

phasefield-accelerator-benchmarks

pre-alpha

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1 Module Index

1.1 Modules

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2 Class Index

2.1 Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

ResidualSumOfSquares2D	
Comparison algorithm for execution on the block of threads	35

3 File Index

3.1 File List

Here is a list of all documented files with brief descriptions:

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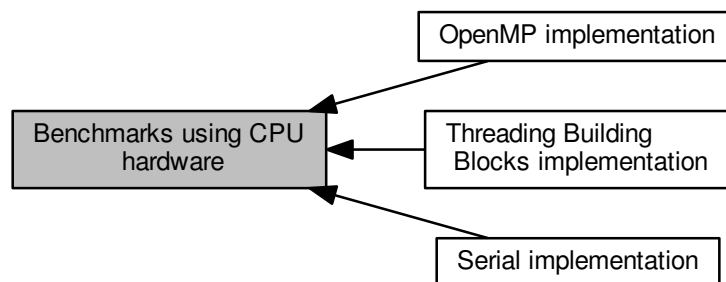
Definition of scalar data type

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4 Module Documentation

4.1 Benchmarks using CPU hardware

Collaboration diagram for Benchmarks using CPU hardware:



Modules

- [OpenMP implementation](#)
- [Serial implementation](#)
- [Threading Building Blocks implementation](#)

Files

- file [cpu/main.c](#)
Implementation of semi-infinite diffusion equation.
- file [cpu/mesh.c](#)
Implementation of mesh handling functions.
- file [cpu/mesh.h](#)
Declaration of mesh function prototypes for CPU benchmarks.
- file [cpu/output.c](#)
Implementation of file output functions.
- file [cpu/output.h](#)
Declaration of output function prototypes for CPU benchmarks.
- file [cpu/timer.c](#)
High-resolution cross-platform machine time reader.
- file [cpu/timer.h](#)
Declaration of timer function prototypes for CPU benchmarks.
- file [cpu/type.h](#)
Definition of scalar data type.

Typedefs

- typedef double `fp_t`

Functions

- int `main` (int argc, char *argv[])
Run simulation using input parameters specified on the command line.
- void `make_arrays` (`fp_t` ***conc_old, `fp_t` ***conc_new, `fp_t` ***conc_lap, `fp_t` ***mask_lap, int nx, int ny, int nm)
Allocate 2D arrays to store scalar composition values.
- void `free_arrays` (`fp_t` **conc_old, `fp_t` **conc_new, `fp_t` **conc_lap, `fp_t` **mask_lap)
Free dynamically allocated memory.
- void `swap_pointers` (`fp_t` ***conc_old, `fp_t` ***conc_new)
Swap pointers to data underlying two arrays.
- void `print_progress` (const int step, const int steps)
Prints timestamps and a 20-point progress bar to stdout.
- void `write_csv` (`fp_t` **conc, int nx, int ny, `fp_t` dx, `fp_t` dy, int step)
Writes scalar composition field to diffusion.???????.csv.
- void `write_png` (`fp_t` **conc, int nx, int ny, int step)
Writes scalar composition field to diffusion.???????.png.
- void `StartTimer` ()
Set CPU frequency and begin timing.
- double `GetTimer` ()
Return elapsed time in seconds.

Variables

- struct timeval `timerStart`

4.1.1 Detailed Description

4.1.2 Typedef Documentation

4.1.2.1 `fp_t`

```
typedef double fp_t
```

Specify the basic data type to achieve the desired accuracy in floating-point arithmetic: float for single-precision, double for double-precision.

Definition at line 41 of file `cpu/type.h`.

4.1.3 Function Documentation

4.1.3.1 main()

```
int main (
    int argc,
    char * argv[] )
```

Run simulation using input parameters specified on the command line.

Program will write a series of PNG image files to visualize scalar composition field, plus a final CSV raw data file and CSV runtime log tabulating the iteration counter (iter), elapsed simulation time (sim_time), system free energy (energy), error relative to analytical solution (wrss), time spent performing convolution (conv_time), time spent updating fields (step_time), time spent writing to disk (IO_time), time spent generating analytical values (soln_time), and total elapsed (run_time).

Definition at line 51 of file cpu/main.c.

4.1.3.2 make_arrays()

```
void make_arrays (
    fp_t *** conc_old,
    fp_t *** conc_new,
    fp_t *** conc_lap,
    fp_t *** mask_lap,
    int nx,
    int ny,
    int nm )
```

Allocate 2D arrays to store scalar composition values.

Arrays are allocated as 1D arrays, then 2D pointer arrays are mapped over the top. This facilitates use of either 1D or 2D data access, depending on whether the task is spatially dependent or not.

Definition at line 41 of file cpu/mesh.c.

4.1.3.3 print_progress()

```
void print_progress (
    const int step,
    const int steps )
```

Prints timestamps and a 20-point progress bar to stdout.

Call inside the timestepping loop, near the top, e.g.

```
for (int step=0; step<steps; step++) {
    print_progress(step, steps);
    take_a_step();
    elapsed += dt;
}
```

Definition at line 49 of file cpu/output.c.

4.1.3.4 swap_pointers()

```
void swap_pointers (
    fp_t *** conc_old,
    fp_t *** conc_new )
```

Swap pointers to data underlying two arrays.

Rather than copy data from `conc_old` into `conc_new`, an expensive operation, simply trade the top-most pointers. New becomes old with no data lost and in almost no time.

Definition at line 95 of file `cpu/mesh.c`.

4.1.4 Variable Documentation

4.1.4.1 timerStart

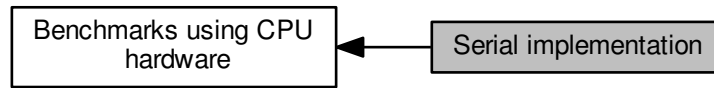
```
struct timeval timerStart
```

Platform-dependent data type of hardware time value

Definition at line 49 of file `cpu/timer.c`.

