim.setPhysicalDimensionsOfLattice(phys_dim,1,1);
        sim.setDiscreteDimensionsOfLattice(disc_dim,1,1);
        sim.initializePatchwork(patches[0], patches[1], patches[2]);

        // Add em-waves
        for (const auto gauss : gaussians)
          sim.icsettings.addGauss1D(gauss.k, gauss.p, gauss.x0, gauss.phig,
                                    gauss.phi);
        for (const auto plane : planes)
          sim.icsettings.addPlaneWave1D(plane.k, plane.p, plane.phi);

        // Check that the patchwork is ready and set the initial conditions
        sim.start();
        sim.addPeriodicICLayerInX();

        // Initialize CVode with abs and rel tolerances
        sim.initializeCVODEobject(CVodeTol[0], CVodeTol[1]);

        // Configure the time evolution function
        TimeEvolution::c = interactions;
        TimeEvolution::TimeEvolver = nonlinear1DProp;

        // Configure the output
        sim.outputManager.generateOutputFolder(outputDirectory);
        if (!myPrc) {
          cout « "Simulation code: " « sim.outputManager.getSimCode() « endl;
        }

        // Conduct the propagation in space and time
        double ts = MPI_Wtime();
        for (int step = 1; step <= numberOfSteps; step++) {
          sim.advanceToTime(endTime / numberOfSteps * step);
          if (step % outputStep == 0) {
            sim.outAllFieldData(step);
          }
```

```
    double tn = MPI_Wtime();
    if (!myPrc) {
      cout « "\rStep " « step « "\t\t" « flush;
      timer(ts, tn);
    }
  }

  return;
}
```

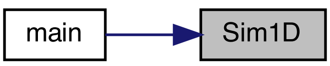
References ICSetter::addGauss1D(), Simulation::addPeriodicICLayerInX(), ICSetter::addPlaneWave1D(), Simulation::advanceToTime(), TimeEvolution::c, errorKill(), OutputManager::generateOutputFolder(), OutputManager::getSimCode(), Simulation::icsettings, Simulation::initializeCVODEobject(), Simulation::initializePatchwork(), nonlinear1DProp(), Simulation::outAllFieldData(), Simulation::outputManager, Simulation::setDiscreteDimensionsOfLattice(), Simulation::setPhysicalDime 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()

```
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 vector< planewave > & planes,
            const vector< gaussian2D > & gaussians )
```

complete 2D Simulation function

Conduct the complete 2D simulation process

Definition at line 95 of file SimulationFunctions.cpp.

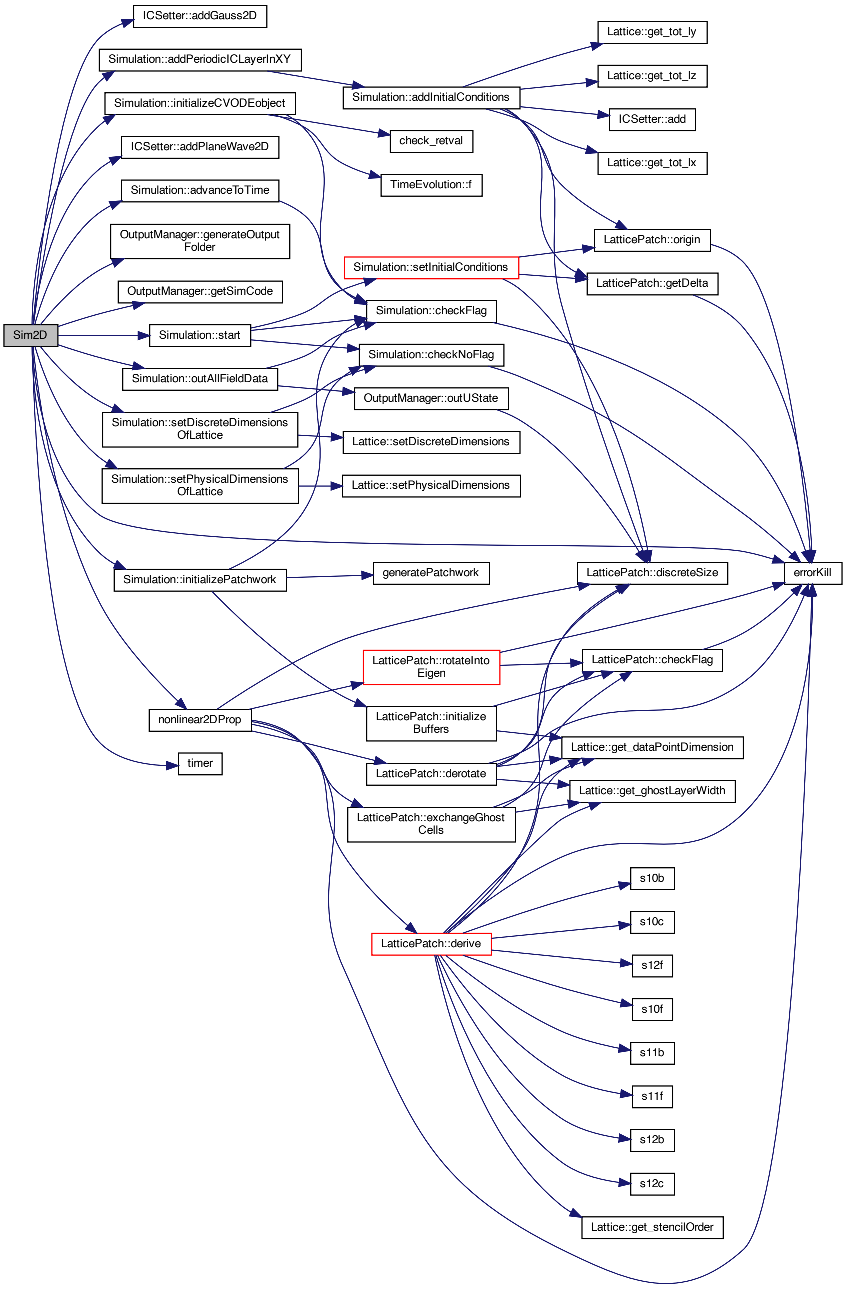
```
                                              {

  // MPI data
  int myPrc = 0, nprc = 0; // Get process rank and number of processes
  MPI_Comm_rank(MPI_COMM_WORLD,
                &myPrc); // Return process rank, number \in [1,nprc]
  MPI_Comm_size(MPI_COMM_WORLD,
                &nprc); // Return number of processes (communicator size)

  // Check feasibility of the patchwork decomposition
  if (myPrc == 0) {
    if (nprc != patches[0] * patches[1]) {
      errorKill(
          "The number of MPI processes must match the number of patches.");
    }
  }

  // Initialize the simulation, set up the cartesian communicator
  Simulation sim(patches[0], patches[1], 1, StencilOrder, periodic);

  // Configure the patchwork
  sim.setPhysicalDimensionsOfLattice(phys_dims[0],
                                     phys_dims[1],
                                     1); // spacing of the lattice
  sim.setDiscreteDimensionsOfLattice(
      disc_dims[0], disc_dims[1], 1); // Spacing equivalence to points
  sim.initializePatchwork(patches[0], patches[1], 1);

  // Add em-waves
  for (const auto gauss : gaussians)
    sim.icsettings.addGauss2D(gauss.x0, gauss.axis, gauss.amp, gauss.phip,
                              gauss.w0, gauss.zr, gauss.ph0, gauss.phA);
  for (const auto plane : planes)
    sim.icsettings.addPlaneWave2D(plane.k, plane.p, plane.phi);

  // Check that the patchwork is ready and set the initial conditions
  sim.start(); // Check if the lattice is set up, set initial field
               // configuration
  sim.addPeriodicICLayerInXY(); // insure periodicity in propagation directions

  // Initialize CVode with rel and abs tolerances
  sim.initializeCVODEobject(CVodeTol[0], CVodeTol[1]);

  // Configure the time evolution function
  TimeEvolution::c = interactions;
  TimeEvolution::TimeEvolver = nonlinear2DProp;

  // Configure the output
  sim.outputManager.generateOutputFolder(outputDirectory);
```

```
  if (!myPrc) {
    cout « "Simulation code: " « sim.outputManager.getSimCode() « endl;
  }
  double ts = MPI_Wtime();

  // Conduct the propagation in space and time
  for (int step = 1; step <= numberOfSteps; step++) {
    sim.advanceToTime(endTime / numberOfSteps * step);
    if (step % outputStep == 0) {
      sim.outAllFieldData(step);
    }
    double tn = MPI_Wtime();
    if (!myPrc) {
      cout « "\rStep " « step « "\t\t" « flush;
      timer(ts, tn);
    }
  }

  return;
}
```

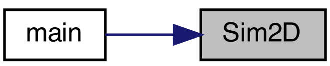
References ICSetter::addGauss2D(), Simulation::addPeriodicICLayerInXY(), ICSetter::addPlaneWave2D(), Simulation::advanceToTime(), TimeEvolution::c, errorKill(), OutputManager::generateOutputFolder(), OutputManager::getSimCode(), Simulation::icsettings, Simulation::initializeCVODEobject(), Simulation::initializePatchwork(), nonlinear2DProp(), Simulation::outAllFieldData(), Simulation::outputManager, Simulation::setDiscreteDimensionsOfLattice(), Simulation::setPhysicalDime 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()

```
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 vector< planewave > & planes,
            const vector< gaussian3D > & gaussians )
```

complete 3D Simulation function

Conduct the complete 3D simulation process

Definition at line 172 of file SimulationFunctions.cpp.

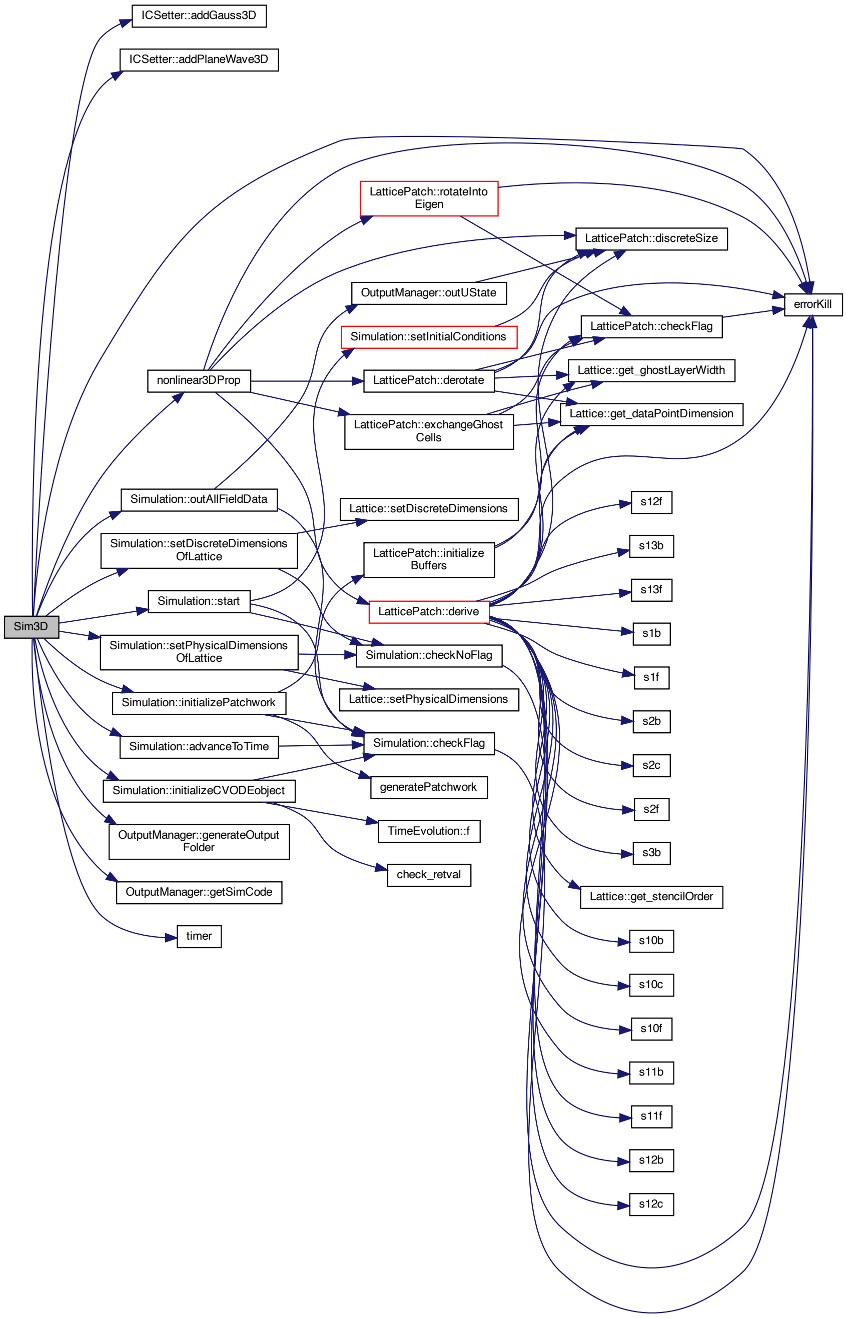
```
                                                   {

  // MPI data
  int myPrc = 0, nprc = 0; // Get process rank and numer of process
  MPI_Comm_rank(MPI_COMM_WORLD,
                &myPrc); // rank of the process inside the world communicator
  MPI_Comm_size(MPI_COMM_WORLD,
                &nprc); // Size of the communicator is the number of processes

  // Check feasibility of the patchwork decomposition
  if (myPrc == 0) {
    if (nprc != patches[0] * patches[1] * patches[2]) {
      errorKill(
          "The number of MPI processes must match the number of patches.");
    }
    if (disc_dims[0] / patches[0] != disc_dims[1] / patches[1] |
        disc_dims[0] / patches[0] != disc_dims[2] / patches[2]) {
      clog
          « "\nWarning: Patches should be cubic in terms of the lattice "
             "points for the computational efficiency of larger simulations.\n";
    }
  }

  // Initialize the simulation, set up the cartesian communicator
  Simulation sim(patches[0], patches[1], patches[2],
                 StencilOrder, periodic); // Simulation object with slicing

  // Create the SUNContext object associated with the thread of execution
  sim.setPhysicalDimensionsOfLattice(phys_dims[0], phys_dims[1],
                                     phys_dims[2]); // spacing of the box
  sim.setDiscreteDimensionsOfLattice(
      disc_dims[0], disc_dims[1],
      disc_dims[2]); // Spacing equivalence to points
  sim.initializePatchwork(patches[0], patches[1], patches[2]);

  // Add em-waves
  for (const auto plane : planes)
    sim.icsettings.addPlaneWave3D(plane.k, plane.p, plane.phi);
  for (const auto gauss : gaussians)
    sim.icsettings.addGauss3D(gauss.x0, gauss.axis, gauss.amp, gauss.phip,
                              gauss.w0, gauss.zr, gauss.ph0, gauss.phA);

  // Check that the patchwork is ready and set the initial conditions
  sim.start();

  // Initialize CVode with abs and rel tolerances
  sim.initializeCVODEobject(CVodeTol[0], CVodeTol[1]);

  // Configure the time evolution function
```

```
  TimeEvolution::c = interactions;
  TimeEvolution::TimeEvolver = nonlinear3DProp;

  // Configure the output
  sim.outputManager.generateOutputFolder(outputDirectory);
  if (!myPrc) {
    cout « "Simulation code: " « sim.outputManager.getSimCode() « endl;
  }
  double ts = MPI_Wtime();

  // Conduct the propagation in space and time
  for (int step = 1; step <= numberOfSteps; step++) {
    sim.advanceToTime(endTime / numberOfSteps * step);
    if (step % outputStep == 0) {
      sim.outAllFieldData(step);
    }
    double tn = MPI_Wtime();
    if (!myPrc) {
      cout « "\rStep " « step « "\t\t" « flush;
      timer(ts, tn);
    }
  }
  return;
}
```

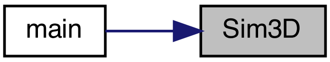
References ICSetter::addGauss3D(), ICSetter::addPlaneWave3D(), Simulation::advanceToTime(), TimeEvolution::c, errorKill(), OutputManager::generateOutputFolder(), OutputManager::getSimCode(), Simulation::icsettings, Simulation::initializeCVODEobject(), Simulation::initializePatchwork(), nonlinear3DProp(), Simulation::outAllFieldData(), Simulation::outputManager, 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 (
            double & t1,
            double & t2 )
```

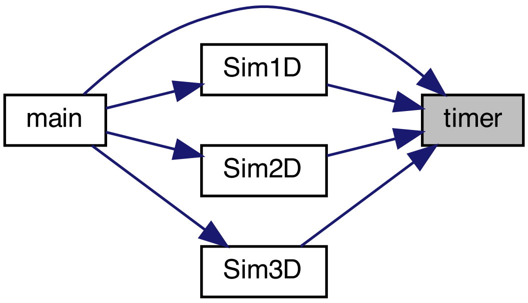
Calculate and print the total simulation time

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.

```
////////////////////////////////////////////////////////////////////////
/// @file SimulationFunctions.cpp
/// @brief Implementation of the complete simulation functions for
/// 1D, 2D, and 3D, as called in the main function
////////////////////////////////////////////////////////////////////////

#include "SimulationFunctions.h"

using namespace std;

/** Calculate and print the total simulation time */
void timer(double &t1, double &t2) {
  printf("Elapsed time:  %fs\n", (t2 - t1));
}

// Instantiate and preliminarily initialize the time evolver
// non-const statics to be defined in actual simulation process
int *TimeEvolution::c = nullptr;
void (*TimeEvolution::TimeEvolver)(LatticePatch *, N_Vector, N_Vector,
                                   int *) = nonlinear1DProp;

/** Conduct the complete 1D simulation process */
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 vector<planewave> &planes,
        const vector<gaussian1D> &gaussians) {

  // MPI data
  int myPrc = 0, nprc = 0;
  MPI_Comm_size(MPI_COMM_WORLD, &nprc);
  MPI_Comm_rank(MPI_COMM_WORLD, &myPrc);

  // Check feasibility of the patchwork decomposition
  if (myPrc == 0) {
      if (disc_dim % nprc != 0) {
        errorKill("The number of lattice points must be "
                  "divisible by the number of processes.");
      }
  }

  // Initialize the simulation, set up the cartesian communicator
  array<int, 3> patches = {nprc, 1, 1};
  Simulation sim(patches[0], patches[1], patches[2], StencilOrder, periodic);

  // Configure the patchwork
  sim.setPhysicalDimensionsOfLattice(phys_dim,1,1);
  sim.setDiscreteDimensionsOfLattice(disc_dim,1,1);
  sim.initializePatchwork(patches[0], patches[1], patches[2]);

  // Add em-waves
  for (const auto gauss : gaussians)
    sim.icsettings.addGauss1D(gauss.k, gauss.p, gauss.x0, gauss.phig,
                              gauss.phi);
  for (const auto plane : planes)
    sim.icsettings.addPlaneWave1D(plane.k, plane.p, plane.phi);

  // Check that the patchwork is ready and set the initial conditions
  sim.start();
  sim.addPeriodicICLayerInX();

  // Initialize CVode with abs and rel tolerances
  sim.initializeCVODEobject(CVodeTol[0], CVodeTol[1]);

  // Configure the time evolution function
  TimeEvolution::c = interactions;
  TimeEvolution::TimeEvolver = nonlinear1DProp;

  // Configure the output
  sim.outputManager.generateOutputFolder(outputDirectory);
  if (!myPrc) {
    cout « "Simulation code: " « sim.outputManager.getSimCode() « endl;
  }

  // Conduct the propagation in space and time
  double ts = MPI_Wtime();
  for (int step = 1; step <= numberOfSteps; step++) {
    sim.advanceToTime(endTime / numberOfSteps * step);
    if (step % outputStep == 0) {
      sim.outAllFieldData(step);
```

```
    }
    double tn = MPI_Wtime();
    if (!myPrc) {
      cout « "\rStep " « step « "\t\t" « flush;
      timer(ts, tn);
    }
  }

  return;
}

/** Conduct the complete 2D simulation process */
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 vector<planewave> &planes,
        const vector<gaussian2D> &gaussians) {

  // MPI data
  int myPrc = 0, nprc = 0; // Get process rank and number of processes
  MPI_Comm_rank(MPI_COMM_WORLD,
                &myPrc); // Return process rank, number \in [1,nprc]
  MPI_Comm_size(MPI_COMM_WORLD,
                &nprc); // Return number of processes (communicator size)

  // Check feasibility of the patchwork decomposition
  if (myPrc == 0) {
    if (nprc != patches[0] * patches[1]) {
      errorKill(
          "The number of MPI processes must match the number of patches.");
    }
  }

  // Initialize the simulation, set up the cartesian communicator
  Simulation sim(patches[0], patches[1], 1, StencilOrder, periodic);

  // Configure the patchwork
  sim.setPhysicalDimensionsOfLattice(phys_dims[0],
                                     phys_dims[1],
                                     1); // spacing of the lattice
  sim.setDiscreteDimensionsOfLattice(
      disc_dims[0], disc_dims[1], 1); // Spacing equivalence to points
  sim.initializePatchwork(patches[0], patches[1], 1);

  // Add em-waves
  for (const auto gauss : gaussians)
    sim.icsettings.addGauss2D(gauss.x0, gauss.axis, gauss.amp, gauss.phip,
                              gauss.w0, gauss.zr, gauss.ph0, gauss.phA);
  for (const auto plane : planes)
    sim.icsettings.addPlaneWave2D(plane.k, plane.p, plane.phi);

  // Check that the patchwork is ready and set the initial conditions
  sim.start(); // Check if the lattice is set up, set initial field
               // configuration
  sim.addPeriodicICLayerInXY(); // insure periodicity in propagation directions

  // Initialize CVode with rel and abs tolerances
  sim.initializeCVODEobject(CVodeTol[0], CVodeTol[1]);

  // Configure the time evolution function
  TimeEvolution::c = interactions;
  TimeEvolution::TimeEvolver = nonlinear2DProp;

  // Configure the output
  sim.outputManager.generateOutputFolder(outputDirectory);
  if (!myPrc) {
    cout « "Simulation code: " « sim.outputManager.getSimCode() « endl;
  }
  double ts = MPI_Wtime();

  // Conduct the propagation in space and time
  for (int step = 1; step <= numberOfSteps; step++) {
    sim.advanceToTime(endTime / numberOfSteps * step);
    if (step % outputStep == 0) {
      sim.outAllFieldData(step);
    }
    double tn = MPI_Wtime();
    if (!myPrc) {
      cout « "\rStep " « step « "\t\t" « flush;
      timer(ts, tn);
    }
  }

  return;
}
```

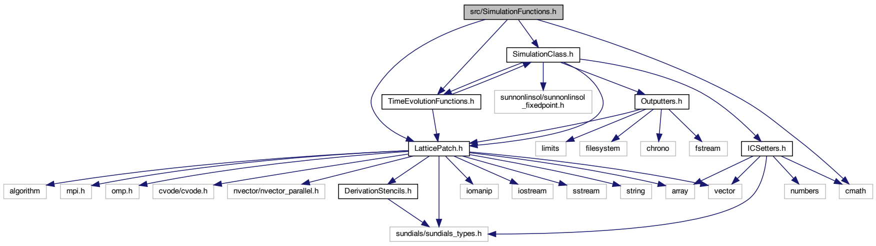
```
/** Conduct the complete 3D simulation process */
void Sim3D(const array<sunrealtype,2> CVodeTol, const int StencilOrder,
        const array<sunrealtype,3> phys_dims,
        const array<sunindextype,3> disc_dims, const array<int,3> patches,
        const bool periodic, int *interactions, const sunrealtype endTime,
        const int numberOfSteps, const string outputDirectory,
        const int outputStep, const vector<planewave> &planes,
        const vector<gaussian3D> &gaussians) {

  // MPI data
  int myPrc = 0, nprc = 0; // Get process rank and numer of process
  MPI_Comm_rank(MPI_COMM_WORLD,
                &myPrc); // rank of the process inside the world communicator
  MPI_Comm_size(MPI_COMM_WORLD,
                &nprc); // Size of the communicator is the number of processes

  // Check feasibility of the patchwork decomposition
  if (myPrc == 0) {
    if (nprc != patches[0] * patches[1] * patches[2]) {
      errorKill(
          "The number of MPI processes must match the number of patches.");
    }
    if (disc_dims[0] / patches[0] != disc_dims[1] / patches[1] |
        disc_dims[0] / patches[0] != disc_dims[2] / patches[2]) {
      clog
          « "\nWarning: Patches should be cubic in terms of the lattice "
             "points for the computational efficiency of larger simulations.\n";
    }
  }

  // Initialize the simulation, set up the cartesian communicator
  Simulation sim(patches[0], patches[1], patches[2],
                 StencilOrder, periodic); // Simulation object with slicing

  // Create the SUNContext object associated with the thread of execution
  sim.setPhysicalDimensionsOfLattice(phys_dims[0], phys_dims[1],
                                     phys_dims[2]); // spacing of the box
  sim.setDiscreteDimensionsOfLattice(
      disc_dims[0], disc_dims[1],
      disc_dims[2]); // Spacing equivalence to points
  sim.initializePatchwork(patches[0], patches[1], patches[2]);

  // Add em-waves
  for (const auto plane : planes)
    sim.icsettings.addPlaneWave3D(plane.k, plane.p, plane.phi);
  for (const auto gauss : gaussians)
    sim.icsettings.addGauss3D(gauss.x0, gauss.axis, gauss.amp, gauss.phip,
                              gauss.w0, gauss.zr, gauss.ph0, gauss.phA);

  // Check that the patchwork is ready and set the initial conditions
  sim.start();

  // Initialize CVode with abs and rel tolerances
  sim.initializeCVODEobject(CVodeTol[0], CVodeTol[1]);

  // Configure the time evolution function
  TimeEvolution::c = interactions;
  TimeEvolution::TimeEvolver = nonlinear3DProp;

  // Configure the output
  sim.outputManager.generateOutputFolder(outputDirectory);
  if (!myPrc) {
    cout « "Simulation code: " « sim.outputManager.getSimCode() « endl;
  }
  double ts = MPI_Wtime();

  // Conduct the propagation in space and time
  for (int step = 1; step <= numberOfSteps; step++) {
    sim.advanceToTime(endTime / numberOfSteps * step);
    if (step % outputStep == 0) {
      sim.outAllFieldData(step);
    }
    double tn = MPI_Wtime();
    if (!myPrc) {
      cout « "\rStep " « step « "\t\t" « flush;
      timer(ts, tn);
    }
  }
  return;
}
```

6.26 src/SimulationFunctions.h File Reference

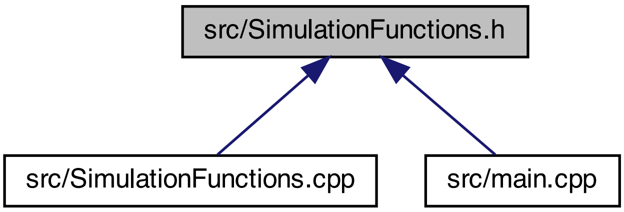
Full simulation functions for 1D, 2D, and 3D used in main.cpp.

```
#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 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 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 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()

```
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 vector< planewave > & planes,
            const vector< gaussian1D > & gaussians )
```

complete 1D Simulation function

Conduct the complete 1D simulation process

Definition at line 23 of file SimulationFunctions.cpp.

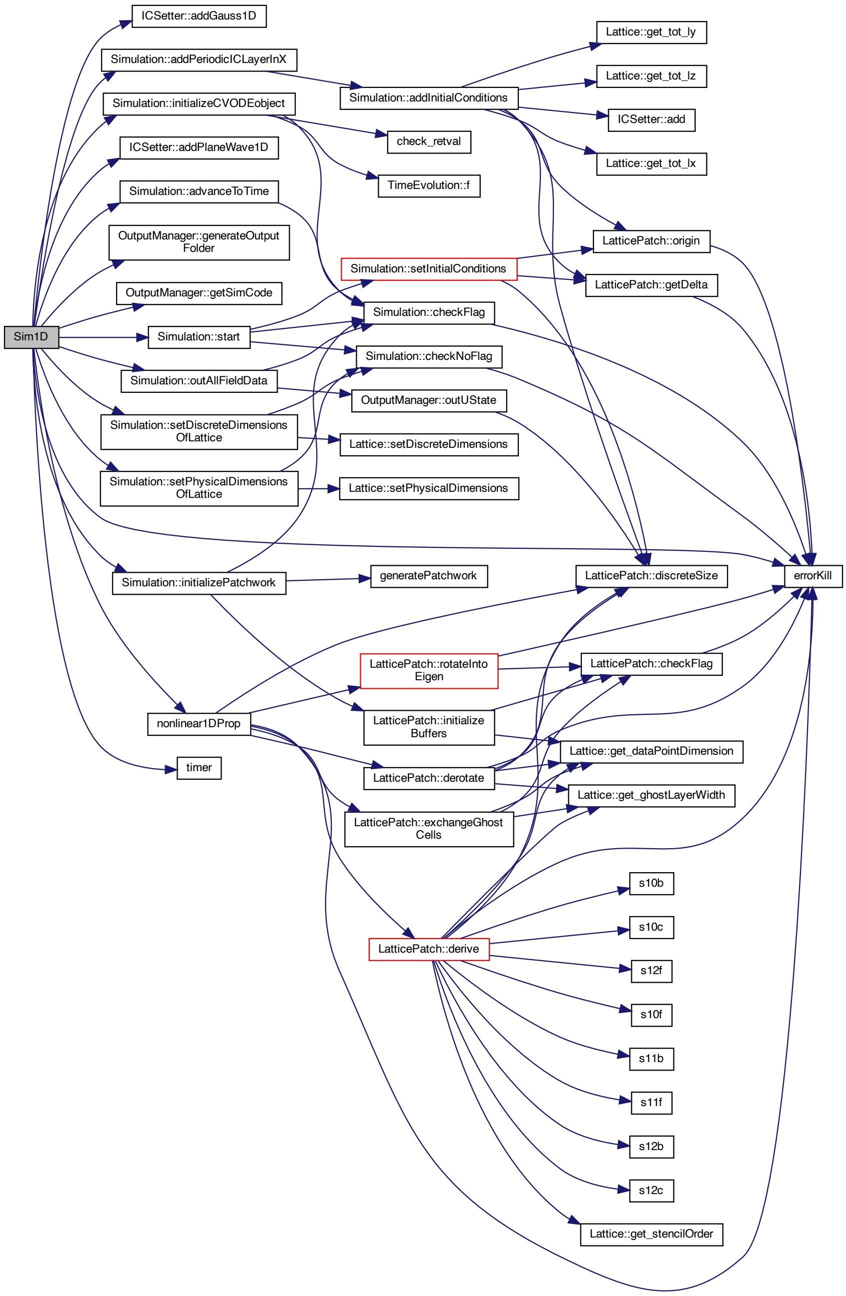
```
00029                                                     {
00030 
00031   // MPI data
00032   int myPrc = 0, nprc = 0;
00033   MPI_Comm_size(MPI_COMM_WORLD, &nprc);
00034   MPI_Comm_rank(MPI_COMM_WORLD, &myPrc);
00035 
00036   // Check feasibility of the patchwork decomposition
```

```
  if (myPrc == 0) {
      if (disc_dim % nprc != 0) {
        errorKill("The number of lattice points must be "
                  "divisible by the number of processes.");
      }
  }

  // Initialize the simulation, set up the cartesian communicator
  array<int, 3> patches = {nprc, 1, 1};
  Simulation sim(patches[0], patches[1], patches[2], StencilOrder, periodic);

  // Configure the patchwork
  sim.setPhysicalDimensionsOfLattice(phys_dim,1,1);
  sim.setDiscreteDimensionsOfLattice(disc_dim,1,1);
  sim.initializePatchwork(patches[0], patches[1], patches[2]);

  // Add em-waves
  for (const auto gauss : gaussians)
    sim.icsettings.addGauss1D(gauss.k, gauss.p, gauss.x0, gauss.phig,
                              gauss.phi);
  for (const auto plane : planes)
    sim.icsettings.addPlaneWave1D(plane.k, plane.p, plane.phi);

  // Check that the patchwork is ready and set the initial conditions
  sim.start();
  sim.addPeriodicICLayerInX();

  // Initialize CVode with abs and rel tolerances
  sim.initializeCVODEobject(CVodeTol[0], CVodeTol[1]);

  // Configure the time evolution function
  TimeEvolution::c = interactions;
  TimeEvolution::TimeEvolver = nonlinear1DProp;

  // Configure the output
  sim.outputManager.generateOutputFolder(outputDirectory);
  if (!myPrc) {
    cout « "Simulation code: " « sim.outputManager.getSimCode() « endl;
  }

  // Conduct the propagation in space and time
  double ts = MPI_Wtime();
  for (int step = 1; step <= numberOfSteps; step++) {
    sim.advanceToTime(endTime / numberOfSteps * step);
    if (step % outputStep == 0) {
      sim.outAllFieldData(step);
    }
    double tn = MPI_Wtime();
    if (!myPrc) {
      cout « "\rStep " « step « "\t\t" « flush;
      timer(ts, tn);
    }
  }

  return;
}
```

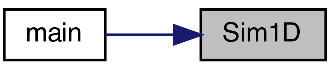
References ICSetter::addGauss1D(), Simulation::addPeriodicICLayerInX(), ICSetter::addPlaneWave1D(), Simulation::advanceToTime(), TimeEvolution::c, errorKill(), OutputManager::generateOutputFolder(), OutputManager::getSimCode(), Simulation::icsettings, Simulation::initializeCVODEobject(), Simulation::initializePatchwork(), nonlinear1DProp(), Simulation::outAllFieldData(), Simulation::outputManager, Simulation::setDiscreteDimensionsOfLattice(), Simulation::setPhysicalDime
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()

```
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 vector< planewave > & planes,
            const vector< gaussian2D > & gaussians )
```

complete 2D Simulation function

Conduct the complete 2D simulation process

Definition at line 95 of file SimulationFunctions.cpp.

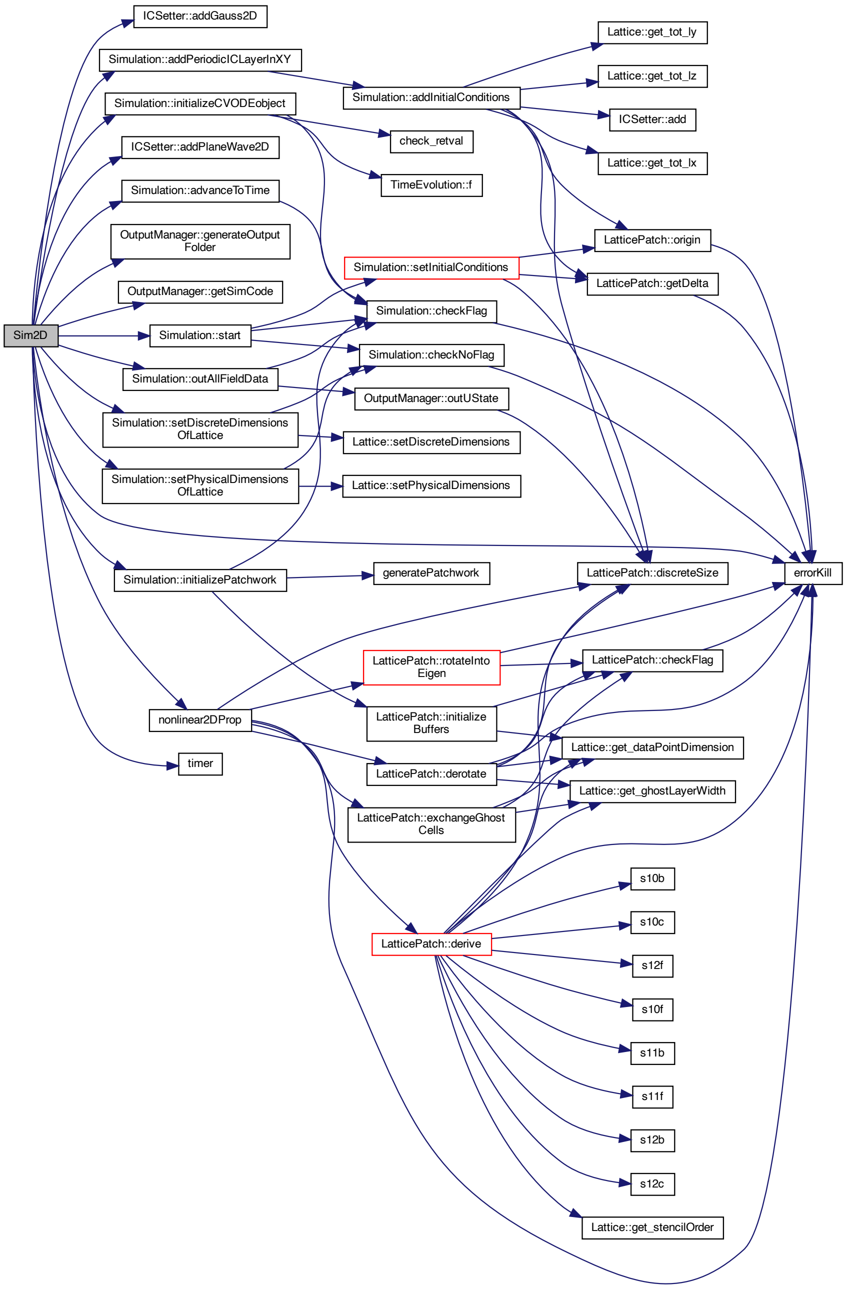
```
                                            {

  // MPI data
  int myPrc = 0, nprc = 0; // Get process rank and number of processes
  MPI_Comm_rank(MPI_COMM_WORLD,
                &myPrc); // Return process rank, number \in [1,nprc]
  MPI_Comm_size(MPI_COMM_WORLD,
                &nprc); // Return number of processes (communicator size)

  // Check feasibility of the patchwork decomposition
  if (myPrc == 0) {
    if (nprc != patches[0] * patches[1]) {
      errorKill(
          "The number of MPI processes must match the number of patches.");
    }
  }

  // Initialize the simulation, set up the cartesian communicator
  Simulation sim(patches[0], patches[1], 1, StencilOrder, periodic);

  // Configure the patchwork
  sim.setPhysicalDimensionsOfLattice(phys_dims[0],
                                     phys_dims[1],
                                     1); // spacing of the lattice
  sim.setDiscreteDimensionsOfLattice(
      disc_dims[0], disc_dims[1], 1); // Spacing equivalence to points
  sim.initializePatchwork(patches[0], patches[1], 1);

  // Add em-waves
  for (const auto gauss : gaussians)
    sim.icsettings.addGauss2D(gauss.x0, gauss.axis, gauss.amp, gauss.phip,
                              gauss.w0, gauss.zr, gauss.ph0, gauss.phA);
  for (const auto plane : planes)
    sim.icsettings.addPlaneWave2D(plane.k, plane.p, plane.phi);

  // Check that the patchwork is ready and set the initial conditions
  sim.start(); // Check if the lattice is set up, set initial field
               // configuration
  sim.addPeriodicICLayerInXY(); // insure periodicity in propagation directions

  // Initialize CVode with rel and abs tolerances
  sim.initializeCVODEobject(CVodeTol[0], CVodeTol[1]);

  // Configure the time evolution function
  TimeEvolution::c = interactions;
  TimeEvolution::TimeEvolver = nonlinear2DProp;