4.2 Serial implementation

Collaboration diagram for Serial implementation:



Files

- file [cpu/serial/boundaries.c](#)
Implementation of boundary condition functions without threading.
- file [cpu/serial/boundaries.h](#)
Declaration of boundary condition function prototypes for CPU benchmarks.
- file [cpu/serial/discretization.c](#)
Implementation of boundary condition functions without threading.
- file [cpu/serial/discretization.h](#)
Declaration of discretized mathematical function prototypes for CPU benchmarks.

Functions

- void [set_boundaries](#) ([fp_t](#) bc[2][2])
Set values to be used along the simulation domain boundaries.
- void [apply_initial_conditions](#) ([fp_t](#) **conc, int nx, int ny, int nm, [fp_t](#) bc[2][2])
Initialize flat composition field with fixed boundary conditions.
- void [apply_boundary_conditions](#) ([fp_t](#) **conc, int nx, int ny, int nm, [fp_t](#) bc[2][2])
Set fixed value (c_{hi}) along left and bottom, zero-flux elsewhere.
- void [set_threads](#) (int n)
Set number of OpenMP threads to use in parallel code sections.
- void [five_point_Laplacian_stencil](#) ([fp_t](#) dx, [fp_t](#) dy, [fp_t](#) **mask_lap)
Write 5-point Laplacian stencil into convolution mask.
- void [nine_point_Laplacian_stencil](#) ([fp_t](#) dx, [fp_t](#) dy, [fp_t](#) **mask_lap)
Write 9-point Laplacian stencil into convolution mask.
- void [slow_nine_point_Laplacian_stencil](#) ([fp_t](#) dx, [fp_t](#) dy, [fp_t](#) **mask_lap)
Write 9-point Laplacian stencil into convolution mask.
- void [set_mask](#) ([fp_t](#) dx, [fp_t](#) dy, int nm, [fp_t](#) **mask_lap)
Specify which stencil to use for the Laplacian.
- void [compute_convolution](#) ([fp_t](#) **conc_old, [fp_t](#) **conc_lap, [fp_t](#) **mask_lap, int nx, int ny, int nm)
Perform the convolution of the mask matrix with the composition matrix.
- void [solve_diffusion_equation](#) ([fp_t](#) **conc_old, [fp_t](#) **conc_new, [fp_t](#) **conc_lap, int nx, int ny, int nm, [fp_t](#) D, [fp_t](#) dt, [fp_t](#) *elapsed)
Update the scalar composition field using old and Laplacian values.
- void [analytical_value](#) ([fp_t](#) x, [fp_t](#) t, [fp_t](#) D, [fp_t](#) bc[2][2], [fp_t](#) *c)
Analytical solution of the diffusion equation for a carburizing process.
- void [check_solution](#) ([fp_t](#) **conc_new, int nx, int ny, [fp_t](#) dx, [fp_t](#) dy, int nm, [fp_t](#) elapsed, [fp_t](#) D, [fp_t](#) bc[2][2], [fp_t](#) *rss)
Compare numerical and analytical solutions of the diffusion equation.

4.2.1 Detailed Description

4.2.2 Function Documentation

4.2.2.1 analytical_value()

```
void analytical_value (
    fp_t x,
    fp_t t,
    fp_t D,
    fp_t bc[2][2],
    fp_t * c )
```

Analytical solution of the diffusion equation for a carburizing process.

For 1D diffusion through a semi-infinite domain with initial and far-field composition c_∞ and boundary value $c(x = 0, t) = c_0$ with constant diffusivity D , the solution to Fick's second law is

$$c(x, t) = c_0 - (c_0 - c_\infty) \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right)$$

which reduces, when $c_\infty = 0$, to

$$c(x, t) = c_0 \left[1 - \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right) \right].$$

Definition at line 166 of file `cpu/serial/discretization.c`.

4.2.2.2 apply_initial_conditions()

```
void apply_initial_conditions (
    fp_t ** conc,
    int nx,
    int ny,
    int nm,
    fp_t bc[2][2] )
```

Initialize flat composition field with fixed boundary conditions.

The boundary conditions are fixed values of c_{hi} along the lower-left half and upper-right half walls, no flux everywhere else, with an initial values of c_{lo} everywhere. These conditions represent a carburizing process, with partial exposure (rather than the entire left and right walls) to produce an inhomogeneous workload and highlight numerical errors at the boundaries.

Definition at line 59 of file `cpu/serial/boundaries.c`.

4.2.2.3 check_solution()

```
void check_solution (
    fp_t ** conc_new,
    int nx,
    int ny,
    fp_t dx,
    fp_t dy,
    int nm,
    fp_t elapsed,
    fp_t D,
    fp_t bc[2][2],
    fp_t * rss )
```

Compare numerical and analytical solutions of the diffusion equation.

Returns

Residual sum of squares (RSS), normalized to the domain size.

Definition at line 175 of file `cpu/serial/discretization.c`.

4.2.2.4 compute_convolution()

```
void compute_convolution (
    fp_t ** conc_old,
    fp_t ** conc_lap,
    fp_t ** mask_lap,
    int nx,
    int ny,
    int nm )
```

Perform the convolution of the mask matrix with the composition matrix.

If the convolution mask is the Laplacian stencil, the convolution evaluates the discrete Laplacian of the composition field. Other masks are possible, for example the Sobel filters for edge detection. This function is general purpose: as long as the dimensions `nx`, `ny`, and `nm` are properly specified, the convolution will be correctly computed.

Definition at line 124 of file `cpu/serial/discretization.c`.

4.2.2.5 five_point_Laplacian_stencil()

```
void five_point_Laplacian_stencil (
    fp_t dx,
    fp_t dy,
    fp_t ** mask_lap )
```

Write 5-point Laplacian stencil into convolution mask.

3×3 mask, 5 values, truncation error $\mathcal{O}(\Delta x^2)$

Definition at line 51 of file `cpu/serial/discretization.c`.

4.2.2.6 `nine_point_Laplacian_stencil()`

```
void nine_point_Laplacian_stencil (
    fp_t dx,
    fp_t dy,
    fp_t ** mask_lap )
```

Write 9-point Laplacian stencil into convolution mask.

3×3 mask, 9 values, truncation error $\mathcal{O}(\Delta x^4)$

Definition at line 65 of file `cpu/serial/discretization.c`.

4.2.2.7 `set_boundaries()`

```
void set_boundaries (
    fp_t bc[2][2] )
```

Set values to be used along the simulation domain boundaries.

Indexing is row-major, i.e. $A[y][x]$, so `bc` = $[[y_{lo}, y_{hi}], [x_{lo}, x_{hi}]]$.

Definition at line 41 of file `cpu/serial/boundaries.c`.

4.2.2.8 `set_threads()`

```
void set_threads (
    int n )
```

Set number of OpenMP threads to use in parallel code sections.

Warning

Serial code contains no parallel sections: this setting has no effect.

Definition at line 41 of file `cpu/serial/discretization.c`.

4.2.2.9 `slow_nine_point_Laplacian_stencil()`

```
void slow_nine_point_Laplacian_stencil (
    fp_t dx,
    fp_t dy,
    fp_t ** mask_lap )
```

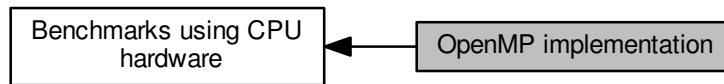
Write 9-point Laplacian stencil into convolution mask.

4×4 mask, 9 values, truncation error $\mathcal{O}(\Delta x^4)$ Provided for testing and demonstration of scalability, only: as the name indicates, this 9-point stencil is computationally more expensive than the 3×3 version. If your code requires $\mathcal{O}(\Delta x^4)$ accuracy, please use [nine_point_Laplacian_stencil\(\)](#).

Definition at line 89 of file `cpu/serial/discretization.c`.

4.3 OpenMP implementation

Collaboration diagram for OpenMP implementation:



Files

- file [cpu/openmp/boundaries.c](#)
Implementation of boundary condition functions with OpenMP threading.
- file [cpu/openmp/boundaries.h](#)
Declaration of boundary condition function prototypes for OpenMP benchmarks.
- file [cpu/openmp/discretization.c](#)
Implementation of boundary condition functions with OpenMP threading.
- file [cpu/openmp/discretization.h](#)
Declaration of discretized mathematical function prototypes for OpenMP benchmarks.

Functions

- void [set_boundaries](#) ([fp_t](#) bc[2][2])
Set values to be used along the simulation domain boundaries.
- void [apply_initial_conditions](#) ([fp_t](#) **conc, int nx, int ny, int nm, [fp_t](#) bc[2][2])
Initialize flat composition field with fixed boundary conditions.
- void [apply_boundary_conditions](#) ([fp_t](#) **conc, int nx, int ny, int nm, [fp_t](#) bc[2][2])
Set fixed value (c_{hi}) along left and bottom, zero-flux elsewhere.
- void [set_threads](#) (int n)
Set number of OpenMP threads to use in parallel code sections.
- void [five_point_Laplacian_stencil](#) ([fp_t](#) dx, [fp_t](#) dy, [fp_t](#) **mask_lap)
Write 5-point Laplacian stencil into convolution mask.
- void [nine_point_Laplacian_stencil](#) ([fp_t](#) dx, [fp_t](#) dy, [fp_t](#) **mask_lap)
Write 9-point Laplacian stencil into convolution mask.
- void [slow_nine_point_Laplacian_stencil](#) ([fp_t](#) dx, [fp_t](#) dy, [fp_t](#) **mask_lap)
Write 9-point Laplacian stencil into convolution mask.
- void [set_mask](#) ([fp_t](#) dx, [fp_t](#) dy, int nm, [fp_t](#) **mask_lap)
Specify which stencil to use for the Laplacian.
- void [compute_convolution](#) ([fp_t](#) **conc_old, [fp_t](#) **conc_lap, [fp_t](#) **mask_lap, int nx, int ny, int nm)
Perform the convolution of the mask matrix with the composition matrix.
- void [solve_diffusion_equation](#) ([fp_t](#) **conc_old, [fp_t](#) **conc_new, [fp_t](#) **conc_lap, int nx, int ny, int nm, [fp_t](#) D, [fp_t](#) dt, [fp_t](#) *elapsed)
Update the scalar composition field using old and Laplacian values.
- void [analytical_value](#) ([fp_t](#) x, [fp_t](#) t, [fp_t](#) D, [fp_t](#) bc[2][2], [fp_t](#) *c)
Analytical solution of the diffusion equation for a carburizing process.
- void [check_solution](#) ([fp_t](#) **conc_new, int nx, int ny, [fp_t](#) dx, [fp_t](#) dy, int nm, [fp_t](#) elapsed, [fp_t](#) D, [fp_t](#) bc[2][2], [fp_t](#) *rss)
Compare numerical and analytical solutions of the diffusion equation.

4.3.1 Detailed Description

4.3.2 Function Documentation

4.3.2.1 analytical_value()

```
void analytical_value (
    fp_t x,
    fp_t t,
    fp_t D,
    fp_t bc[2][2],
    fp_t * c )
```

Analytical solution of the diffusion equation for a carburizing process.

For 1D diffusion through a semi-infinite domain with initial and far-field composition c_∞ and boundary value $c(x = 0, t) = c_0$ with constant diffusivity D , the solution to Fick's second law is

$$c(x, t) = c_0 - (c_0 - c_\infty) \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right)$$

which reduces, when $c_\infty = 0$, to

$$c(x, t) = c_0 \left[1 - \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right) \right].$$

Definition at line 173 of file `cpu/openmp/discretization.c`.

4.3.2.2 apply_initial_conditions()

```
void apply_initial_conditions (
    fp_t ** conc,
    int nx,
    int ny,
    int nm,
    fp_t bc[2][2] )
```

Initialize flat composition field with fixed boundary conditions.