  // Configure the output
  sim.outputManager.generateOutputFolder(outputDirectory);
```

```
  if (!myPrc) {
    cout « "Simulation code: " « sim.outputManager.getSimCode() « endl;
  }
  double ts = MPI_Wtime();

  // Conduct the propagation in space and time
  for (int step = 1; step <= numberOfSteps; step++) {
    sim.advanceToTime(endTime / numberOfSteps * step);
    if (step % outputStep == 0) {
      sim.outAllFieldData(step);
    }
    double tn = MPI_Wtime();
    if (!myPrc) {
      cout « "\rStep " « step « "\t\t" « flush;
      timer(ts, tn);
    }
  }

  return;
}
```

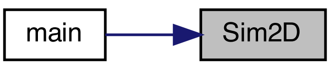
References ICSetter::addGauss2D(), Simulation::addPeriodicICLayerInXY(), ICSetter::addPlaneWave2D(), Simulation::advanceToTime(), TimeEvolution::c, errorKill(), OutputManager::generateOutputFolder(), OutputManager::getSimCode(), Simulation::icsettings, Simulation::initializeCVODEobject(), Simulation::initializePatchwork(), nonlinear2DProp(), Simulation::outAllFieldData(), Simulation::outputManager, Simulation::setDiscreteDimensionsOfLattice(), Simulation::setPhysicalDime 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()

```
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 vector< planewave > & planes,
            const vector< gaussian3D > & gaussians )
```

complete 3D Simulation function

Conduct the complete 3D simulation process

Definition at line 172 of file SimulationFunctions.cpp.

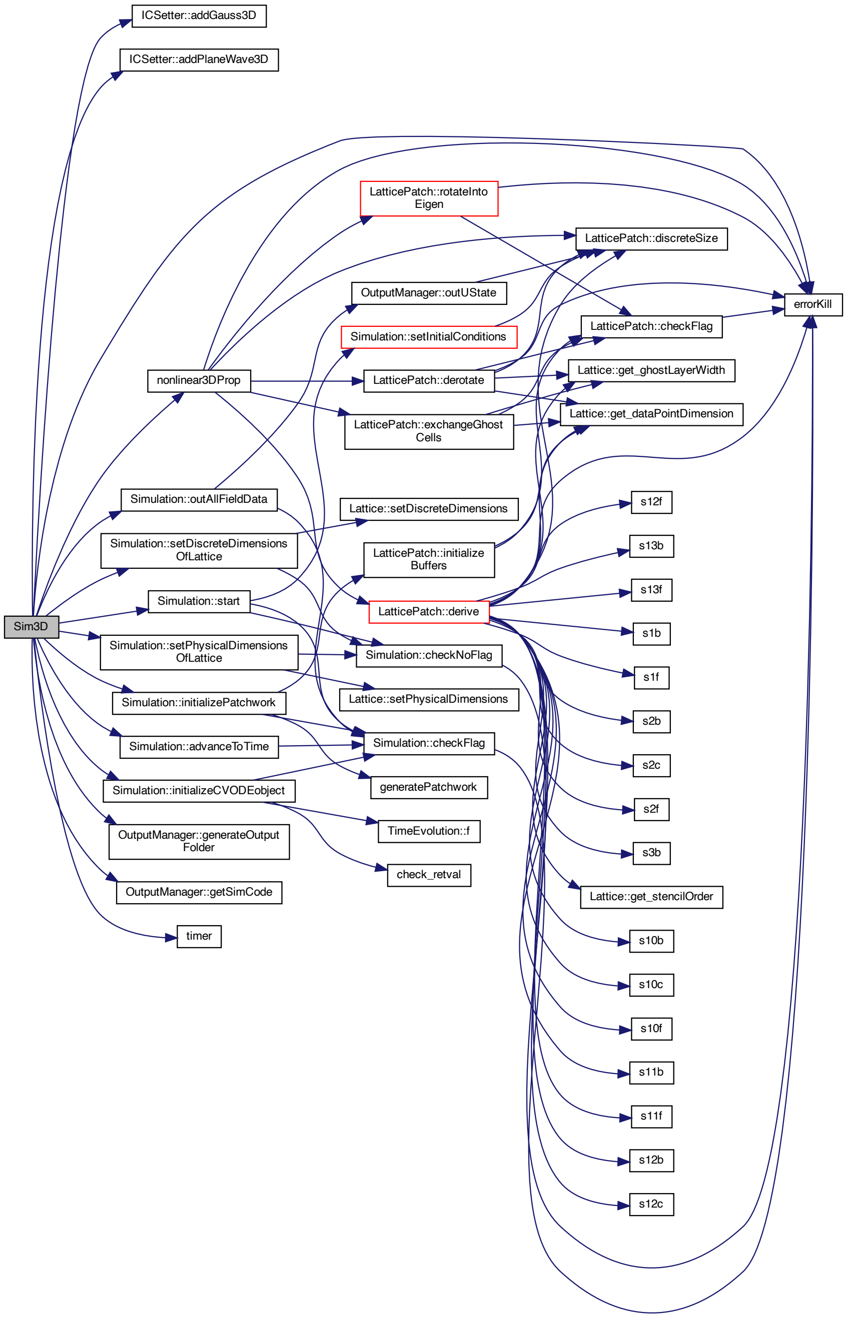
```
                                            {

  // MPI data
  int myPrc = 0, nprc = 0; // Get process rank and numer of process
  MPI_Comm_rank(MPI_COMM_WORLD,
                &myPrc); // rank of the process inside the world communicator
  MPI_Comm_size(MPI_COMM_WORLD,
                &nprc); // Size of the communicator is the number of processes

  // Check feasibility of the patchwork decomposition
  if (myPrc == 0) {
    if (nprc != patches[0] * patches[1] * patches[2]) {
      errorKill(
          "The number of MPI processes must match the number of patches.");
    }
    if (disc_dims[0] / patches[0] != disc_dims[1] / patches[1] |
        disc_dims[0] / patches[0] != disc_dims[2] / patches[2]) {
      clog
          « "\nWarning: Patches should be cubic in terms of the lattice "
             "points for the computational efficiency of larger simulations.\n";
    }
  }

  // Initialize the simulation, set up the cartesian communicator
  Simulation sim(patches[0], patches[1], patches[2],
                 StencilOrder, periodic); // Simulation object with slicing

  // Create the SUNContext object associated with the thread of execution
  sim.setPhysicalDimensionsOfLattice(phys_dims[0], phys_dims[1],
                                     phys_dims[2]); // spacing of the box
  sim.setDiscreteDimensionsOfLattice(
      disc_dims[0], disc_dims[1],
      disc_dims[2]); // Spacing equivalence to points
  sim.initializePatchwork(patches[0], patches[1], patches[2]);

  // Add em-waves
  for (const auto plane : planes)
    sim.icsettings.addPlaneWave3D(plane.k, plane.p, plane.phi);
  for (const auto gauss : gaussians)
    sim.icsettings.addGauss3D(gauss.x0, gauss.axis, gauss.amp, gauss.phip,
                              gauss.w0, gauss.zr, gauss.ph0, gauss.phA);

  // Check that the patchwork is ready and set the initial conditions
  sim.start();

  // Initialize CVode with abs and rel tolerances
  sim.initializeCVODEobject(CVodeTol[0], CVodeTol[1]);

  // Configure the time evolution function
```

```
  TimeEvolution::c = interactions;
  TimeEvolution::TimeEvolver = nonlinear3DProp;

  // Configure the output
  sim.outputManager.generateOutputFolder(outputDirectory);
  if (!myPrc) {
    cout « "Simulation code: " « sim.outputManager.getSimCode() « endl;
  }
  double ts = MPI_Wtime();

  // Conduct the propagation in space and time
  for (int step = 1; step <= numberOfSteps; step++) {
    sim.advanceToTime(endTime / numberOfSteps * step);
    if (step % outputStep == 0) {
      sim.outAllFieldData(step);
    }
    double tn = MPI_Wtime();
    if (!myPrc) {
      cout « "\rStep " « step « "\t\t" « flush;
      timer(ts, tn);
    }
  }
  return;
}
```

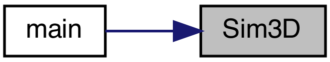
References ICSetter::addGauss3D(), ICSetter::addPlaneWave3D(), Simulation::advanceToTime(), TimeEvolution::c, errorKill(), OutputManager::generateOutputFolder(), OutputManager::getSimCode(), Simulation::icsettings, Simulation::initializeCVODEobject(), Simulation::initializePatchwork(), nonlinear3DProp(), Simulation::outAllFieldData(), Simulation::outputManager, 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 (
            double & t1,
            double & t2 )
```

MPI timer function

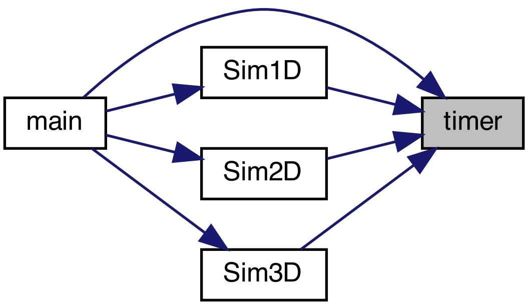
Calculate and print the total simulation time

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:



6.27 SimulationFunctions.h

Go to the documentation of this file.

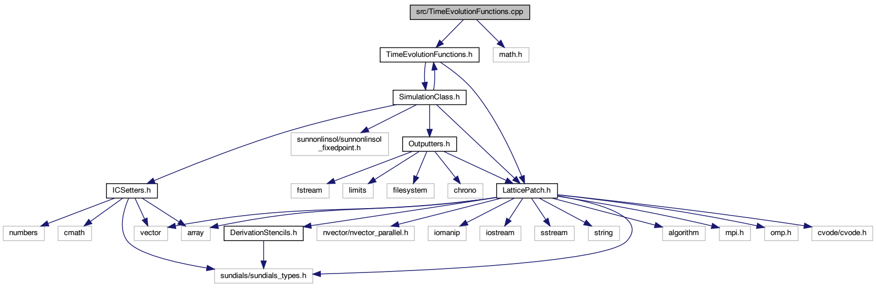
```
///////////////////////////////////////////////////////////////////////////////
/// @file SimulationFunctions.h
/// @brief Full simulation functions for 1D, 2D, and 3D used in main.cpp
///////////////////////////////////////////////////////////////////////////////

// math
#include <cmath>
//#include <mathimf.h>

// project subfile headers
#include "LatticePatch.h"
#include "SimulationClass.h"
#include "TimeEvolutionFunctions.h"

/****** EM-wave structures ******/

/// plane wave structure
struct planewave {
  vector<sunrealtype> k;   /**< wavevector (normalized to \f$ 1/\lambda \f$) */
  vector<sunrealtype> p;   /**< amplitde & polarization vector */
  vector<sunrealtype> phi; /**< phase shift */
};

/// 1D Gaussian wave structure
struct gaussian1D {
  vector<sunrealtype> k;   /**< wavevector (normalized to \f$ 1/\lambda \f$) */
  vector<sunrealtype> p;   /**< amplitude & polarization vector */
  vector<sunrealtype> x0;  /**< shift from origin */
  sunrealtype phig;        /**< width */
  vector<sunrealtype> phi; /**< phase shift */
};

/// 2D Gaussian wave structure
struct gaussian2D {
  vector<sunrealtype> x0;   /**< center */
  vector<sunrealtype> axis; /**< direction to center */
  sunrealtype amp;          /**< amplitude */
  sunrealtype phip;         /**< polarization rotation */
  sunrealtype w0;           /**< taille */
  sunrealtype zr;           /**< Rayleigh length */
  sunrealtype ph0;          /**< beam center */
  sunrealtype phA;          /**< beam length */
};

/// 3D Gaussian wave structure
struct gaussian3D {
  vector<sunrealtype> x0;   /**< center */
  vector<sunrealtype> axis; /**< direction to center */
  sunrealtype amp;          /**< amplitude */
  sunrealtype phip;         /**< polarization rotation */
  sunrealtype w0;           /**< taille */
  sunrealtype zr;           /**< Rayleigh length */
  sunrealtype ph0;          /**< beam center */
  sunrealtype phA;          /**< beam length */
};

/****** simulation function declarations ******/

/// complete 1D Simulation function
void Sim1D(const array<sunrealtype,2>, const int, const sunrealtype,
        const sunindextype, const bool, int *, const sunrealtype, const int,
        const string, const int, const vector<planewave> &,
        const vector<gaussian1D> &);
/// complete 2D 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 vector<planewave> &, const vector<gaussian2D> &);
/// complete 3D 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 vector<planewave> &, const vector<gaussian3D> &);

/** MPI timer function */
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()

```
void linear1DProp (
            LatticePatch * data,
            N_Vector u,
            N_Vector udot,
            int * c )
```

only under-the-hood-callable Maxwell propagation in 1D

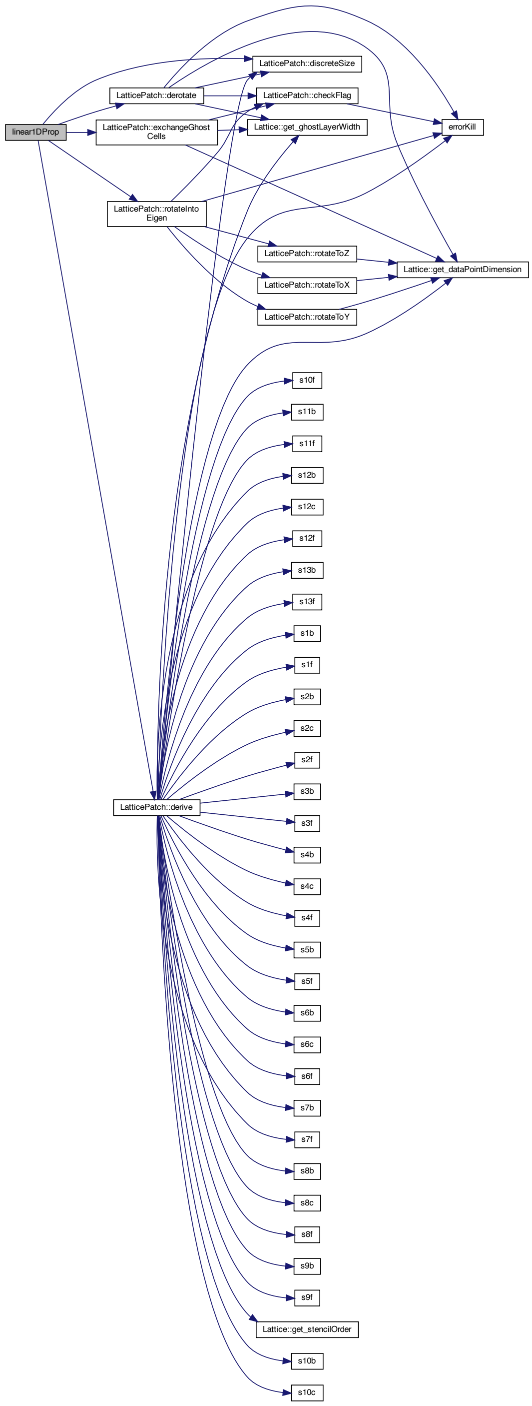
Maxwell propagation function for 1D – only for reference.

Definition at line 46 of file TimeEvolutionFunctions.cpp.

```
00046                                                                        {
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:
00053   data->exchangeGhostCells(1); // exchange halos
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   for (int i = 0; i < totalNP; i++) {
00063     pp = i * 6;
00064     /*
00065      simple vacuum Maxwell equations for spatial deriative only in x-direction
00066      temporal derivative is approximated by spatial derivative according to the
00067      numerical scheme with Jacobi=0 -> no polarization or magnetization terms
00068     */
00069     duData[pp + 0] = 0;
00070     duData[pp + 1] = -dxData[pp + 5];
00071     duData[pp + 2] = dxData[pp + 4];
00072     duData[pp + 3] = 0;
00073     duData[pp + 4] = dxData[pp + 2];
00074     duData[pp + 5] = -dxData[pp + 1];
00075   }
00076 }
```

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()

```
void linear2DProp (
            LatticePatch * data,
```

```
N_Vector u,
N_Vector udot,
int * c )
```

only under-the-hood-callable Maxwell propagation in 2D

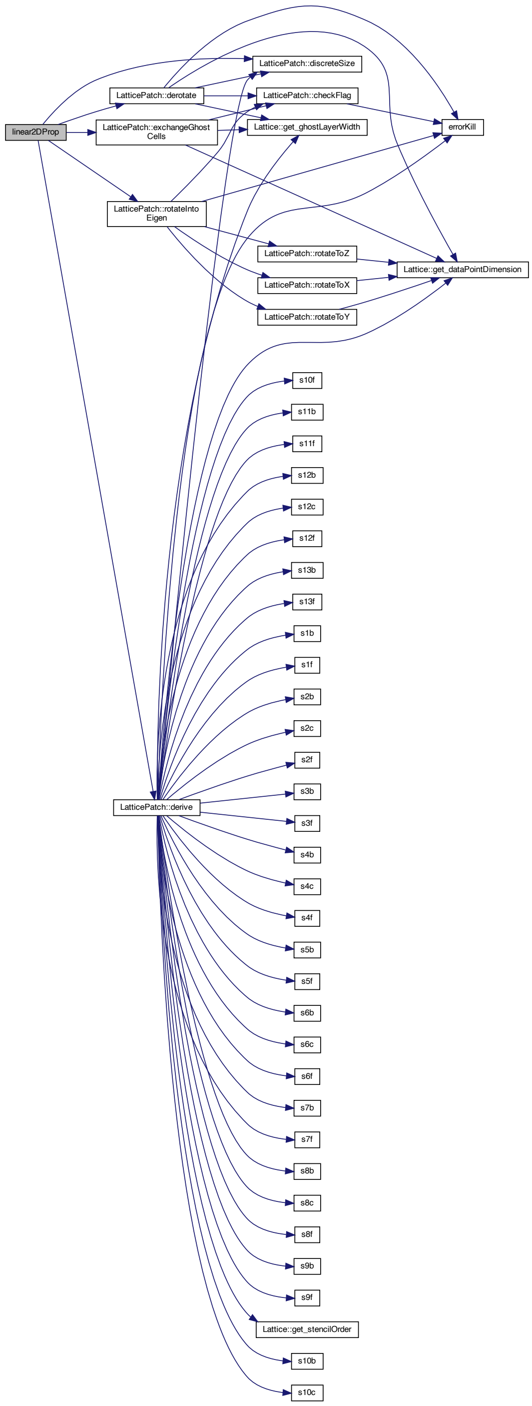
Maxwell propagation function for 2D – only for reference.

Definition at line 265 of file TimeEvolutionFunctions.cpp.