The boundary conditions are fixed values of c_{hi} along the lower-left half and upper-right half walls, no flux everywhere else, with an initial values of c_{lo} everywhere. These conditions represent a carburizing process, with partial exposure (rather than the entire left and right walls) to produce an inhomogeneous workload and highlight numerical errors at the boundaries.

Definition at line 60 of file `cpu/openmp/boundaries.c`.

4.3.2.3 check_solution()

```
void check_solution (
    fp_t ** conc_new,
    int nx,
    int ny,
    fp_t dx,
    fp_t dy,
    int nm,
    fp_t elapsed,
    fp_t D,
    fp_t bc[2][2],
    fp_t * rss )
```

Compare numerical and analytical solutions of the diffusion equation.

Returns the residual sum of squares (RSS), normalized to the domain size.

Definition at line 183 of file `cpu/openmp/discretization.c`.

4.3.2.4 compute_convolution()

```
void compute_convolution (
    fp_t ** conc_old,
    fp_t ** conc_lap,
    fp_t ** mask_lap,
    int nx,
    int ny,
    int nm )
```

Perform the convolution of the mask matrix with the composition matrix.

If the convolution mask is the Laplacian stencil, the convolution evaluates the discrete Laplacian of the composition field. Other masks are possible, for example the Sobel filters for edge detection. This function is general purpose: as long as the dimensions `nx`, `ny`, and `nm` are properly specified, the convolution will be correctly computed.

Definition at line 122 of file `cpu/openmp/discretization.c`.

4.3.2.5 five_point_Laplacian_stencil()

```
void five_point_Laplacian_stencil (
    fp_t dx,
    fp_t dy,
    fp_t ** mask_lap )
```

Write 5-point Laplacian stencil into convolution mask.

3×3 mask, 5 values, truncation error $\mathcal{O}(\Delta x^2)$

Definition at line 50 of file `cpu/openmp/discretization.c`.

4.3.2.6 `nine_point_Laplacian_stencil()`

```
void nine_point_Laplacian_stencil (
    fp_t dx,
    fp_t dy,
    fp_t ** mask_lap )
```

Write 9-point Laplacian stencil into convolution mask.

3×3 mask, 9 values, truncation error $\mathcal{O}(\Delta x^4)$

Definition at line 64 of file `cpu/openmp/discretization.c`.

4.3.2.7 `set_boundaries()`

```
void set_boundaries (
    fp_t bc[2][2] )
```

Set values to be used along the simulation domain boundaries.

Indexing is row-major, i.e. $A[y][x]$, so `bc` = $[[y_{lo}, y_{hi}], [x_{lo}, x_{hi}]]$.

Definition at line 42 of file `cpu/openmp/boundaries.c`.

4.3.2.8 `slow_nine_point_Laplacian_stencil()`

```
void slow_nine_point_Laplacian_stencil (
    fp_t dx,
    fp_t dy,
    fp_t ** mask_lap )
```

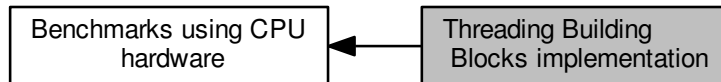
Write 9-point Laplacian stencil into convolution mask.

4×4 mask, 9 values, truncation error $\mathcal{O}(\Delta x^4)$ Provided for testing and demonstration of scalability, only: as the name indicates, this 9-point stencil is computationally more expensive than the 3×3 version. If your code requires $\mathcal{O}(\Delta x^4)$ accuracy, please use [nine_point_Laplacian_stencil\(\)](#).

Definition at line 88 of file `cpu/openmp/discretization.c`.

4.4 Threading Building Blocks implementation

Collaboration diagram for Threading Building Blocks implementation:



Files

- file [boundaries.cpp](#)
Implementation of boundary condition functions with TBB threading.
- file [cpu/tbb/boundaries.h](#)
Declaration of boundary condition function prototypes for TBB benchmarks.
- file [discretization.cpp](#)
Implementation of boundary condition functions with TBB threading.
- file [cpu/tbb/discretization.h](#)
Declaration of discretized mathematical function prototypes for TBB benchmarks.

Classes

- class [ResidualSumOfSquares2D](#)
Comparison algorithm for execution on the block of threads.

Functions

- void [set_boundaries](#) ([fp_t](#) bc[2][2])
Set values to be used along the simulation domain boundaries.
- void [apply_initial_conditions](#) ([fp_t](#) **conc, int nx, int ny, int nm, [fp_t](#) bc[2][2])
Initialize flat composition field with fixed boundary conditions.
- void [apply_boundary_conditions](#) ([fp_t](#) **conc, int nx, int ny, int nm, [fp_t](#) bc[2][2])
Set fixed value (c_{hi}) along left and bottom, zero-flux elsewhere.
- void [set_threads](#) (int n)
Requested number of TBB threads to use in parallel code sections.
- void [five_point_Laplacian_stencil](#) ([fp_t](#) dx, [fp_t](#) dy, [fp_t](#) **mask_lap)
Write 5-point Laplacian stencil into convolution mask.
- void [nine_point_Laplacian_stencil](#) ([fp_t](#) dx, [fp_t](#) dy, [fp_t](#) **mask_lap)
Write 9-point Laplacian stencil into convolution mask.
- void [slow_nine_point_Laplacian_stencil](#) ([fp_t](#) dx, [fp_t](#) dy, [fp_t](#) **mask_lap)
Write 9-point Laplacian stencil into convolution mask.
- void [set_mask](#) ([fp_t](#) dx, [fp_t](#) dy, int nm, [fp_t](#) **mask_lap)
Specify which stencil to use for the Laplacian.
- void [compute_convolution](#) ([fp_t](#) **conc_old, [fp_t](#) **conc_lap, [fp_t](#) **mask_lap, int nx, int ny, int nm)

Perform the convolution of the mask matrix with the composition matrix.