```
{

  sunrealtype *duData = data->duData;
  sunrealtype *dxData = data->buffData[1 - 1];
  sunrealtype *dyData = data->buffData[2 - 1];

  data->exchangeGhostCells(1);
  data->rotateIntoEigen(1);
  data->derive(1);
  data->derotate(1, dxData);
  data->exchangeGhostCells(2);
  data->rotateIntoEigen(2);
  data->derive(2);
  data->derotate(2, dyData);

  int totalNP = data->discreteSize();
  int pp = 0;
  for (int i = 0; i < totalNP; i++) {
    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];
    duData[pp + 5] = dyData[pp + 0] - dxData[pp + 1];
  }
}
```

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()

```
void linear3DProp (
            LatticePatch * data,
```

```
N_Vector u,
N_Vector udot,
int * c )
```

only under-the-hood-callable Maxwell propagation in 3D

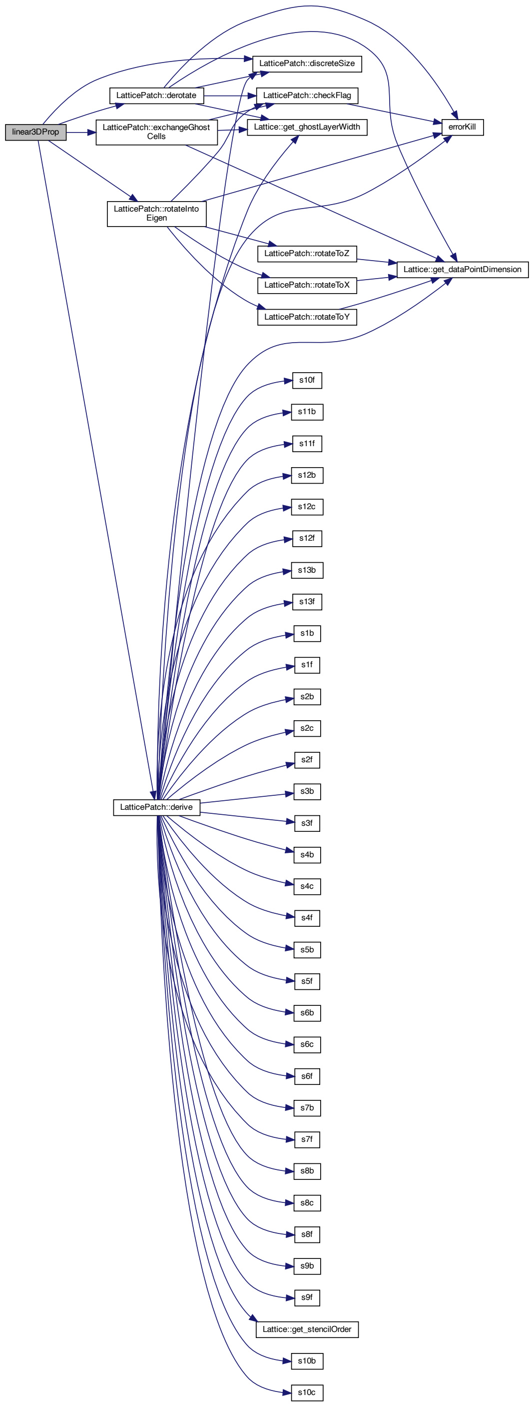
Maxwell propagation function for 3D – only for reference.

Definition at line 476 of file TimeEvolutionFunctions.cpp.

```
00476                                                                               {
00477
00478   sunrealtype *duData = data->duData;
00479   sunrealtype *dxData = data->buffData[1 - 1];
00480   sunrealtype *dyData = data->buffData[2 - 1];
00481   sunrealtype *dzData = data->buffData[3 - 1];
00482
00483   data->exchangeGhostCells(1);
00484   data->rotateIntoEigen(1);
00485   data->derive(1);
00486   data->derotate(1, dxData);
00487   data->exchangeGhostCells(2);
00488   data->rotateIntoEigen(2);
00489   data->derive(2);
00490   data->derotate(2, dyData);
00491   data->exchangeGhostCells(3);
00492   data->rotateIntoEigen(3);
00493   data->derive(3);
00494   data->derotate(3, dzData);
00495
00496   int totalNP = data->discreteSize();
00497   int pp = 0;
00498   for (int i = 0; i < totalNP; i++) {
00499     pp = i * 6;
00500     duData[pp + 0] = dyData[pp + 5] - dzData[pp + 4];
00501     duData[pp + 1] = dzData[pp + 3] - dxData[pp + 5];
00502     duData[pp + 2] = dxData[pp + 4] - dyData[pp + 3];
00503     duData[pp + 3] = -dyData[pp + 2] + dzData[pp + 1];
00504     duData[pp + 4] = -dzData[pp + 0] + dxData[pp + 2];
00505     duData[pp + 5] = -dxData[pp + 1] + dyData[pp + 0];
00506   }
00507 }
```

References LatticePatch::buffData, LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::discreteSize(), LatticePatch::duData, LatticePatch::exchangeGhostCells(), and LatticePatch::rotateIntoEigen().

Here is the call graph for this function:



6.28.2.4 nonlinear1DProp()

```
void nonlinear1DProp (
            LatticePatch * data,
```

```
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 79 of file TimeEvolutionFunctions.cpp.

```
00079                                                                       {
00080
00081   // pointer to spatial derivative data sufficient, temporal derivative data
00082   // provided with udot
00083   sunrealtype *dxData = data->buffData[1 - 1];
00084
00085   // same sequence as in the linear case
00086   data->exchangeGhostCells(1);
00087   data->rotateIntoEigen(1);
00088   data->derive(1);
00089   data->derotate(1, dxData);
00090
00091   /*
00092   F and G are nonzero in the nonlinear case,
00093   polarization and magnetization contributions in Jacobi matrix style
00094   with derivatives of polarization and magnetization
00095   w.r.t. E- and B-field
00096   */
00097   sunrealtype f = NAN, g = NAN; // em field invariants F, G
00098   sunrealtype lf = NAN, lff = NAN, lfg = NAN, lg = NAN,
00099               lgg = NAN; // derivatives of Lagrangian w.r.t. field invariants
00100   array<sunrealtype, 36> JMM; // Jacobi matrix
00101   array<sunrealtype, 6> Quad; // array to hold E^2 and B^2 components
00102   array<sunrealtype, 6> h; // holding temporal derivatives of E and B components
00103                          // before operating (1+Z)^-1
00104   sunrealtype pseudoDenom = NAN; // needed for inversion of 1+Z
00105   sunrealtype *udata = nullptr,
00106               *dudata = nullptr; // pointers to data and temp. derivative data
00107   udata = NV_DATA_P(u);
00108   dudata = NV_DATA_P(udot);
00109   int totalNP = data->discreteSize(); // number of points in the patch
00110   for (int pp = 0; pp < totalNP * 6;
00111        pp += 6) { // loops through all 6dim points in the patch
00112             //     for(int ppB=0;ppB<totalNP*6;ppB+=6*6){
00113             //       for(int pp=ppB;pp<min(totalNP*6,ppB+6*6);pp+=6){
00114     /// Calculation of the Jacobi matrix
00115     // 1. Calculate F and G
00116     f = 0.5 * ((Quad[0] = udata[pp] * udata[pp]) +
00117                (Quad[1] = udata[pp + 1] * udata[pp + 1]) +
00118                (Quad[2] = udata[pp + 2] * udata[pp + 2]) -
00119                (Quad[3] = udata[pp + 3] * udata[pp + 3]) -
00120                (Quad[4] = udata[pp + 4] * udata[pp + 4]) -
00121                (Quad[5] = udata[pp + 5] * udata[pp + 5]));
00122     g = udata[pp] * udata[pp + 3] + udata[pp + 1] * udata[pp + 4] +
00123         udata[pp + 2] * udata[pp + 5];
00124     // 2. Choose process/expansion order and assign derivative values of L
00125     // w.r.t. F, G
00126     switch (*c) {
00127     case 0:
00128       lf = 0;
00129       lff = 0;
00130       lfg = 0;
00131       lg = 0;
00132       lgg = 0;
00133       break;
00134     case 2:
00135       lf = 0.000354046449700427580438254 * f * f +
00136            0.000191775160254398272737387 * g * g;
00137       lff = 0.000708092899400855160876507 * f;
00138       lfg = 0.000383550320508796545474749 * g;
00139       lg = 0.000383550320508796545474749 * f * g;
00140       lgg = 0.000383550320508796545474749 * f;
00141       break;
00142     case 1:
00143       lf = 0.000206527095658582755255648 * f;
00144       lff = 0.000206527095658582755255648;
00145       lfg = 0;
00146       lg = 0.000361422417402519821697384 1 * g;
00147       lgg = 0.000361422417402519821697384 1;
00148       break;
00149     case 3:
00150       lf = (0.000206527095658582755255648 + 0.000354046449700427580438254 * f) *
00151                f +
00152            0.000191775160254398272737387 * g * g;
```

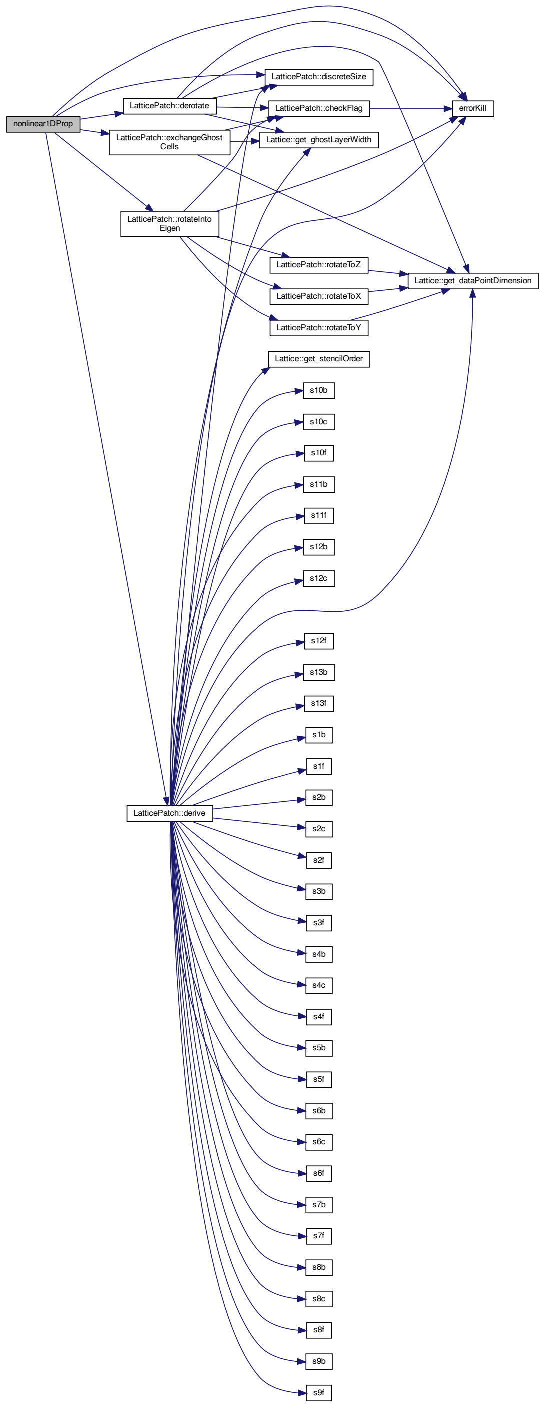
```
      lff = 0.000206527095658582755255648 + 0.0007080928994008551608765075 * f;
      lfg = 0.0003835503205087965454747749 * g;
      lg = (0.0003614224174025198216973841 +
            0.0003835503205087965454747749 * f) *
           g;
      lgg = 0.0003614224174025198216973841 + 0.0003835503205087965454747749 * f;
      break;
    default:
      errorKill(
          "You need to specify a correct order in the weak-field expansion.");
    }
    // 3. Assign Jacobi components
    JMM[0] = lf + lff * Quad[0] +
             udata[3 + pp] * (2 * lfg * udata[pp] + lgg * udata[3 + pp]);
    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];
    JMM[7] = lf + lff * Quad[1] +
             udata[4 + pp] * (2 * lfg * udata[1 + pp] + lgg * udata[4 + pp]);
    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];
    JMM[13] = lff * udata[1 + pp] * udata[2 + pp] +
              lfg * udata[2 + pp] * udata[4 + pp] +
              lfg * udata[1 + pp] * udata[5 + pp] +
              lgg * udata[4 + pp] * udata[5 + pp];
    JMM[14] = lf + lff * Quad[2] +
              udata[5 + pp] * (2 * lfg * udata[2 + pp] + lgg * udata[5 + pp]);
    JMM[18] = lg + lfg * (Quad[0] - Quad[3 + 0]) +
              (-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]);
    JMM[20] = -(udata[3 + pp] * (lff * udata[2 + pp] + lfg * udata[5 + pp])) +
              udata[pp] * (lfg * udata[2 + pp] + lgg * udata[5 + pp]);
    JMM[21] = -lf + lgg * Quad[0] +
              udata[3 + pp] * (-2 * lfg * udata[pp] + lff * udata[3 + pp]);
    JMM[24] = udata[1 + pp] * (lfg * udata[pp] + lgg * udata[3 + pp]) -
              (lff * udata[pp] + lfg * udata[3 + pp]) * udata[4 + pp];
    JMM[25] = lg + lfg * (Quad[1] - Quad[4 + 0]) +
              (-lff + lgg) * udata[1 + 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]);
    JMM[27] = lgg * udata[pp] * udata[1 + pp] +
              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]);
    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]) -
              (lff * udata[1 + pp] + lfg * udata[4 + pp]) * udata[5 + pp];
    JMM[32] = lg + lfg * (Quad[2] - Quad[5 + 0]) +
              (-lff + lgg) * udata[2 + pp] * udata[5 + pp];
    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]);
    JMM[34] =
        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]);
    JMM[35] = -lf + lgg * Quad[2] +
              udata[5 + pp] * (-2 * lfg * udata[2 + pp] + lff * udata[5 + pp]);
    for (int i = 0; i < 6; i++) {
      for (int j = i + 1; j < 6; j++) {
        JMM[i * 6 + j] = JMM[j * 6 + i];
      }
    }
    // 4. Final values for temporal derivatives of field values
    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]);
    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];
    h[3] = 0;
    h[4] = dxData[2 + pp];
    h[5] = -dxData[1 + 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];
    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] =
        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] =
```

```
        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]));
    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]);
    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]));
    dudata[pp + 0] /= pseudoDenom;
    dudata[pp + 1] /= pseudoDenom;
    dudata[pp + 2] /= pseudoDenom;
    dudata[pp + 3] = h[3];
    dudata[pp + 4] = h[4];
    dudata[pp + 5] = h[5];
  }
  return;
}
```

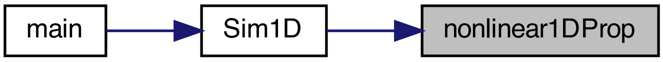
References LatticePatch::buffData, LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::discreteSize(), errorKill(), LatticePatch::exchangeGhostCells(), and LatticePatch::rotateIntoEigen().

Referenced by Sim1D().

Here is the call graph for this function:



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 294 of file TimeEvolutionFunctions.cpp.

```
00294                                                                  {
00295
00296   sunrealtype *dxData = data->buffData[1 - 1];
00297   sunrealtype *dyData = data->buffData[2 - 1];
00298
00299   data->exchangeGhostCells(1);
00300   data->rotateIntoEigen(1);
00301   data->derive(1);
00302   data->derotate(1, dxData);
00303   data->exchangeGhostCells(2);
00304   data->rotateIntoEigen(2);
00305   data->derive(2);
00306   data->derotate(2, dyData);
00307
00308   sunrealtype f = NAN, g = NAN;
00309   sunrealtype lf = NAN, lff = NAN, lfg = NAN, lg = NAN, lgg = NAN;
00310   array<sunrealtype, 36> JMM;
00311   array<sunrealtype, 6> Quad;
00312   array<sunrealtype, 6> h;
00313   sunrealtype pseudoDenom = NAN;
00314   sunrealtype *udata = nullptr, *dudata = nullptr;
00315   udata = NV_DATA_P(u);
00316   dudata = NV_DATA_P(udot);
00317   int totalNP = data->discreteSize();
00318   for (int pp = 0; pp < totalNP * 6; pp += 6) {
00319     // 1
00320     f = 0.5 * ((Quad[0] = udata[pp] * udata[pp]) +
00321                (Quad[1] = udata[pp + 1] * udata[pp + 1]) +
00322                (Quad[2] = udata[pp + 2] * udata[pp + 2]) -
00323                (Quad[3] = udata[pp + 3] * udata[pp + 3]) -
00324                (Quad[4] = udata[pp + 4] * udata[pp + 4]) -
00325                (Quad[5] = udata[pp + 5] * udata[pp + 5]));
00326     g = udata[pp] * udata[pp + 3] + udata[pp + 1] * udata[pp + 4] +
00327         udata[pp + 2] * udata[pp + 5];
00328     // 2
00329     switch (*c) {
00330     case 0:
00331       lf = 0;
00332       lff = 0;
00333       lfg = 0;
00334       lg = 0;
00335       lgg = 0;
00336       break;
```

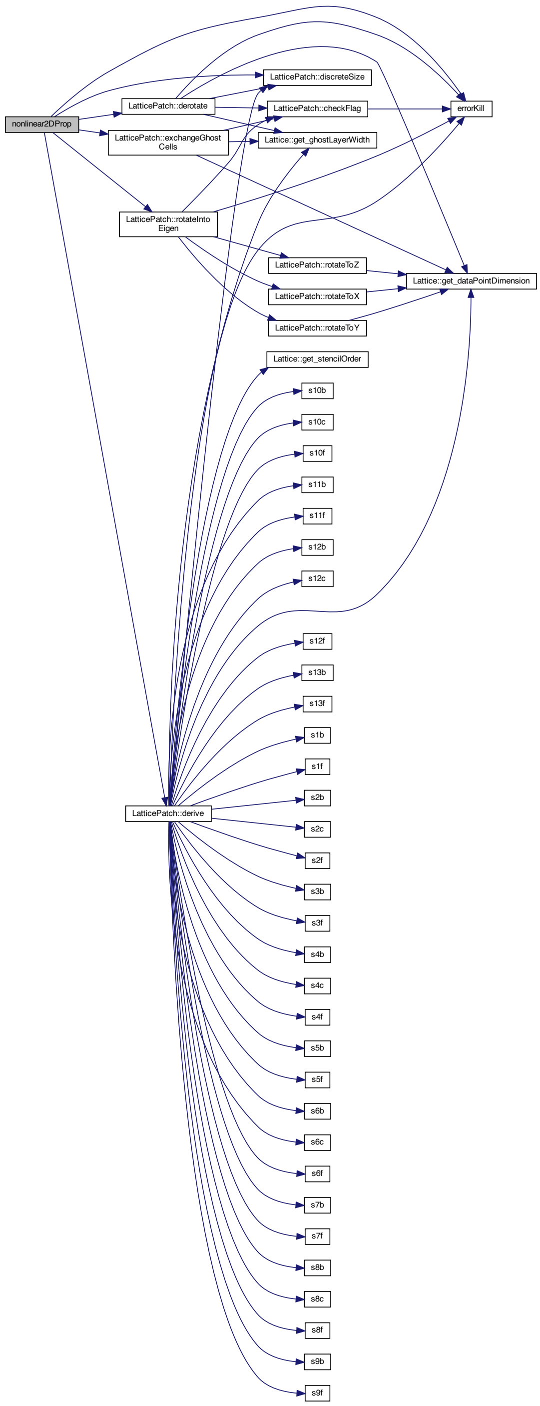
```
    case 2:
      lf = 0.00035404644970042758043825 4 * f * f +
           0.0001917751602543982727373 87 * g * g;
      lff = 0.00070809289940085516087650 75 * f;
      lfg = 0.00038355032050879654547477 49 * g;
      lg = 0.00038355032050879654547477 49 * f * g;
      lgg = 0.00038355032050879654547477 49 * f;
      break;
    case 1:
      lf = 0.00020652709565858275525564 8 * f;
      lff = 0.00020652709565858275525564 8;
      lfg = 0;
      lg = 0.00036142241740251982169738 41 * g;
      lgg = 0.00036142241740251982169738 41;
      break;
    case 3:
      lf = (0.0002065270956585827552556 48 + 0.00035404644970042758043825 4 * f) *
               f +
           0.0001917751602543982727373 87 * g * g;
      lff = 0.0002065270956585827552556 48 + 0.0007080928994008551608765 08 * f;
      lfg = 0.00038355032050879654547477 49 * g;
      lg = (0.0003614224174025198216973 84 + 0.0003835503205087965454747 75 * f) *
           g;
      lgg = 0.0003614224174025198216973 84 + 0.0003835503205087965454747 75 * f;
      break;
    default:
      errorKill(
          "You need to specify a correct order in the weak-field expansion.");
    }
    // 3
    JMM[0] = lf + lff * Quad[0] +
             udata[3 + pp] * (2 * lfg * udata[pp] + lgg * udata[3 + pp]);
    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];
    JMM[7] = lf + lff * Quad[1] +
             udata[4 + pp] * (2 * lfg * udata[1 + pp] + lgg * udata[4 + pp]);
    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];
    JMM[13] = lff * udata[1 + pp] * udata[2 + pp] +
              lfg * udata[2 + pp] * udata[4 + pp] +
              lfg * udata[1 + pp] * udata[5 + pp] +
              lgg * udata[4 + pp] * udata[5 + pp];
    JMM[14] = lf + lff * Quad[2] +
              udata[5 + pp] * (2 * lfg * udata[2 + pp] + lgg * udata[5 + pp]);
    JMM[18] = lg + lfg * (Quad[0] - Quad[3 + 0]) +
              (-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]);
    JMM[20] = -(udata[3 + pp] * (lff * udata[2 + pp] + lfg * udata[5 + pp])) +
              udata[pp] * (lfg * udata[2 + pp] + lgg * udata[5 + pp]);
    JMM[21] = -lf + lgg * Quad[0] +
              udata[3 + pp] * (-2 * lfg * udata[pp] + lff * udata[3 + pp]);
    JMM[24] = udata[1 + pp] * (lfg * udata[pp] + lgg * udata[3 + pp]) -
              (lff * udata[pp] + lfg * udata[3 + pp]) * udata[4 + pp];
    JMM[25] = lg + lfg * (Quad[1] - Quad[4 + 0]) +
              (-lff + lgg) * udata[1 + 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]);
    JMM[27] = lgg * udata[pp] * udata[1 + pp] +
              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]);
    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]) -
              (lff * udata[1 + pp] + lfg * udata[4 + pp]) * udata[5 + pp];
    JMM[32] = lg + lfg * (Quad[2] - Quad[5 + 0]) +
              (-lff + lgg) * udata[2 + pp] * udata[5 + pp];
    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]);
    JMM[34] =
        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]);
    JMM[35] = -lf + lgg * Quad[2] +
              udata[5 + pp] * (-2 * lfg * udata[2 + pp] + lff * udata[5 + pp]);
    // 4
    for (int i = 0; i < 6; i++) {
      for (int j = i + 1; j < 6; j++) {
        JMM[i * 6 + j] = JMM[j * 6 + i];
      }
    }
    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]);
    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];
    h[3] = 0;
    h[4] = dxData[2 + pp];
    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]);
    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];
    h[3] += -dyData[2 + pp];
    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];
    h[2] -= h[3] * JMM[15] + h[4] * JMM[16] + h[5] * JMM[17];
    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]));
    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]));
    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]);
    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]));
    dudata[pp + 0] /= pseudoDenom;
    dudata[pp + 1] /= pseudoDenom;
    dudata[pp + 2] /= pseudoDenom;
    dudata[pp + 3] = h[3];
    dudata[pp + 4] = h[4];
    dudata[pp + 5] = h[5];
  }
  return;
}
```

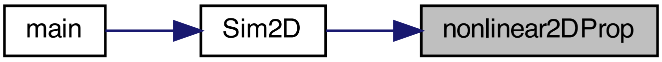
References LatticePatch::buffData, LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::discreteSize(), errorKill(), LatticePatch::exchangeGhostCells(), and LatticePatch::rotateIntoEigen().

Referenced by Sim2D().

Here is the call graph for this function:



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 510 of file TimeEvolutionFunctions.cpp.

```
00510                                                                      {
00511
00512   sunrealtype *dxData = data->buffData[1 - 1];
00513   sunrealtype *dyData = data->buffData[2 - 1];
00514   sunrealtype *dzData = data->buffData[3 - 1];
00515
00516   data->exchangeGhostCells(1);
00517   data->rotateIntoEigen(1);
00518   data->derive(1);
00519   data->derotate(1,dxData);
00520   data->exchangeGhostCells(2);
00521   data->rotateIntoEigen(2);
00522   data->derive(2);
00523   data->derotate(2,dyData);
00524   data->exchangeGhostCells(3);
00525   data->rotateIntoEigen(3);
00526   data->derive(3);
00527   data->derotate(3,dzData);
00528
00529   sunrealtype f = NAN, g = NAN;
00530   sunrealtype lf = NAN, lff = NAN, lfg = NAN, lg = NAN, lgg = NAN;
00531   array<sunrealtype, 36> JMM;
00532   array<sunrealtype, 6> Quad;
00533   array<sunrealtype, 6> h;
00534   sunrealtype pseudoDenom = NAN;
00535   sunrealtype *udata = nullptr, *dudata = nullptr;
00536   udata = NV_DATA_P(u);
00537   dudata = NV_DATA_P(udot);
00538   int totalNP = data->discreteSize();
00539   for (int pp = 0; pp < totalNP * 6; pp += 6) {
00540     // 1
00541     f = 0.5 * ((Quad[0] = udata[pp] * udata[pp]) +
00542                (Quad[1] = udata[pp + 1] * udata[pp + 1]) +
00543                (Quad[2] = udata[pp + 2] * udata[pp + 2]) -
00544                (Quad[3] = udata[pp + 3] * udata[pp + 3]) -
00545                (Quad[4] = udata[pp + 4] * udata[pp + 4]) -
00546                (Quad[5] = udata[pp + 5] * udata[pp + 5]));
00547     g = udata[pp] * udata[pp + 3] + udata[pp + 1] * udata[pp + 4] +
00548         udata[pp + 2] * udata[pp + 5];
00549     // 2
00550     switch (*c) {
00551     case 0:
00552       lf = 0;
```

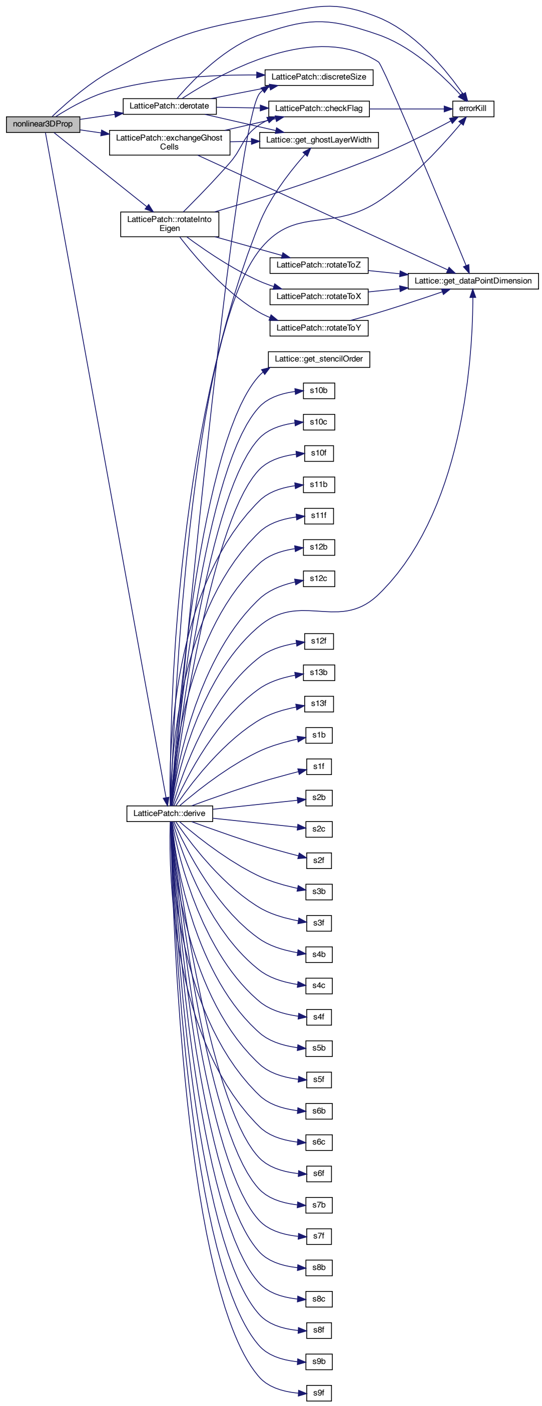
```
      lff = 0;
      lfg = 0;
      lg = 0;
      lgg = 0;
      break;
    case 2:
      lf = 0.00035404644970042758043825 4 * f * f +
           0.000191775160254398272737387 * g * g;
      lff = 0.00070809289940085516087650 75 * f;
      lfg = 0.000383550320508796545474774 9 * g;
      lg = 0.000383550320508796545474774 9 * f * g;
      lgg = 0.000383550320508796545474774 9 * f;
      break;
    case 1:
      lf = 0.000206527095658582755255648 * f;
      lff = 0.000206527095658582755255648;
      lfg = 0;
      lg = 0.000361422417402519821697384 1 * g;
      lgg = 0.000361422417402519821697384 1;
      break;
    case 3:
      lf = (0.000206527095658582755255648 + 0.00035404644970042758043825 4 * f) *
               f +
           0.000191775160254398272737387 * g * g;
      lff = 0.000206527095658582755255648 + 0.00070809289940085516087650 8 * f;
      lfg = 0.000383550320508796545474774 9 * g;
      lg = (0.000361422417402519821697384 + 0.000383550320508796545474775 * f) *
           g;
      lgg = 0.000361422417402519821697384 + 0.000383550320508796545474775 * f;
      break;
    default:
      errorKill(
          "You need to specify a correct order in the weak-field expansion.");
    }
    // 3
    JMM[0] = lf + lff * Quad[0] +
             udata[3 + pp] * (2 * lfg * udata[pp] + lgg * udata[3 + pp]);
    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];
    JMM[7] = lf + lff * Quad[1] +
             udata[4 + pp] * (2 * lfg * udata[1 + pp] + lgg * udata[4 + pp]);
    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];
    JMM[13] = lff * udata[1 + pp] * udata[2 + pp] +
              lfg * udata[2 + pp] * udata[4 + pp] +
              lfg * udata[1 + pp] * udata[5 + pp] +
              lgg * udata[4 + pp] * udata[5 + pp];
    JMM[14] = lf + lff * Quad[2] +
              udata[5 + pp] * (2 * lfg * udata[2 + pp] + lgg * udata[5 + pp]);
    JMM[18] = lg + lfg * (Quad[0] - Quad[3 + 0]) +
              (-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]);
    JMM[20] = -(udata[3 + pp] * (lff * udata[2 + pp] + lfg * udata[5 + pp])) +
              udata[pp] * (lfg * udata[2 + pp] + lgg * udata[5 + pp]);
    JMM[21] = -lf + lgg * Quad[0] +
              udata[3 + pp] * (-2 * lfg * udata[pp] + lff * udata[3 + pp]);
    JMM[24] = udata[1 + pp] * (lfg * udata[pp] + lgg * udata[3 + pp]) -
              (lff * udata[pp] + lfg * udata[3 + pp]) * udata[4 + pp];
    JMM[25] = lg + lfg * (Quad[1] - Quad[4 + 0]) +
              (-lff + lgg) * udata[1 + 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]);
    JMM[27] = lgg * udata[pp] * udata[1 + pp] +
              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]);
    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]) -
              (lff * udata[1 + pp] + lfg * udata[4 + pp]) * udata[5 + pp];
    JMM[32] = lg + lfg * (Quad[2] - Quad[5 + 0]) +
              (-lff + lgg) * udata[2 + pp] * udata[5 + pp];
    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]);
    JMM[34] =
        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]);
    JMM[35] = -lf + lgg * Quad[2] +
              udata[5 + pp] * (-2 * lfg * udata[2 + pp] + lff * udata[5 + pp]);
    // 4
    for (int i = 0; i < 6; i++) {
```

```
      for (int j = i + 1; j < 6; j++) {
        JMM[i * 6 + j] = JMM[j * 6 + i];
      }
    }
    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]);
    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];
    h[3] = 0;
    h[4] = dxData[2 + pp];
    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]);
    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];
    h[3] += -dyData[2 + pp];
    h[4] += 0;
    h[5] += dyData[pp];
    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];
    h[2] += 0;
    h[3] += dzData[1 + pp];
    h[4] += -dzData[pp];
    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];
    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]));
    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]));
    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]);
    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]));
    dudata[pp + 0] /= pseudoDenom;
    dudata[pp + 1] /= pseudoDenom;
    dudata[pp + 2] /= pseudoDenom;
    dudata[pp + 3] = h[3];
    dudata[pp + 4] = h[4];
    dudata[pp + 5] = h[5];
  }
  return;
}
```

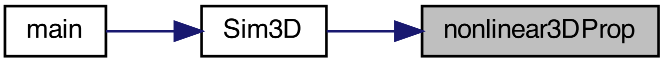
References LatticePatch::buffData, LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::discreteSize(), errorKill(), LatticePatch::exchangeGhostCells(), and LatticePatch::rotateIntoEigen().

Referenced by Sim3D().

Here is the call graph for this function:



Here is the caller graph for this function:



6.29 TimeEvolutionFunctions.cpp

Go to the documentation of this file.

```
////////////////////////////////////////////////////////////
/// @file TimeEvolutionFunctions.cpp
/// @brief 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>

/// CVode right-hand-side function (CVRhsFn)
int TimeEvolution::f(sunrealtype t, N_Vector u, N_Vector udot, void *data_loc) {
  // Set recover pointer to provided lattice patch where the data resides
  LatticePatch *data = nullptr;
  data = static_cast<LatticePatch *>(data_loc);

  // pointers for update circle
  sunrealtype *udata = nullptr, *dudata = nullptr;
  sunrealtype *originaluData = nullptr, *originalduData = nullptr;

  // Access NVECTOR_PARALLEL argument data with pointers
  udata = NV_DATA_P(u);
  dudata = NV_DATA_P(udot);

  // Store original data location of the patch
  originaluData = data->uData;
  originalduData = data->duData;
  // Point patch data to arguments of f
  data->uData = udata;
  data->duData = dudata;

  // Time-evolve these arguments (the field data) with specific propagator below
  TimeEvolver(data, u, udot, c);

  // Refer patch data back to original location
  data->uData = originaluData;
  data->duData = originalduData;

  return (0);
}

/// only under-the-hood-callable Maxwell propagation in 1D
// unused parameters 2-4 for compliance with CVRhsFn
// same as the respective nonlinear function without nonlinear terms
void linear1DProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c) {

  // pointers to temporal and spatial derivative data
  sunrealtype *duData = data->duData;
  sunrealtype *dxData = data->buffData[1 - 1];

  // sequence along any dimension:
  data->exchangeGhostCells(1); // exchange halos
  data->rotateIntoEigen(
      1);           // -> rotate all data to prepare derivative operation
  data->derive(1); // -> perform derivative on it
  data->derotate(
      1, dxData); // -> derotate derivative data to x-space for further use

  int totalNP = data->discreteSize();
  int pp = 0;
```

```
  for (int i = 0; i < totalNP; i++) {
    pp = i * 6;
    /*
     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
    */
    duData[pp + 0] = 0;
    duData[pp + 1] = -dxData[pp + 5];
    duData[pp + 2] = dxData[pp + 4];
    duData[pp + 3] = 0;
    duData[pp + 4] = dxData[pp + 2];
    duData[pp + 5] = -dxData[pp + 1];
  }
}

/// nonlinear 1D HE propagation
void nonlinear1DProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c) {

  // pointer to spatial derivative data sufficient, temporal derivative data
  // provided with udot
  sunrealtype *dxData = data->buffData[1 - 1];

  // same sequence as in the linear case
  data->exchangeGhostCells(1);
  data->rotateIntoEigen(1);
  data->derive(1);
  data->derotate(1, dxData);

  /*
  F and G are nonzero in the nonlinear case,
  polarization and magnetization contributions in Jacobi matrix style
  with derivatives of polarization and magnetization
  w.r.t. E- and B-field
  */
  sunrealtype f = NAN, g = NAN; // em field invariants F, G
  sunrealtype lf = NAN, lff = NAN, lfg = NAN, lg = NAN,
              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
  sunrealtype pseudoDenom = NAN; // needed for inversion of 1+Z
  sunrealtype *udata = nullptr,
              *dudata = nullptr; // pointers to data and temp. derivative data
  udata = NV_DATA_P(u);
  dudata = NV_DATA_P(udot);
  int totalNP = data->discreteSize(); // number of points in the patch
  for (int pp = 0; pp < totalNP * 6;
       pp += 6) { // loops through all 6dim points in the patch
                  //    for(int ppB=0;ppB<totalNP*6;ppB+=6*6){
                  //      for(int pp=ppB;pp<min(totalNP*6,ppB+6*6);pp+=6){
    /// Calculation of the Jacobi matrix
    // 1. Calculate F and G
    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]) -
               (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];
    // 2. Choose process/expansion order and assign derivative values of L
    // w.r.t. F, G
    switch (*c) {
    case 0:
      lf = 0;
      lff = 0;
      lfg = 0;
      lg = 0;
      lgg = 0;
      break;
    case 2:
      lf = 0.000354046449700427580438254 * f * f +
           0.000191775160254398272737387 * g * g;
      lff = 0.000708092899400855160876507 5 * f;
      lfg = 0.000383550320508796545474774 9 * g;
      lg = 0.000383550320508796545474774 9 * f * g;
      lgg = 0.000383550320508796545474774 9 * f;
      break;
    case 1:
      lf = 0.000206527095658582755255648 * f;
      lff = 0.000206527095658582755255648;
      lfg = 0;
      lg = 0.000361422417402519821697384 1 * g;
      lgg = 0.000361422417402519821697384 1;
      break;
```

```
case 3:
  lf = (0.000206527095658582755255648 + 0.000354046449700427580438254 * f) *
           f +
       0.000191775160254398272737387 * g * g;
  lff = 0.000206527095658582755255648 + 0.000708092899400855160876507 * f;
  lfg = 0.000383550320508796545474774 * g;
  lg = (0.000361422417402519821697384 +
        0.000383550320508796545474774 * f) *
       g;
  lgg = 0.000361422417402519821697384 + 0.000383550320508796545474774 * f;
  break;
default:
  errorKill(
      "You need to specify a correct order in the weak-field expansion.");
}
// 3. Assign Jacobi components
JMM[0] = lf + lff * Quad[0] +
         udata[3 + pp] * (2 * lfg * udata[pp] + lgg * udata[3 + pp]);
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];
JMM[7] = lf + lff * Quad[1] +
         udata[4 + pp] * (2 * lfg * udata[1 + pp] + lgg * udata[4 + pp]);
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];
JMM[13] = lff * udata[1 + pp] * udata[2 + pp] +
          lfg * udata[2 + pp] * udata[4 + pp] +
          lfg * udata[1 + pp] * udata[5 + pp] +
          lgg * udata[4 + pp] * udata[5 + pp];
JMM[14] = lf + lff * Quad[2] +
          udata[5 + pp] * (2 * lfg * udata[2 + pp] + lgg * udata[5 + pp]);
JMM[18] = lg + lfg * (Quad[0] - Quad[3 + 0]) +
          (-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]);
JMM[20] = -(udata[3 + pp] * (lff * udata[2 + pp] + lfg * udata[5 + pp])) +
          udata[pp] * (lfg * udata[2 + pp] + lgg * udata[5 + pp]);
JMM[21] = -lf + lgg * Quad[0] +
          udata[3 + pp] * (-2 * lfg * udata[pp] + lff * udata[3 + pp]);
JMM[24] = udata[1 + pp] * (lfg * udata[pp] + lgg * udata[3 + pp]) -
          (lff * udata[pp] + lfg * udata[3 + pp]) * udata[4 + pp];
JMM[25] = lg + lfg * (Quad[1] - Quad[4 + 0]) +
          (-lff + lgg) * udata[1 + 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]);
JMM[27] = lgg * udata[pp] * udata[1 + pp] +
          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]);
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]) -
          (lff * udata[1 + pp] + lfg * udata[4 + pp]) * udata[5 + pp];
JMM[32] = lg + lfg * (Quad[2] - Quad[5 + 0]) +
          (-lff + lgg) * udata[2 + pp] * udata[5 + pp];
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]);
JMM[34] =
    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]);
JMM[35] = -lf + lgg * Quad[2] +
          udata[5 + pp] * (-2 * lfg * udata[2 + pp] + lff * udata[5 + pp]);
for (int i = 0; i < 6; i++) {
  for (int j = i + 1; j < 6; j++) {
    JMM[i * 6 + j] = JMM[j * 6 + i];
  }
}
// 4. Final values for temporal derivatives of field values
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]);
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];
h[3] = 0;
h[4] = dxData[2 + pp];
h[5] = -dxData[1 + 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];
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] =
```

```
        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] =
        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]));
    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]);
    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]));
    dudata[pp + 0] /= pseudoDenom;
    dudata[pp + 1] /= pseudoDenom;
    dudata[pp + 2] /= pseudoDenom;
    dudata[pp + 3] = h[3];
    dudata[pp + 4] = h[4];
    dudata[pp + 5] = h[5];
  }
  return;
}

/// only under-the-hood-callable Maxwell propagation in 2D
// unused parameters 2-4 for compliance with CVRhsFn
// same as the respective nonlinear function without nonlinear terms
void linear2DProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c) {

  sunrealtype *duData = data->duData;
  sunrealtype *dxData = data->buffData[1 - 1];
  sunrealtype *dyData = data->buffData[2 - 1];

  data->exchangeGhostCells(1);
  data->rotateIntoEigen(1);
  data->derive(1);
  data->derotate(1, dxData);
  data->exchangeGhostCells(2);
  data->rotateIntoEigen(2);
  data->derive(2);
  data->derotate(2, dyData);

  int totalNP = data->discreteSize();
  int pp = 0;
  for (int i = 0; i < totalNP; i++) {
    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];
    duData[pp + 5] = dyData[pp + 0] - dxData[pp + 1];
  }
}

/// nonlinear 2D HE propagation
void nonlinear2DProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c) {

  sunrealtype *dxData = data->buffData[1 - 1];
  sunrealtype *dyData = data->buffData[2 - 1];

  data->exchangeGhostCells(1);
  data->rotateIntoEigen(1);
  data->derive(1);
  data->derotate(1, dxData);
  data->exchangeGhostCells(2);
  data->rotateIntoEigen(2);
  data->derive(2);
  data->derotate(2, dyData);

  sunrealtype f = NAN, g = NAN;
  sunrealtype lf = NAN, lff = NAN, lfg = NAN, lg = NAN, lgg = NAN;
  array<sunrealtype, 36> JMM;
  array<sunrealtype, 6> Quad;
  array<sunrealtype, 6> h;
  sunrealtype pseudoDenom = NAN;
  sunrealtype *udata = nullptr, *dudata = nullptr;
  udata = NV_DATA_P(u);
  dudata = NV_DATA_P(udot);
  int totalNP = data->discreteSize();
  for (int pp = 0; pp < totalNP * 6; pp += 6) {
    // 1
    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]) -
```

```
                (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];
      // 2
      switch (*c) {
      case 0:
        lf = 0;
        lff = 0;
        lfg = 0;
        lg = 0;
        lgg = 0;
        break;
      case 2:
        lf = 0.00035404644970042758043825 4 * f * f +
             0.00019177516025439827273738 7 * g * g;
        lff = 0.000708092899400855160876507 5 * f;
        lfg = 0.00038355032050879654547474 9 * g;
        lg = 0.00038355032050879654547474 9 * f * g;
        lgg = 0.00038355032050879654547474 9 * f;
        break;
      case 1:
        lf = 0.000206527095658582755255648 * f;
        lff = 0.000206527095658582755255648;
        lfg = 0;
        lg = 0.000361422417402519821697384 1 * g;
        lgg = 0.000361422417402519821697384 1;
        break;
      case 3:
        lf = (0.000206527095658582755255648 + 0.000354046449700427580438254 * f) *
                 f +
             0.000191775160254398272737387 * g * g;
        lff = 0.000206527095658582755255648 + 0.000708092899400855160876508 * f;
        lfg = 0.000383550320508796545474774 9 * g;
        lg = (0.000361422417402519821697384 + 0.000383550320508796545474775 * f) *
             g;
        lgg = 0.000361422417402519821697384 + 0.000383550320508796545474775 * f;
        break;
      default:
        errorKill(
            "You need to specify a correct order in the weak-field expansion.");
      }
      // 3
      JMM[0] = lf + lff * Quad[0] +
               udata[3 + pp] * (2 * lfg * udata[pp] + lgg * udata[3 + pp]);
      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];
      JMM[7] = lf + lff * Quad[1] +
               udata[4 + pp] * (2 * lfg * udata[1 + pp] + lgg * udata[4 + pp]);
      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];
      JMM[13] = lff * udata[1 + pp] * udata[2 + pp] +
                lfg * udata[2 + pp] * udata[4 + pp] +
                lfg * udata[1 + pp] * udata[5 + pp] +
                lgg * udata[4 + pp] * udata[5 + pp];
      JMM[14] = lf + lff * Quad[2] +
                udata[5 + pp] * (2 * lfg * udata[2 + pp] + lgg * udata[5 + pp]);
      JMM[18] = lg + lfg * (Quad[0] - Quad[3 + 0]) +
                (-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]);
      JMM[20] = -(udata[3 + pp] * (lff * udata[2 + pp] + lfg * udata[5 + pp])) +
                udata[pp] * (lfg * udata[2 + pp] + lgg * udata[5 + pp]);
      JMM[21] = -lf + lgg * Quad[0] +
                udata[3 + pp] * (-2 * lfg * udata[pp] + lff * udata[3 + pp]);
      JMM[24] = udata[1 + pp] * (lfg * udata[pp] + lgg * udata[3 + pp]) -
                (lff * udata[pp] + lfg * udata[3 + pp]) * udata[4 + pp];
      JMM[25] = lg + lfg * (Quad[1] - Quad[4 + 0]) +
                (-lff + lgg) * udata[1 + 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]);
      JMM[27] = lgg * udata[pp] * udata[1 + pp] +
                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]);
      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]) -
                (lff * udata[1 + pp] + lfg * udata[4 + pp]) * udata[5 + pp];
      JMM[32] = lg + lfg * (Quad[2] - Quad[5 + 0]) +
                (-lff + lgg) * udata[2 + pp] * udata[5 + pp];
      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]);
    JMM[34] =
        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]);
    JMM[35] = -lf + lgg * Quad[2] +
              udata[5 + pp] * (-2 * lfg * udata[2 + pp] + lff * udata[5 + pp]);
    // 4
    for (int i = 0; i < 6; i++) {
      for (int j = i + 1; j < 6; j++) {
        JMM[i * 6 + j] = JMM[j * 6 + i];
      }
    }
    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]);
    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];
    h[3] = 0;
    h[4] = dxData[2 + pp];
    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]);
    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];
    h[3] += -dyData[2 + pp];
    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];
    h[2] -= h[3] * JMM[15] + h[4] * JMM[16] + h[5] * JMM[17];
    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]));
    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]));
    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]);
    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]));
    dudata[pp + 0] /= pseudoDenom;
    dudata[pp + 1] /= pseudoDenom;
    dudata[pp + 2] /= pseudoDenom;
    dudata[pp + 3] = h[3];
    dudata[pp + 4] = h[4];
    dudata[pp + 5] = h[5];
  }
  return;
}

/// only under-the-hood-callable Maxwell propagation in 3D
// unused parameters 2-4 for compliance with CVRhsFn
// same as the respective nonlinear function without nonlinear terms
void linear3DProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c) {

  sunrealtype *duData = data->duData;
  sunrealtype *dxData = data->buffData[1 - 1];
  sunrealtype *dyData = data->buffData[2 - 1];
  sunrealtype *dzData = data->buffData[3 - 1];

  data->exchangeGhostCells(1);
  data->rotateIntoEigen(1);
  data->derive(1);
  data->derotate(1, dxData);
  data->exchangeGhostCells(2);
  data->rotateIntoEigen(2);
  data->derive(2);
  data->derotate(2, dyData);
  data->exchangeGhostCells(3);
  data->rotateIntoEigen(3);
  data->derive(3);
  data->derotate(3, dzData);

  int totalNP = data->discreteSize();
```

```
  int pp = 0;
  for (int i = 0; i < totalNP; i++) {
    pp = i * 6;
    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];
    duData[pp + 4] = -dzData[pp + 0] + dxData[pp + 2];
    duData[pp + 5] = -dxData[pp + 1] + dyData[pp + 0];
  }
}

/// nonlinear 3D HE propagation
void nonlinear3DProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c) {

  sunrealtype *dxData = data->buffData[1 - 1];
  sunrealtype *dyData = data->buffData[2 - 1];
  sunrealtype *dzData = data->buffData[3 - 1];

  data->exchangeGhostCells(1);
  data->rotateIntoEigen(1);
  data->derive(1);
  data->derotate(1,dxData);
  data->exchangeGhostCells(2);
  data->rotateIntoEigen(2);
  data->derive(2);
  data->derotate(2,dyData);
  data->exchangeGhostCells(3);
  data->rotateIntoEigen(3);
  data->derive(3);
  data->derotate(3,dzData);

  sunrealtype f = NAN, g = NAN;
  sunrealtype lf = NAN, lff = NAN, lfg = NAN, lg = NAN, lgg = NAN;
  array<sunrealtype, 36> JMM;
  array<sunrealtype, 6> Quad;
  array<sunrealtype, 6> h;
  sunrealtype pseudoDenom = NAN;
  sunrealtype *udata = nullptr, *dudata = nullptr;
  udata = NV_DATA_P(u);
  dudata = NV_DATA_P(udot);
  int totalNP = data->discreteSize();
  for (int pp = 0; pp < totalNP * 6; pp += 6) {
    // 1
    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]) -
               (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];
    // 2
    switch (*c) {
    case 0:
      lf = 0;
      lff = 0;
      lfg = 0;
      lg = 0;
      lgg = 0;
      break;
    case 2:
      lf = 0.000354046449700427580438254 * f * f +
           0.000191775160254398272737387 * g * g;
      lff = 0.0007080928994008551608765075 * f;
      lfg = 0.0003835503205087965454747749 * g;
      lg = 0.0003835503205087965454747749 * f * g;
      lgg = 0.0003835503205087965454747749 * f;
      break;
    case 1:
      lf = 0.000206527095658582755255648 * f;
      lff = 0.000206527095658582755255648;
      lfg = 0;
      lg = 0.0003614224174025198216973841 * g;
      lgg = 0.0003614224174025198216973841;
      break;
    case 3:
      lf = (0.000206527095658582755255648 + 0.000354046449700427580438254 * f) *
               f +
           0.000191775160254398272737387 * g * g;
      lff = 0.000206527095658582755255648 + 0.000708092899400855160876508 * f;
      lfg = 0.0003835503205087965454747749 * g;
      lg = (0.000361422417402519821697384 + 0.000383550320508796545474775 * f) *
           g;
      lgg = 0.000361422417402519821697384 + 0.000383550320508796545474775 * f;
      break;
    default:
```

```
    errorKill(
        "You need to specify a correct order in the weak-field expansion.");
  }
  // 3
  JMM[0] = lf + lff * Quad[0] +
           udata[3 + pp] * (2 * lfg * udata[pp] + lgg * udata[3 + pp]);
  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];
  JMM[7] = lf + lff * Quad[1] +
           udata[4 + pp] * (2 * lfg * udata[1 + pp] + lgg * udata[4 + pp]);
  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];
  JMM[13] = lff * udata[1 + pp] * udata[2 + pp] +
            lfg * udata[2 + pp] * udata[4 + pp] +
            lfg * udata[1 + pp] * udata[5 + pp] +
            lgg * udata[4 + pp] * udata[5 + pp];
  JMM[14] = lf + lff * Quad[2] +
            udata[5 + pp] * (2 * lfg * udata[2 + pp] + lgg * udata[5 + pp]);
  JMM[18] = lg + lfg * (Quad[0] - Quad[3 + 0]) +
            (-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]);
  JMM[20] = -(udata[3 + pp] * (lff * udata[2 + pp] + lfg * udata[5 + pp])) +
            udata[pp] * (lfg * udata[2 + pp] + lgg * udata[5 + pp]);
  JMM[21] = -lf + lgg * Quad[0] +
            udata[3 + pp] * (-2 * lfg * udata[pp] + lff * udata[3 + pp]);
  JMM[24] = udata[1 + pp] * (lfg * udata[pp] + lgg * udata[3 + pp]) -
            (lff * udata[pp] + lfg * udata[3 + pp]) * udata[4 + pp];
  JMM[25] = lg + lfg * (Quad[1] - Quad[4 + 0]) +
            (-lff + lgg) * udata[1 + 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]);
  JMM[27] = lgg * udata[pp] * udata[1 + pp] +
            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]);
  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]) -
            (lff * udata[1 + pp] + lfg * udata[4 + pp]) * udata[5 + pp];
  JMM[32] = lg + lfg * (Quad[2] - Quad[5 + 0]) +
            (-lff + lgg) * udata[2 + pp] * udata[5 + pp];
  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]);
  JMM[34] =
      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]);
  JMM[35] = -lf + lgg * Quad[2] +
            udata[5 + pp] * (-2 * lfg * udata[2 + pp] + lff * udata[5 + pp]);
  // 4
  for (int i = 0; i < 6; i++) {
    for (int j = i + 1; j < 6; j++) {
      JMM[i * 6 + j] = JMM[j * 6 + i];
    }
  }
  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]);
  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];
  h[3] = 0;
  h[4] = dxData[2 + pp];
  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]);
  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];
  h[3] += -dyData[2 + pp];
  h[4] += 0;
  h[5] += dyData[pp];
  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];
  h[2] += 0;
```

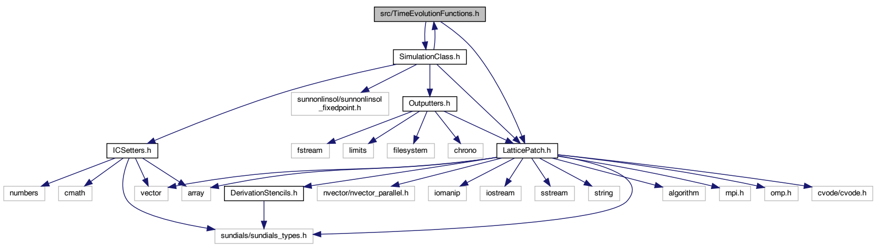
```
    h[3] += dzData[1 + pp];
    h[4] += -dzData[pp];
    h[5] += 0;
    h[0] -= h[3] * JMM[3] + h[4] * JMM[4] + h[5] * JMM[5];
    h[1] -= h[3] * JMM[9] + h[4] * JMM[10] + h[5] * JMM[11];
    h[2] -= h[3] * JMM[15] + h[4] * JMM[16] + h[5] * JMM[17];
    dudata[pp + 0] =
        h[2] * (-(JMM[2] * (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]));
    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]));
    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]);
    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]));
    dudata[pp + 0] /= pseudoDenom;
    dudata[pp + 1] /= pseudoDenom;
    dudata[pp + 2] /= pseudoDenom;
    dudata[pp + 3] = h[3];
    dudata[pp + 4] = h[4];
    dudata[pp + 5] = h[5];
  }
  return;
}
```

6.30 src/TimeEvolutionFunctions.h File Reference

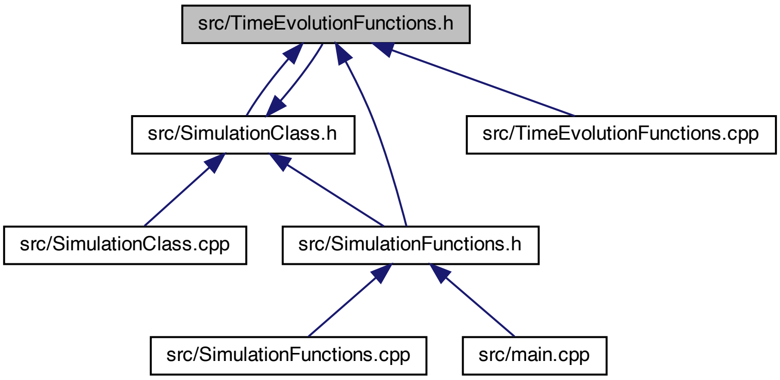
Functions to propagate data vectors in time according to Maxwell's equations, and various orders in the HE weak-field expansion.

```
#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.

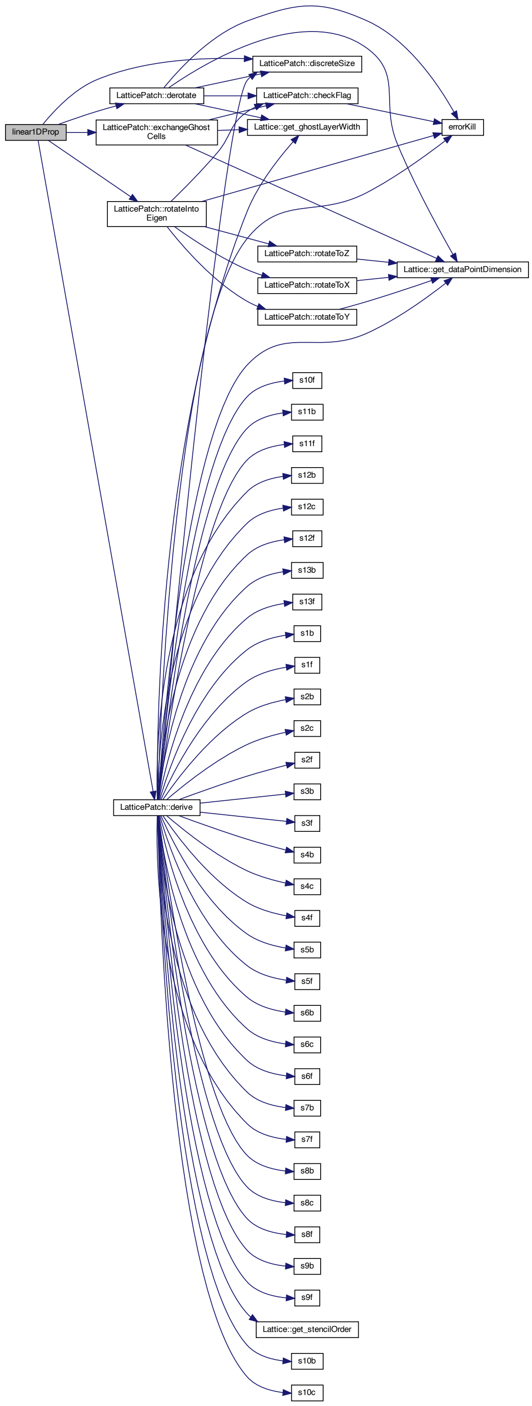
Maxwell propagation function for 1D – only for reference.

Definition at line 46 of file TimeEvolutionFunctions.cpp.