- void `solve_diffusion_equation` (`fp_t **conc_old`, `fp_t **B`, `fp_t **conc_lap`, `int nx`, `int ny`, `int nm`, `fp_t D`, `fp_t dt`, `fp_t *elapsed`)

Update the scalar composition field using old and Laplacian values.

- void `analytical_value` (`fp_t x`, `fp_t t`, `fp_t D`, `fp_t chi`, `fp_t *c`)

Analytical solution of the diffusion equation for a carburizing process.

- void `check_solution` (`fp_t **conc_new`, `int nx`, `int ny`, `fp_t dx`, `fp_t dy`, `int nm`, `fp_t elapsed`, `fp_t D`, `fp_t bc[2][2]`, `fp_t *rss`)

Compare numerical and analytical solutions of the diffusion equation.

- void `analytical_value` (`fp_t x`, `fp_t t`, `fp_t D`, `fp_t bc[2][2]`, `fp_t *c`)

Analytical solution of the diffusion equation for a carburizing process.

4.4.1 Detailed Description

4.4.2 Function Documentation

4.4.2.1 `analytical_value()` [1/2]

```
void analytical_value (
    fp_t x,
    fp_t t,
    fp_t D,
    fp_t bc[2][2],
    fp_t * c )
```

Analytical solution of the diffusion equation for a carburizing process.

For 1D diffusion through a semi-infinite domain with initial and far-field composition c_∞ and boundary value $c(x = 0, t) = c_0$ with constant diffusivity D , the solution to Fick's second law is

$$c(x, t) = c_0 - (c_0 - c_\infty) \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right)$$

which reduces, when $c_\infty = 0$, to

$$c(x, t) = c_0 \left[1 - \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right) \right].$$

Definition at line 173 of file `cpu/openmp/discretization.c`.

4.4.2.2 analytical_value() [2/2]

```
void analytical_value (
    fp_t x,
    fp_t t,
    fp_t D,
    fp_t chi,
    fp_t * c )
```

Analytical solution of the diffusion equation for a carburizing process.

For 1D diffusion through a semi-infinite domain with initial and far-field composition c_∞ and boundary value $c(x = 0, t) = c_0$ with constant diffusivity D , the solution to Fick's second law is

$$c(x, t) = c_0 - (c_0 - c_\infty) \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right)$$

which reduces, when $c_\infty = 0$, to

$$c(x, t) = c_0 \left[1 - \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right) \right].$$

Definition at line 176 of file discretization.cpp.

4.4.2.3 apply_initial_conditions()

```
void apply_initial_conditions (
    fp_t ** conc,
    int nx,
    int ny,
    int nm,
    fp_t bc[2][2] )
```

Initialize flat composition field with fixed boundary conditions.

The boundary conditions are fixed values of c_{hi} along the lower-left half and upper-right half walls, no flux everywhere else, with an initial values of c_{lo} everywhere. These conditions represent a carburizing process, with partial exposure (rather than the entire left and right walls) to produce an inhomogeneous workload and highlight numerical errors at the boundaries.

Definition at line 63 of file boundaries.cpp.

4.4.2.4 check_solution()

```
void check_solution (
    fp_t ** conc_new,
    int nx,
    int ny,
    fp_t dx,
    fp_t dy,
    int nm,
    fp_t elapsed,
    fp_t D,
    fp_t bc[2][2],
    fp_t * rss )
```

Compare numerical and analytical solutions of the diffusion equation.

Returns the residual sum of squares (RSS), normalized to the domain size.

Definition at line 259 of file discretization.cpp.

4.4.2.5 compute_convolution()

```
void compute_convolution (
    fp_t ** conc_old,
    fp_t ** conc_lap,
    fp_t ** mask_lap,
    int nx,
    int ny,
    int nm )
```

Perform the convolution of the mask matrix with the composition matrix.

If the convolution mask is the Laplacian stencil, the convolution evaluates the discrete Laplacian of the composition field. Other masks are possible, for example the Sobel filters for edge detection. This function is general purpose: as long as the dimensions `nx`, `ny`, and `nm` are properly specified, the convolution will be correctly computed.

Definition at line 128 of file `discretization.cpp`.

4.4.2.6 five_point_Laplacian_stencil()

```
void five_point_Laplacian_stencil (
    fp_t dx,
    fp_t dy,
    fp_t ** mask_lap )
```

Write 5-point Laplacian stencil into convolution mask.

3×3 mask, 5 values, truncation error $\mathcal{O}(\Delta x^2)$

Definition at line 56 of file `discretization.cpp`.

4.4.2.7 nine_point_Laplacian_stencil()

```
void nine_point_Laplacian_stencil (
    fp_t dx,
    fp_t dy,
    fp_t ** mask_lap )
```

Write 9-point Laplacian stencil into convolution mask.

3×3 mask, 9 values, truncation error $\mathcal{O}(\Delta x^4)$

Definition at line 70 of file `discretization.cpp`.

4.4.2.8 set_boundaries()

```
void set_boundaries (
    fp_t bc[2][2] )
```

Set values to be used along the simulation domain boundaries.

Indexing is row-major, i.e. $A[y][x]$, so `bc` = $[[y_{lo}, y_{hi}], [x_{lo}, x_{hi}]]$.

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

4.4.2.9 `set_threads()`

```
void set_threads (
    int n )
```

Requested number of TBB threads to use in parallel code sections.

Warning

This setting does not appear to have any effect.

Definition at line 46 of file discretization.cpp.

4.4.2.10 `slow_nine_point_Laplacian_stencil()`

```
void slow_nine_point_Laplacian_stencil (
    fp_t dx,
    fp_t dy,
    fp_t ** mask_lap )
```

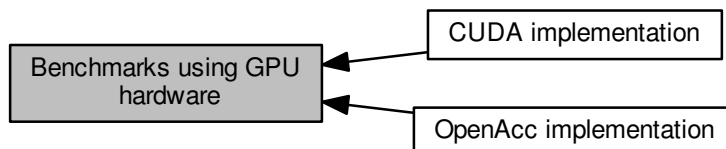
Write 9-point Laplacian stencil into convolution mask.