```
00046                                                                           {
00047
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:
00053   data->exchangeGhostCells(1); // exchange halos
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   for (int i = 0; i < totalNP; i++) {
00063     pp = i * 6;
00064     /*
00065      simple vacuum Maxwell equations for spatial deriative only in x-direction
00066      temporal derivative is approximated by spatial derivative according to the
00067      numerical scheme with Jacobi=0 -> no polarization or magnetization terms
00068     */
00069     duData[pp + 0] = 0;
00070     duData[pp + 1] = -dxData[pp + 5];
00071     duData[pp + 2] = dxData[pp + 4];
00072     duData[pp + 3] = 0;
00073     duData[pp + 4] = dxData[pp + 2];
00074     duData[pp + 5] = -dxData[pp + 1];
00075   }
00076 }
```

References LatticePatch::buffData, LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::discreteSize(), LatticePatch::duData, LatticePatch::exchangeGhostCells(), and LatticePatch::rotateIntoEigen().

Here is the call graph for this function:



6.30.2.2 linear2DProp()

```
void linear2DProp (
            LatticePatch * data,
```

```
N_Vector u,
N_Vector udot,
int * c )
```

Maxwell propagation function for 2D – only for reference.

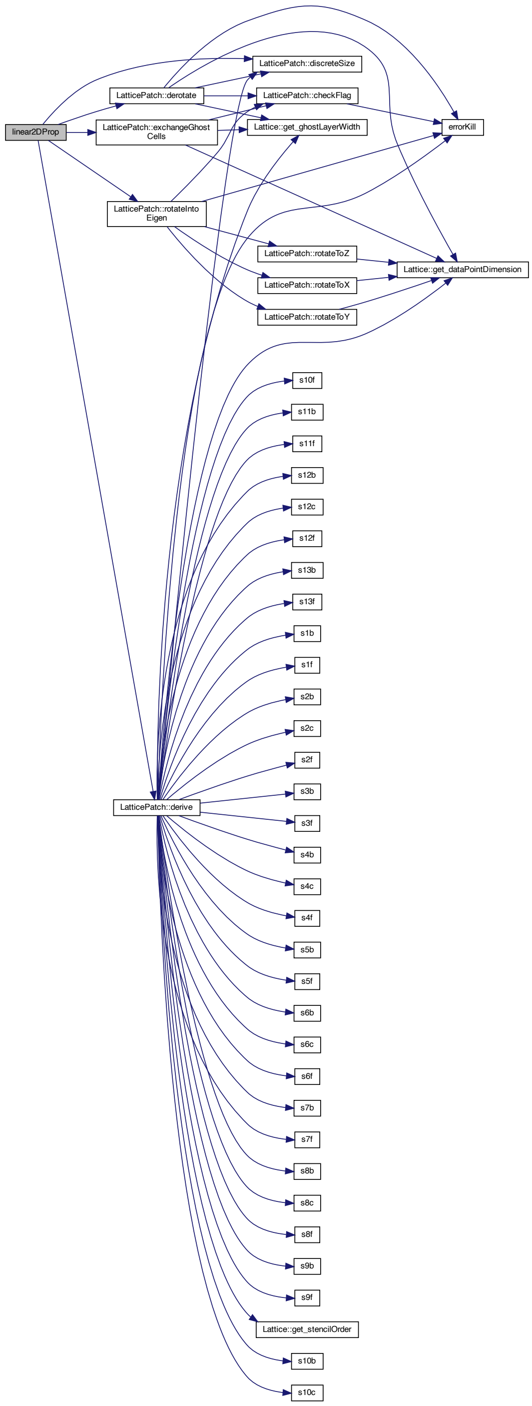
Maxwell propagation function for 2D – only for reference.

Definition at line 265 of file TimeEvolutionFunctions.cpp.

```
00265                                                                                                {
00266
00267   sunrealtype *duData = data->duData;
00268   sunrealtype *dxData = data->buffData[1 - 1];
00269   sunrealtype *dyData = data->buffData[2 - 1];
00270
00271   data->exchangeGhostCells(1);
00272   data->rotateIntoEigen(1);
00273   data->derive(1);
00274   data->derotate(1, dxData);
00275   data->exchangeGhostCells(2);
00276   data->rotateIntoEigen(2);
00277   data->derive(2);
00278   data->derotate(2, dyData);
00279
00280   int totalNP = data->discreteSize();
00281   int pp = 0;
00282   for (int i = 0; i < totalNP; i++) {
00283     pp = i * 6;
00284     duData[pp + 0] = dyData[pp + 5];
00285     duData[pp + 1] = -dxData[pp + 5];
00286     duData[pp + 2] = -dyData[pp + 3] + dxData[pp + 4];
00287     duData[pp + 3] = -dyData[pp + 2];
00288     duData[pp + 4] = dxData[pp + 2];
00289     duData[pp + 5] = dyData[pp + 0] - dxData[pp + 1];
00290   }
00291 }
```

References LatticePatch::buffData, LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::discreteSize(), LatticePatch::duData, LatticePatch::exchangeGhostCells(), and LatticePatch::rotateIntoEigen().

Here is the call graph for this function:



6.30.2.3 linear3DProp()

```
void linear3DProp (
            LatticePatch * data,
```

```
N_Vector u,
N_Vector udot,
int * c )
```

Maxwell propagation function for 3D – only for reference.

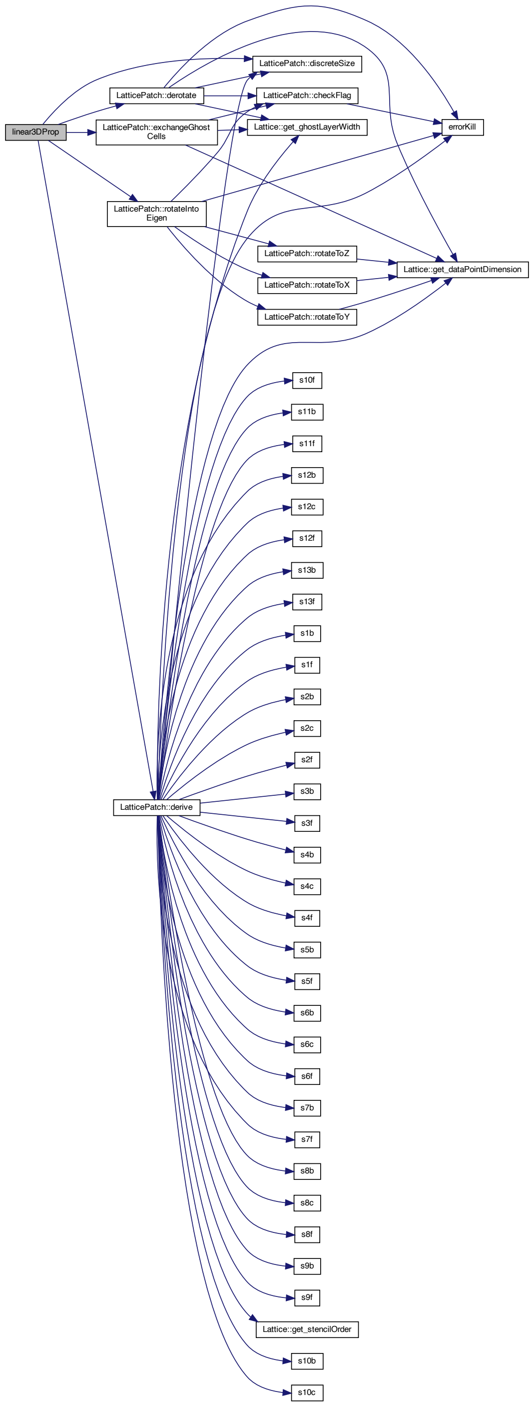
Maxwell propagation function for 3D – only for reference.

Definition at line 476 of file TimeEvolutionFunctions.cpp.

```
00476                                                                      {
00477
00478   sunrealtype *duData = data->duData;
00479   sunrealtype *dxData = data->buffData[1 - 1];
00480   sunrealtype *dyData = data->buffData[2 - 1];
00481   sunrealtype *dzData = data->buffData[3 - 1];
00482
00483   data->exchangeGhostCells(1);
00484   data->rotateIntoEigen(1);
00485   data->derive(1);
00486   data->derotate(1, dxData);
00487   data->exchangeGhostCells(2);
00488   data->rotateIntoEigen(2);
00489   data->derive(2);
00490   data->derotate(2, dyData);
00491   data->exchangeGhostCells(3);
00492   data->rotateIntoEigen(3);
00493   data->derive(3);
00494   data->derotate(3, dzData);
00495
00496   int totalNP = data->discreteSize();
00497   int pp = 0;
00498   for (int i = 0; i < totalNP; i++) {
00499     pp = i * 6;
00500     duData[pp + 0] = dyData[pp + 5] - dzData[pp + 4];
00501     duData[pp + 1] = dzData[pp + 3] - dxData[pp + 5];
00502     duData[pp + 2] = dxData[pp + 4] - dyData[pp + 3];
00503     duData[pp + 3] = -dyData[pp + 2] + dzData[pp + 1];
00504     duData[pp + 4] = -dzData[pp + 0] + dxData[pp + 2];
00505     duData[pp + 5] = -dxData[pp + 1] + dyData[pp + 0];
00506   }
00507 }
```

References LatticePatch::buffData, LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::discreteSize(), LatticePatch::duData, LatticePatch::exchangeGhostCells(), and LatticePatch::rotateIntoEigen().

Here is the call graph for this function:



6.30.2.4 nonlinear1DProp()

```
void nonlinear1DProp (
            LatticePatch * data,
```

```
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 79 of file TimeEvolutionFunctions.cpp.

```
00079                                                                                {
00080
00081     // pointer to spatial derivative data sufficient, temporal derivative data
00082     // provided with udot
00083     sunrealtype *dxData = data->buffData[1 - 1];
00084
00085     // same sequence as in the linear case
00086     data->exchangeGhostCells(1);
00087     data->rotateIntoEigen(1);
00088     data->derive(1);
00089     data->derotate(1, dxData);
00090
00091     /*
00092     F and G are nonzero in the nonlinear case,
00093     polarization and magnetization contributions in Jacobi matrix style
00094     with derivatives of polarization and magnetization
00095     w.r.t. E- and B-field
00096     */
00097     sunrealtype f = NAN, g = NAN; // em field invariants F, G
00098     sunrealtype lf = NAN, lff = NAN, lfg = NAN, lg = NAN,
00099                 lgg = NAN; // derivatives of Lagrangian w.r.t. field invariants
00100     array<sunrealtype, 36> JMM; // Jacobi matrix
00101     array<sunrealtype, 6> Quad; // array to hold E^2 and B^2 components
00102     array<sunrealtype, 6> h; // holding temporal derivatives of E and B components
00103                              // before operating (1+Z)^-1
00104     sunrealtype pseudoDenom = NAN; // needed for inversion of 1+Z
00105     sunrealtype *udata = nullptr,
00106                 *dudata = nullptr; // pointers to data and temp. derivative data
00107     udata = NV_DATA_P(u);
00108     dudata = NV_DATA_P(udot);
00109     int totalNP = data->discreteSize(); // number of points in the patch
00110     for (int pp = 0; pp < totalNP * 6;
00111          pp += 6) { // loops through all 6dim points in the patch
00112                  //    for(int ppB=0;ppB<totalNP*6;ppB+=6*6){
00113                  //      for(int pp=ppB;pp<min(totalNP*6,ppB+6*6);pp+=6){
00114       /// Calculation of the Jacobi matrix
00115       // 1. Calculate F and G
00116       f = 0.5 * ((Quad[0] = udata[pp] * udata[pp]) +
00117                  (Quad[1] = udata[pp + 1] * udata[pp + 1]) +
00118                  (Quad[2] = udata[pp + 2] * udata[pp + 2]) -
00119                  (Quad[3] = udata[pp + 3] * udata[pp + 3]) -
00120                  (Quad[4] = udata[pp + 4] * udata[pp + 4]) -
00121                  (Quad[5] = udata[pp + 5] * udata[pp + 5]));
00122       g = udata[pp] * udata[pp + 3] + udata[pp + 1] * udata[pp + 4] +
00123           udata[pp + 2] * udata[pp + 5];
00124       // 2. Choose process/expansion order and assign derivative values of L
00125       // w.r.t. F, G
00126       switch (*c) {
00127       case 0:
00128         lf = 0;
00129         lff = 0;
00130         lfg = 0;
00131         lg = 0;
00132         lgg = 0;
00133         break;
00134       case 2:
00135         lf = 0.000354046449700427580438254 * f * f +
00136              0.000191775160254398272737387 * g * g;
00137         lff = 0.000708092899400855160876507 5 * f;
00138         lfg = 0.000383550320508796545474774 9 * g;
00139         lg = 0.000383550320508796545474774 9 * f * g;
00140         lgg = 0.000383550320508796545474774 9 * f;
00141         break;
00142       case 1:
00143         lf = 0.000206527095658582755255648 * f;
00144         lff = 0.000206527095658582755255648;
00145         lfg = 0;
00146         lg = 0.000361422417402519821697384 1 * g;
00147         lgg = 0.000361422417402519821697384 1;
00148         break;
00149       case 3:
00150         lf = (0.000206527095658582755255648 + 0.000354046449700427580438254 * f) *
00151                f +
00152              0.000191775160254398272737387 * g * g;
```

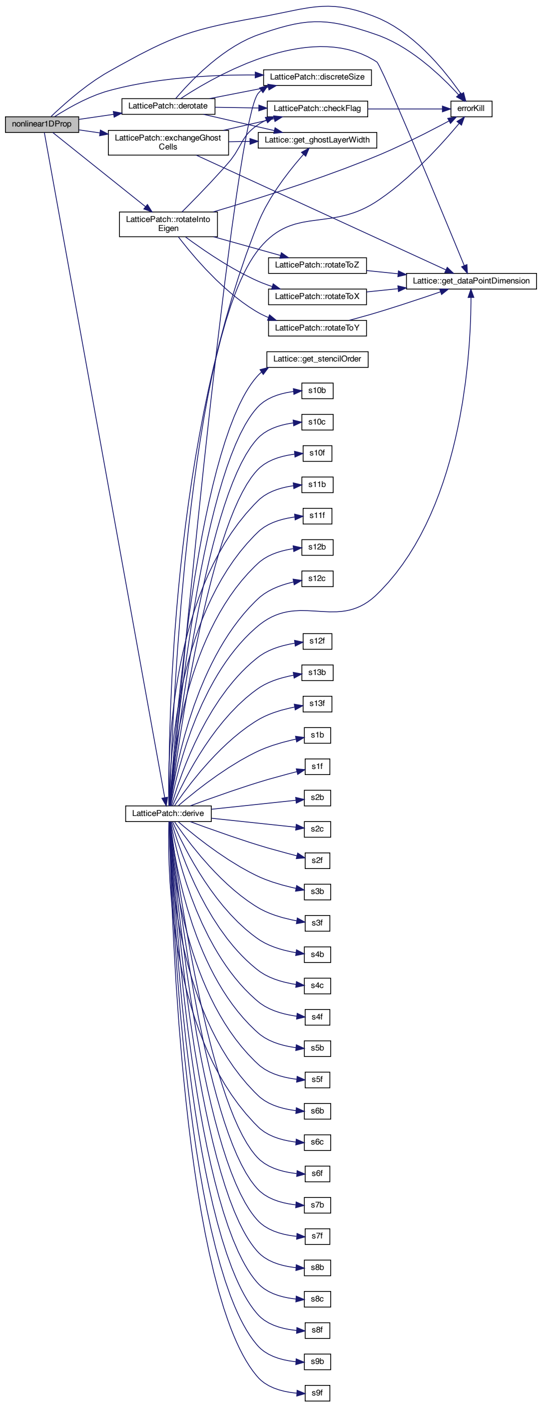
```
      lff = 0.000206527095658582755255648 + 0.0007080928994008551608765075 * f;
      lfg = 0.0003835503205087965454747749 * g;
      lg = (0.0003614224174025198216973841 +
            0.0003835503205087965454747749 * f) *
           g;
      lgg = 0.0003614224174025198216973841 + 0.0003835503205087965454747749 * f;
      break;
    default:
      errorKill(
          "You need to specify a correct order in the weak-field expansion.");
    }
    // 3. Assign Jacobi components
    JMM[0] = lf + lff * Quad[0] +
             udata[3 + pp] * (2 * lfg * udata[pp] + lgg * udata[3 + pp]);
    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];
    JMM[7] = lf + lff * Quad[1] +
             udata[4 + pp] * (2 * lfg * udata[1 + pp] + lgg * udata[4 + pp]);
    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];
    JMM[13] = lff * udata[1 + pp] * udata[2 + pp] +
              lfg * udata[2 + pp] * udata[4 + pp] +
              lfg * udata[1 + pp] * udata[5 + pp] +
              lgg * udata[4 + pp] * udata[5 + pp];
    JMM[14] = lf + lff * Quad[2] +
              udata[5 + pp] * (2 * lfg * udata[2 + pp] + lgg * udata[5 + pp]);
    JMM[18] = lg + lfg * (Quad[0] - Quad[3 + 0]) +
              (-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]);
    JMM[20] = -(udata[3 + pp] * (lff * udata[2 + pp] + lfg * udata[5 + pp])) +
              udata[pp] * (lfg * udata[2 + pp] + lgg * udata[5 + pp]);
    JMM[21] = -lf + lgg * Quad[0] +
              udata[3 + pp] * (-2 * lfg * udata[pp] + lff * udata[3 + pp]);
    JMM[24] = udata[1 + pp] * (lfg * udata[pp] + lgg * udata[3 + pp]) -
              (lff * udata[pp] + lfg * udata[3 + pp]) * udata[4 + pp];
    JMM[25] = lg + lfg * (Quad[1] - Quad[4 + 0]) +
              (-lff + lgg) * udata[1 + 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]);
    JMM[27] = lgg * udata[pp] * udata[1 + pp] +
              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]);
    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]) -
              (lff * udata[1 + pp] + lfg * udata[4 + pp]) * udata[5 + pp];
    JMM[32] = lg + lfg * (Quad[2] - Quad[5 + 0]) +
              (-lff + lgg) * udata[2 + pp] * udata[5 + pp];
    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]);
    JMM[34] =
        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]);
    JMM[35] = -lf + lgg * Quad[2] +
              udata[5 + pp] * (-2 * lfg * udata[2 + pp] + lff * udata[5 + pp]);
    for (int i = 0; i < 6; i++) {
      for (int j = i + 1; j < 6; j++) {
        JMM[i * 6 + j] = JMM[j * 6 + i];
      }
    }
    // 4. Final values for temporal derivatives of field values
    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]);
    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];
    h[3] = 0;
    h[4] = dxData[2 + pp];
    h[5] = -dxData[1 + 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];
    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] =
        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] =
```

```
        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]));
    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]);
    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]));
    dudata[pp + 0] /= pseudoDenom;
    dudata[pp + 1] /= pseudoDenom;
    dudata[pp + 2] /= pseudoDenom;
    dudata[pp + 3] = h[3];
    dudata[pp + 4] = h[4];
    dudata[pp + 5] = h[5];
  }
  return;
}
```

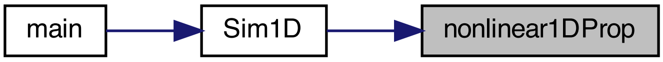
References LatticePatch::buffData, LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::discreteSize(), errorKill(), LatticePatch::exchangeGhostCells(), and LatticePatch::rotateIntoEigen().

Referenced by Sim1D().

Here is the call graph for this function:



Here is the caller graph for this function:



6.30.2.5 nonlinear2DProp()

```
void nonlinear2DProp (
            LatticePatch * data,
            N_Vector u,
            N_Vector udot,
            int * c )
```

HE propagation function for 2D.

HE propagation function for 2D.

Definition at line 294 of file TimeEvolutionFunctions.cpp.

```
00294                                                                  {
00295
00296   sunrealtype *dxData = data->buffData[1 - 1];
00297   sunrealtype *dyData = data->buffData[2 - 1];
00298
00299   data->exchangeGhostCells(1);
00300   data->rotateIntoEigen(1);
00301   data->derive(1);
00302   data->derotate(1, dxData);
00303   data->exchangeGhostCells(2);
00304   data->rotateIntoEigen(2);
00305   data->derive(2);
00306   data->derotate(2, dyData);
00307
00308   sunrealtype f = NAN, g = NAN;
00309   sunrealtype lf = NAN, lff = NAN, lfg = NAN, lg = NAN, lgg = NAN;
00310   array<sunrealtype, 36> JMM;
00311   array<sunrealtype, 6> Quad;
00312   array<sunrealtype, 6> h;
00313   sunrealtype pseudoDenom = NAN;
00314   sunrealtype *udata = nullptr, *dudata = nullptr;
00315   udata = NV_DATA_P(u);
00316   dudata = NV_DATA_P(udot);
00317   int totalNP = data->discreteSize();
00318   for (int pp = 0; pp < totalNP * 6; pp += 6) {
00319     // 1
00320     f = 0.5 * ((Quad[0] = udata[pp] * udata[pp]) +
00321                (Quad[1] = udata[pp + 1] * udata[pp + 1]) +
00322                (Quad[2] = udata[pp + 2] * udata[pp + 2]) -
00323                (Quad[3] = udata[pp + 3] * udata[pp + 3]) -
00324                (Quad[4] = udata[pp + 4] * udata[pp + 4]) -
00325                (Quad[5] = udata[pp + 5] * udata[pp + 5]));
00326     g = udata[pp] * udata[pp + 3] + udata[pp + 1] * udata[pp + 4] +
00327         udata[pp + 2] * udata[pp + 5];
00328     // 2
00329     switch (*c) {
00330     case 0:
00331       lf = 0;
00332       lff = 0;
00333       lfg = 0;
00334       lg = 0;
00335       lgg = 0;
00336       break;
```

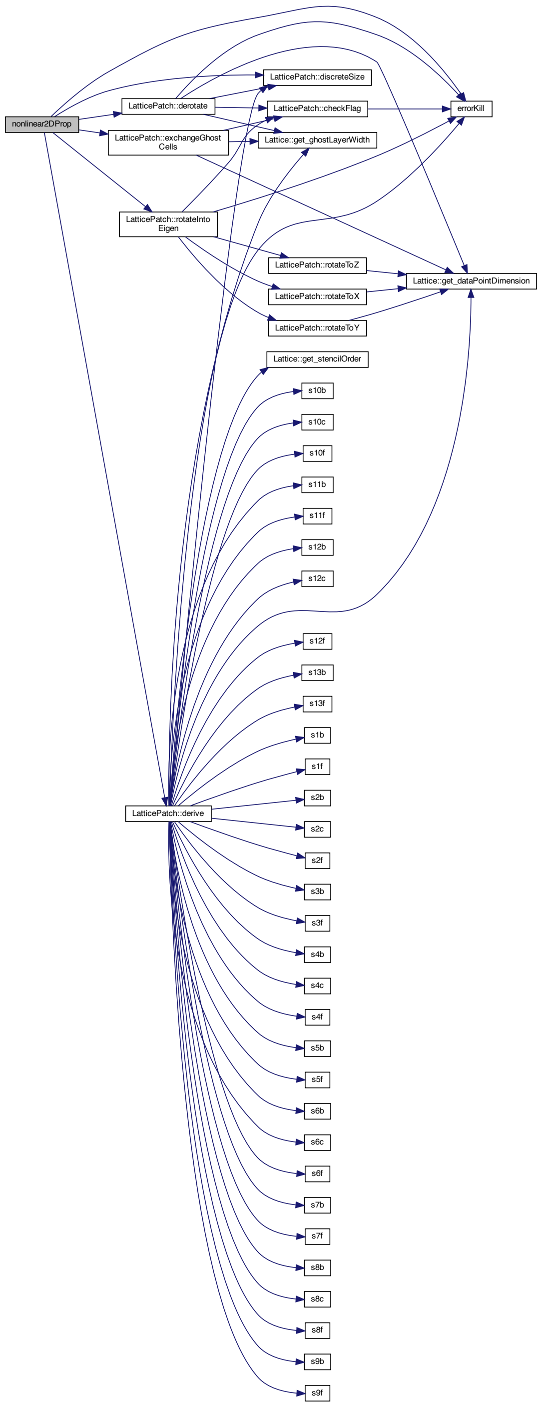
```
    case 2:
      lf = 0.00035404644970042758043825 4 * f * f +
           0.00019177516025439827273738 7 * g * g;
      lff = 0.0007080928994008551608765075 * f;
      lfg = 0.0003835503205087965454747749 * g;
      lg = 0.0003835503205087965454747749 * f * g;
      lgg = 0.0003835503205087965454747749 * f;
      break;
    case 1:
      lf = 0.0002065270956585827552556 48 * f;
      lff = 0.000206527095658582755255648;
      lfg = 0;
      lg = 0.0003614224174025198216973841 * g;
      lgg = 0.0003614224174025198216973841;
      break;
    case 3:
      lf = (0.000206527095658582755255648 + 0.000354046449700427580438254 * f) *
               f +
           0.000191775160254398272737387 * g * g;
      lff = 0.000206527095658582755255648 + 0.000708092899400855160876508 * f;
      lfg = 0.0003835503205087965454747749 * g;
      lg = (0.000361422417402519821697384 + 0.000383550320508796545474775 * f) *
           g;
      lgg = 0.000361422417402519821697384 + 0.000383550320508796545474775 * f;
      break;
    default:
      errorKill(
          "You need to specify a correct order in the weak-field expansion.");
    }
    // 3
    JMM[0] = lf + lff * Quad[0] +
             udata[3 + pp] * (2 * lfg * udata[pp] + lgg * udata[3 + pp]);
    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];
    JMM[7] = lf + lff * Quad[1] +
             udata[4 + pp] * (2 * lfg * udata[1 + pp] + lgg * udata[4 + pp]);
    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];
    JMM[13] = lff * udata[1 + pp] * udata[2 + pp] +
              lfg * udata[2 + pp] * udata[4 + pp] +
              lfg * udata[1 + pp] * udata[5 + pp] +
              lgg * udata[4 + pp] * udata[5 + pp];
    JMM[14] = lf + lff * Quad[2] +
              udata[5 + pp] * (2 * lfg * udata[2 + pp] + lgg * udata[5 + pp]);
    JMM[18] = lg + lfg * (Quad[0] - Quad[3 + 0]) +
              (-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]);
    JMM[20] = -(udata[3 + pp] * (lff * udata[2 + pp] + lfg * udata[5 + pp])) +
              udata[pp] * (lfg * udata[2 + pp] + lgg * udata[5 + pp]);
    JMM[21] = -lf + lgg * Quad[0] +
              udata[3 + pp] * (-2 * lfg * udata[pp] + lff * udata[3 + pp]);
    JMM[24] = udata[1 + pp] * (lfg * udata[pp] + lgg * udata[3 + pp]) -
              (lff * udata[pp] + lfg * udata[3 + pp]) * udata[4 + pp];
    JMM[25] = lg + lfg * (Quad[1] - Quad[4 + 0]) +
              (-lff + lgg) * udata[1 + 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]);
    JMM[27] = lgg * udata[pp] * udata[1 + pp] +
              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]);
    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]) -
              (lff * udata[1 + pp] + lfg * udata[4 + pp]) * udata[5 + pp];
    JMM[32] = lg + lfg * (Quad[2] - Quad[5 + 0]) +
              (-lff + lgg) * udata[2 + pp] * udata[5 + pp];
    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]);
    JMM[34] =
        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]);
    JMM[35] = -lf + lgg * Quad[2] +
              udata[5 + pp] * (-2 * lfg * udata[2 + pp] + lff * udata[5 + pp]);
    // 4
    for (int i = 0; i < 6; i++) {
      for (int j = i + 1; j < 6; j++) {
        JMM[i * 6 + j] = JMM[j * 6 + i];
      }
    }
    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]);
    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];
    h[3] = 0;
    h[4] = dxData[2 + pp];
    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]);
    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];
    h[3] += -dyData[2 + pp];
    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];
    h[2] -= h[3] * JMM[15] + h[4] * JMM[16] + h[5] * JMM[17];
    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]));
    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]));
    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]);
    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]));
    dudata[pp + 0] /= pseudoDenom;
    dudata[pp + 1] /= pseudoDenom;
    dudata[pp + 2] /= pseudoDenom;
    dudata[pp + 3] = h[3];
    dudata[pp + 4] = h[4];
    dudata[pp + 5] = h[5];
  }
  return;
}
```

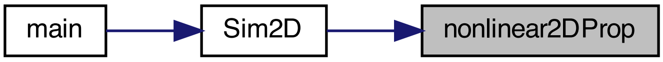
References LatticePatch::buffData, LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::discreteSize(), errorKill(), LatticePatch::exchangeGhostCells(), and LatticePatch::rotateIntoEigen().

Referenced by Sim2D().

Here is the call graph for this function:



Here is the caller graph for this function:



6.30.2.6 nonlinear3DProp()

```
void nonlinear3DProp (
            LatticePatch * data,
            N_Vector u,
            N_Vector udot,
            int * c )
```

HE propagation function for 3D.

HE propagation function for 3D.

Definition at line 510 of file TimeEvolutionFunctions.cpp.

```
00510                                                                          {
00511
00512   sunrealtype *dxData = data->buffData[1 - 1];
00513   sunrealtype *dyData = data->buffData[2 - 1];
00514   sunrealtype *dzData = data->buffData[3 - 1];
00515
00516   data->exchangeGhostCells(1);
00517   data->rotateIntoEigen(1);
00518   data->derive(1);
00519   data->derotate(1,dxData);
00520   data->exchangeGhostCells(2);
00521   data->rotateIntoEigen(2);
00522   data->derive(2);
00523   data->derotate(2,dyData);
00524   data->exchangeGhostCells(3);
00525   data->rotateIntoEigen(3);
00526   data->derive(3);
00527   data->derotate(3,dzData);
00528
00529   sunrealtype f = NAN, g = NAN;
00530   sunrealtype lf = NAN, lff = NAN, lfg = NAN, lg = NAN, lgg = NAN;
00531   array<sunrealtype, 36> JMM;
00532   array<sunrealtype, 6> Quad;
00533   array<sunrealtype, 6> h;
00534   sunrealtype pseudoDenom = NAN;
00535   sunrealtype *udata = nullptr, *dudata = nullptr;
00536   udata = NV_DATA_P(u);
00537   dudata = NV_DATA_P(udot);
00538   int totalNP = data->discreteSize();
00539   for (int pp = 0; pp < totalNP * 6; pp += 6) {
00540     // 1
00541     f = 0.5 * ((Quad[0] = udata[pp] * udata[pp]) +
00542                (Quad[1] = udata[pp + 1] * udata[pp + 1]) +
00543                (Quad[2] = udata[pp + 2] * udata[pp + 2]) -
00544                (Quad[3] = udata[pp + 3] * udata[pp + 3]) -
00545                (Quad[4] = udata[pp + 4] * udata[pp + 4]) -
00546                (Quad[5] = udata[pp + 5] * udata[pp + 5]));
00547     g = udata[pp] * udata[pp + 3] + udata[pp + 1] * udata[pp + 4] +
00548         udata[pp + 2] * udata[pp + 5];
00549     // 2
00550     switch (*c) {
00551     case 0:
00552       lf = 0;
```

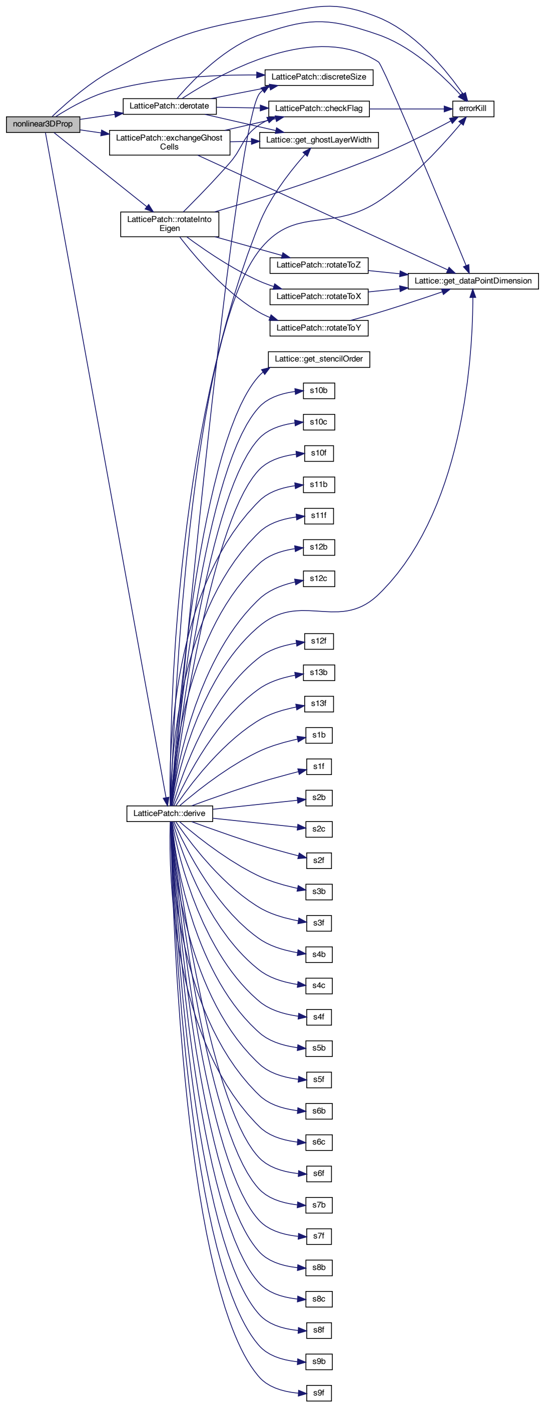
```
        lff = 0;
        lfg = 0;
        lg = 0;
        lgg = 0;
        break;
      case 2:
        lf = 0.00035404644970042758043825 4 * f * f +
             0.000191775160254398272737387 * g * g;
        lff = 0.00070809289940085516087650 75 * f;
        lfg = 0.000383550320508796545474774 9 * g;
        lg = 0.000383550320508796545474774 9 * f * g;
        lgg = 0.000383550320508796545474774 9 * f;
        break;
      case 1:
        lf = 0.000206527095658582755255648 * f;
        lff = 0.000206527095658582755255648;
        lfg = 0;
        lg = 0.000361422417402519821697384 1 * g;
        lgg = 0.000361422417402519821697384 1;
        break;
      case 3:
        lf = (0.000206527095658582755255648 + 0.000354046449700427580438254 * f) *
                 f +
             0.000191775160254398272737387 * g * g;
        lff = 0.000206527095658582755255648 + 0.000708092899400855160876508 * f;
        lfg = 0.000383550320508796545474774 9 * g;
        lg = (0.000361422417402519821697384 + 0.000383550320508796545474775 * f) *
             g;
        lgg = 0.000361422417402519821697384 + 0.000383550320508796545474775 * f;
        break;
      default:
        errorKill(
            "You need to specify a correct order in the weak-field expansion.");
      }
      // 3
      JMM[0] = lf + lff * Quad[0] +
               udata[3 + pp] * (2 * lfg * udata[pp] + lgg * udata[3 + pp]);
      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];
      JMM[7] = lf + lff * Quad[1] +
               udata[4 + pp] * (2 * lfg * udata[1 + pp] + lgg * udata[4 + pp]);
      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];
      JMM[13] = lff * udata[1 + pp] * udata[2 + pp] +
                lfg * udata[2 + pp] * udata[4 + pp] +
                lfg * udata[1 + pp] * udata[5 + pp] +
                lgg * udata[4 + pp] * udata[5 + pp];
      JMM[14] = lf + lff * Quad[2] +
                udata[5 + pp] * (2 * lfg * udata[2 + pp] + lgg * udata[5 + pp]);
      JMM[18] = lg + lfg * (Quad[0] - Quad[3 + 0]) +
                (-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]);
      JMM[20] = -(udata[3 + pp] * (lff * udata[2 + pp] + lfg * udata[5 + pp])) +
                udata[pp] * (lfg * udata[2 + pp] + lgg * udata[5 + pp]);
      JMM[21] = -lf + lgg * Quad[0] +
                udata[3 + pp] * (-2 * lfg * udata[pp] + lff * udata[3 + pp]);
      JMM[24] = udata[1 + pp] * (lfg * udata[pp] + lgg * udata[3 + pp]) -
                (lff * udata[pp] + lfg * udata[3 + pp]) * udata[4 + pp];
      JMM[25] = lg + lfg * (Quad[1] - Quad[4 + 0]) +
                (-lff + lgg) * udata[1 + 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]);
      JMM[27] = lgg * udata[pp] * udata[1 + pp] +
                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]);
      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]) -
                (lff * udata[1 + pp] + lfg * udata[4 + pp]) * udata[5 + pp];
      JMM[32] = lg + lfg * (Quad[2] - Quad[5 + 0]) +
                (-lff + lgg) * udata[2 + pp] * udata[5 + pp];
      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]);
      JMM[34] =
          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]);
      JMM[35] = -lf + lgg * Quad[2] +
                udata[5 + pp] * (-2 * lfg * udata[2 + pp] + lff * udata[5 + pp]);
      // 4
      for (int i = 0; i < 6; i++) {
```

```
      for (int j = i + 1; j < 6; j++) {
        JMM[i * 6 + j] = JMM[j * 6 + i];
      }
    }
    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]);
    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];
    h[3] = 0;
    h[4] = dxData[2 + pp];
    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]);
    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];
    h[3] += -dyData[2 + pp];
    h[4] += 0;
    h[5] += dyData[pp];
    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];
    h[2] += 0;
    h[3] += dzData[1 + pp];
    h[4] += -dzData[pp];
    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];
    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]));
    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]));
    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]);
    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]));
    dudata[pp + 0] /= pseudoDenom;
    dudata[pp + 1] /= pseudoDenom;
    dudata[pp + 2] /= pseudoDenom;
    dudata[pp + 3] = h[3];
    dudata[pp + 4] = h[4];
    dudata[pp + 5] = h[5];
  }
  return;
}
```

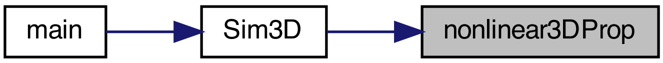
References LatticePatch::buffData, LatticePatch::derive(), LatticePatch::derotate(), LatticePatch::discreteSize(), errorKill(), LatticePatch::exchangeGhostCells(), and LatticePatch::rotateIntoEigen().

Referenced by Sim3D().

Here is the call graph for this function:



Here is the caller graph for this function:



6.31 TimeEvolutionFunctions.h

Go to the documentation of this file.

```
/////////////////////////////////////////////////////////
/// @file TimeEvolutionFunctions.h
/// @brief Functions to propagate data vectors in time
/// according to Maxwell's equations, and various
/// orders in the HE weak-field expansion
/////////////////////////////////////////////////////////

// Include Guard
#ifndef TIMEEVOLVER
#define TIMEEVOLVER

#include "LatticePatch.h"
#include "SimulationClass.h"

/** @brief monostate TimeEvolution Class to propagate the field data in time in
 * a given order of the HE weak-field expansion */
class TimeEvolution {
public:
  /// choice which processes of the weak field expansion are included
  static int *c;

  /// Pointer to functions for differentiation and time evolution
  static void (*TimeEvolver)(LatticePatch *, N_Vector, N_Vector, int *);

  /// CVODE right hand side function (CVRhsFn) to provide IVP of the ODE
  static int f(sunrealtype t, N_Vector u, N_Vector udot, void *data_loc);
};

/// Maxwell propagation function for 1D - only for reference
void linear1DProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c);
/// HE propagation function for 1D
void nonlinear1DProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c);
/// Maxwell propagation function for 2D - only for reference
void linear2DProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c);
/// HE propagation function for 2D
void nonlinear2DProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c);
/// Maxwell propagation function for 3D - only for reference
void linear3DProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c);
/// HE propagation function for 3D
void nonlinear3DProp(LatticePatch *data, N_Vector u, N_Vector udot, int *c);

// End of Includeguard
#endif
```

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