4×4 mask, 9 values, truncation error $\mathcal{O}(\Delta x^4)$ Provided for testing and demonstration of scalability, only: as the name indicates, this 9-point stencil is computationally more expensive than the 3×3 version. If your code requires $\mathcal{O}(\Delta x^4)$ accuracy, please use [nine_point_Laplacian_stencil\(\)](#).

Definition at line 94 of file discretization.cpp.

4.5 Benchmarks using GPU hardware

Collaboration diagram for Benchmarks using GPU hardware:



Modules

- [CUDA implementation](#)
- [OpenAcc implementation](#)

Files

- file [gpu/main.c](#)
Implementation of semi-infinite diffusion equation.
- file [gpu/mesh.c](#)
Implementation of mesh handling functions.
- file [gpu/mesh.h](#)
Declaration of mesh function prototypes for GPU benchmarks.
- file [gpu/output.c](#)
Implementation of file output functions.
- file [gpu/output.h](#)
Declaration of output function prototypes for GPU benchmarks.
- file [gpu/timer.c](#)
High-resolution cross-platform machine time reader.
- file [gpu/timer.h](#)
Declaration of timer function prototypes for GPU benchmarks.
- file [gpu/type.h](#)
Definition of scalar data type.

Typedefs

- typedef double [fp_t](#)

Functions

- int `main` (int argc, char *argv[])
Run simulation using input parameters specified on the command line.
- void `make_arrays` (fp_t ***conc_old, fp_t ***conc_new, fp_t ***conc_lap, fp_t ***mask_lap, int nx, int ny, int nm)
Allocate 2D arrays to store scalar composition values.
- void `free_arrays` (fp_t **conc_old, fp_t **conc_new, fp_t **conc_lap, fp_t **mask_lap)
Free dynamically allocated memory.
- void `swap_pointers` (fp_t ***conc_old, fp_t ***conc_new)
Swap pointers to data underlying two arrays.
- void `print_progress` (const int step, const int steps)
Prints timestamps and a 20-point progress bar to stdout.
- void `write_csv` (fp_t **conc, int nx, int ny, fp_t dx, fp_t dy, int step)
Writes scalar composition field to diffusion.?????.csv.
- void `write_png` (fp_t **conc, int nx, int ny, int step)
Writes scalar composition field to diffusion.?????.png.
- void `StartTimer` ()
Set CPU frequency and begin timing.
- double `GetTimer` ()
Return elapsed time in seconds.

Variables

- struct timeval `timerStart`

4.5.1 Detailed Description

4.5.2 Typedef Documentation

4.5.2.1 fp_t

```
typedef double fp_t
```

Specify the basic data type to achieve the desired accuracy in floating-point arithmetic: float for single-precision, double for double-precision.

Definition at line 40 of file gpu/type.h.

4.5.3 Function Documentation

4.5.3.1 main()

```
int main (
    int argc,
    char * argv[] )
```

Run simulation using input parameters specified on the command line.

Program will write a series of PNG image files to visualize scalar composition field, plus a final CSV raw data file and CSV runtime log tabulating the iteration counter (iter), elapsed simulation time (sim_time), system free energy (energy), error relative to analytical solution (wrss), time spent performing convolution (conv_time), time spent updating fields (step_time), time spent writing to disk (IO_time), time spent generating analytical values (soln_time), and total elapsed (run_time).

Definition at line 50 of file gpu/main.c.

4.5.3.2 make_arrays()

```
void make_arrays (
    fp_t *** conc_old,
    fp_t *** conc_new,
    fp_t *** conc_lap,
    fp_t *** mask_lap,
    int nx,
    int ny,
    int nm )
```

Allocate 2D arrays to store scalar composition values.

Arrays are allocated as 1D arrays, then 2D pointer arrays are mapped over the top. This facilitates use of either 1D or 2D data access, depending on whether the task is spatially dependent or not.

Definition at line 40 of file gpu/mesh.c.

4.5.3.3 print_progress()

```
void print_progress (
    const int step,
    const int steps )
```

Prints timestamps and a 20-point progress bar to stdout.

Call inside the timestepping loop, near the top, e.g.

```
for (int step=0; step<steps; step++) {
    print_progress(step, steps);
    take_a_step();
    elapsed += dt;
}
```

Definition at line 48 of file gpu/output.c.

4.5.3.4 swap_pointers()

```
void swap_pointers (
    fp_t *** conc_old,
    fp_t *** conc_new )
```

Swap pointers to data underlying two arrays.

Rather than copy data from `conc_old` into `conc_new`, an expensive operation, simply trade the top-most pointers. New becomes old with no data lost and in almost no time.

Definition at line 98 of file `gpu/mesh.c`.

4.5.4 Variable Documentation

4.5.4.1 timerStart

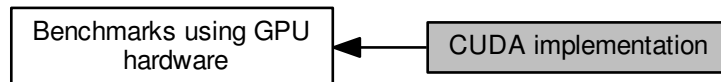
```
struct timeval timerStart
```

Platform-dependent data type of hardware time value

Definition at line 49 of file `gpu/timer.c`.

4.6 CUDA implementation

Collaboration diagram for CUDA implementation:



Files

- file [gpu/cuda/boundaries.c](#)
Implementation of boundary condition functions with OpenMP threading.
- file [gpu/cuda/boundaries.h](#)
Declaration of boundary condition function prototypes for CUDA benchmarks.
- file [discretization.cu](#)
Implementation of boundary condition functions with CUDA acceleration.
- file [gpu/cuda/discretization.h](#)
Declaration of discretized mathematical function prototypes for CUDA benchmarks.

Macros

- `#define MAX_TILE_W 32`
- `#define MAX_TILE_H 32`
- `#define MAX_MASK_W 3`

Functions

- void [set_boundaries](#) ([fp_t](#) bc[2][2])
Set values to be used along the simulation domain boundaries.
- void [apply_initial_conditions](#) ([fp_t](#) **conc, int nx, int ny, int nm, [fp_t](#) bc[2][2])
Initialize flat composition field with fixed boundary conditions.
- void [apply_boundary_conditions](#) ([fp_t](#) **conc, int nx, int ny, int nm, [fp_t](#) bc[2][2])
Set fixed value (c_{hi}) along left and bottom, zero-flux elsewhere.
- void [set_threads](#) (int n)
Set number of OpenMP threads to use in CPU code sections.
- void [five_point_Laplacian_stencil](#) ([fp_t](#) dx, [fp_t](#) dy, [fp_t](#) **mask_lap)
Write 5-point Laplacian stencil into convolution mask.
- void [nine_point_Laplacian_stencil](#) ([fp_t](#) dx, [fp_t](#) dy, [fp_t](#) **mask_lap)
Write 9-point Laplacian stencil into convolution mask.
- void [slow_nine_point_Laplacian_stencil](#) ([fp_t](#) dx, [fp_t](#) dy, [fp_t](#) **mask_lap)
Write 9-point Laplacian stencil into convolution mask.
- void [set_mask](#) ([fp_t](#) dx, [fp_t](#) dy, int nm, [fp_t](#) **mask_lap)
Specify which stencil to use for the Laplacian.

- `__global__ void convolution_kernel (fp_t *conc_old, fp_t *conc_lap, int nx, int ny, int nm)`
Tiled convolution algorithm for execution on the GPU.
- `void compute_convolution (fp_t **conc_old, fp_t **conc_lap, fp_t **mask_lap, int nx, int ny, int nm, int bs)`
Perform the convolution of the mask matrix with the composition matrix.
- `__global__ void diffusion_kernel (fp_t *conc_old, fp_t *conc_new, fp_t *conc_lap, int nx, int ny, int nm, fp_t D, fp_t dt)`
Vector addition algorithm for execution on the GPU.
- `void solve_diffusion_equation (fp_t **conc_old, fp_t **conc_new, fp_t **conc_lap, int nx, int ny, int nm, int bs, fp_t D, fp_t dt, fp_t *elapsed)`
Update the scalar composition field using old and Laplacian values.
- `void analytical_value (fp_t x, fp_t t, fp_t D, fp_t bc[2][2], fp_t *c)`
Analytical solution of the diffusion equation for a carburizing process.
- `void check_solution (fp_t **conc_new, int nx, int ny, fp_t dx, fp_t dy, int nm, int bs, fp_t elapsed, fp_t D, fp_t bc[2][2], fp_t *rss)`
Compare numerical and analytical solutions of the diffusion equation.
- `void check_solution (fp_t **conc_new, int nx, int ny, fp_t dx, fp_t dy, int nm, fp_t elapsed, fp_t D, fp_t bc[2][2], fp_t *rss)`
Compare numerical and analytical solutions of the diffusion equation.

Variables

- `__constant__ fp_t Mc [MAX_MASK_W * MAX_MASK_W]`

4.6.1 Detailed Description

4.6.2 Macro Definition Documentation

4.6.2.1 MAX_MASK_W

```
#define MAX_MASK_W 3
```

Maximum height and width of the mask array, for GPU memory allocation

Definition at line 55 of file discretization.cu.

4.6.2.2 MAX_TILE_H

```
#define MAX_TILE_H 32
```

Maximum height of an input tile, including halo cells, for GPU memory allocation

Definition at line 50 of file discretization.cu.

4.6.2.3 MAX_TILE_W

```
#define MAX_TILE_W 32
```

Maximum width of an input tile, including halo cells, for GPU memory allocation

Definition at line 45 of file discretization.cu.

4.6.3 Function Documentation

4.6.3.1 analytical_value()

```
void analytical_value (
    fp_t x,
    fp_t t,
    fp_t D,
    fp_t bc[2][2],
    fp_t * c )
```

Analytical solution of the diffusion equation for a carburizing process.

For 1D diffusion through a semi-infinite domain with initial and far-field composition c_∞ and boundary value $c(x = 0, t) = c_0$ with constant diffusivity D , the solution to Fick's second law is

$$c(x, t) = c_0 - (c_0 - c_\infty) \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right)$$

which reduces, when $c_\infty = 0$, to

$$c(x, t) = c_0 \left[1 - \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right) \right].$$

Definition at line 325 of file discretization.cu.

4.6.3.2 apply_initial_conditions()

```
void apply_initial_conditions (
    fp_t ** conc,
    int nx,
    int ny,
    int nm,
    fp_t bc[2][2] )
```

Initialize flat composition field with fixed boundary conditions.

The boundary conditions are fixed values of c_{hi} along the lower-left half and upper-right half walls, no flux everywhere else, with an initial values of c_{lo} everywhere. These conditions represent a carburizing process, with partial exposure (rather than the entire left and right walls) to produce an inhomogeneous workload and highlight numerical errors at the boundaries.

Definition at line 60 of file gpu/cuda/boundaries.c.

4.6.3.3 `check_solution()` [1/2]

```
void check_solution (
    fp_t ** conc_new,
    int nx,
    int ny,
    fp_t dx,
    fp_t dy,
    int nm,
    fp_t elapsed,
    fp_t D,
    fp_t bc[2][2],
    fp_t * rss )
```

Compare numerical and analytical solutions of the diffusion equation.

Returns the residual sum of squares (RSS), normalized to the domain size.

Returns

Residual sum of squares (RSS), normalized to the domain size.

Definition at line 183 of file `cpu/openmp/discretization.c`.

4.6.3.4 `check_solution()` [2/2]

```
void check_solution (
    fp_t ** conc_new,
    int nx,
    int ny,
    fp_t dx,
    fp_t dy,
    int nm,
    int bs,
    fp_t elapsed,
    fp_t D,
    fp_t bc[2][2],
    fp_t * rss )
```

Compare numerical and analytical solutions of the diffusion equation.

Returns the residual sum of squares (RSS), normalized to the domain size.

Definition at line 335 of file `discretization.cu`.

4.6.3.5 compute_convolution()

```
void compute_convolution (
    fp_t ** conc_old,
    fp_t ** conc_lap,
    fp_t ** mask_lap,
    int nx,
    int ny,
    int nm,
    int bs )
```

Perform the convolution of the mask matrix with the composition matrix.

If the convolution mask is the Laplacian stencil, the convolution evaluates the discrete Laplacian of the composition field. Other masks are possible, for example the Sobel filters for edge detection. This function is general purpose: as long as the dimensions `nx`, `ny`, and `nm` are properly specified, the convolution will be correctly computed.

Definition at line 219 of file discretization.cu.

4.6.3.6 convolution_kernel()

```
__global__ void convolution_kernel (
    fp_t * conc_old,
    fp_t * conc_lap,
    int nx,
    int ny,
    int nm )
```

Tiled convolution algorithm for execution on the GPU.

This function accesses 1D data rather than the 2D array representation of the scalar composition field, mapping into 2D tiles on the GPU with halo cells before computing the convolution

Definition at line 145 of file discretization.cu.

4.6.3.7 diffusion_kernel()

```
__global__ void diffusion_kernel (
    fp_t * conc_old,
    fp_t * conc_new,
    fp_t * conc_lap,
    int nx,
    int ny,
    int nm,
    fp_t D,
    fp_t dt )
```

Vector addition algorithm for execution on the GPU.

This function accesses 1D data rather than the 2D array representation of the scalar composition field

Definition at line 259 of file discretization.cu.

4.6.3.8 five_point_Laplacian_stencil()

```
void five_point_Laplacian_stencil (
    fp_t dx,
    fp_t dy,
    fp_t ** mask_lap )
```

Write 5-point Laplacian stencil into convolution mask.

3×3 mask, 5 values, truncation error $\mathcal{O}(\Delta x^2)$

Definition at line 75 of file discretization.cu.

4.6.3.9 nine_point_Laplacian_stencil()

```
void nine_point_Laplacian_stencil (
    fp_t dx,
    fp_t dy,
    fp_t ** mask_lap )
```

Write 9-point Laplacian stencil into convolution mask.

3×3 mask, 9 values, truncation error $\mathcal{O}(\Delta x^4)$

Definition at line 89 of file discretization.cu.

4.6.3.10 set_boundaries()

```
void set_boundaries (
    fp_t bc[2][2] )
```

Set values to be used along the simulation domain boundaries.

Indexing is row-major, i.e. $A[y][x]$, so $bc = [[y_{lo}, y_{hi}], [x_{lo}, x_{hi}]]$.

Definition at line 42 of file gpu/cuda/boundaries.c.

4.6.3.11 slow_nine_point_Laplacian_stencil()

```
void slow_nine_point_Laplacian_stencil (
    fp_t dx,
    fp_t dy,
    fp_t ** mask_lap )
```

Write 9-point Laplacian stencil into convolution mask.

4×4 mask, 9 values, truncation error $\mathcal{O}(\Delta x^4)$ Provided for testing and demonstration of scalability, only: as the name indicates, this 9-point stencil is computationally more expensive than the 3×3 version. If your code requires $\mathcal{O}(\Delta x^4)$ accuracy, please use [nine_point_Laplacian_stencil\(\)](#).

Definition at line 113 of file discretization.cu.

4.6.4 Variable Documentation

4.6.4.1 Mc

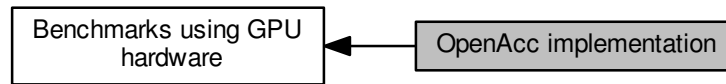
```
__constant__ fp_t Mc[MAX_MASK_W * MAX_MASK_W]
```

Allocate constant memory on the GPU for the convolution mask

Definition at line 60 of file discretization.cu.

4.7 OpenAcc implementation

Collaboration diagram for OpenAcc implementation:



Files

- file [gpu/openacc/boundaries.c](#)
Implementation of boundary condition functions with OpenMP threading.
- file [gpu/openacc/boundaries.h](#)
Declaration of boundary condition function prototypes for OpenAcc benchmarks.
- file [gpu/openacc/discretization.c](#)
Implementation of boundary condition functions with OpenACC threading.
- file [gpu/openacc/discretization.h](#)
Declaration of discretized mathematical function prototypes for OpenAcc benchmarks.

Functions

- void [set_boundaries](#) ([fp_t](#) bc[2][2])
Set values to be used along the simulation domain boundaries.
- void [apply_initial_conditions](#) ([fp_t](#) **conc, int nx, int ny, int nm, [fp_t](#) bc[2][2])
Initialize flat composition field with fixed boundary conditions.
- void [apply_boundary_conditions](#) ([fp_t](#) **conc, int nx, int ny, int nm, [fp_t](#) bc[2][2])
Set fixed value (c_{hi}) along left and bottom, zero-flux elsewhere.
- void [set_threads](#) (int n)
Set number of OpenMP threads to use in CPU code sections.
- void [five_point_Laplacian_stencil](#) ([fp_t](#) dx, [fp_t](#) dy, [fp_t](#) **mask_lap)
Write 5-point Laplacian stencil into convolution mask.
- void [nine_point_Laplacian_stencil](#) ([fp_t](#) dx, [fp_t](#) dy, [fp_t](#) **mask_lap)
Write 9-point Laplacian stencil into convolution mask.
- void [slow_nine_point_Laplacian_stencil](#) ([fp_t](#) dx, [fp_t](#) dy, [fp_t](#) **mask_lap)
Write 9-point Laplacian stencil into convolution mask.
- void [set_mask](#) ([fp_t](#) dx, [fp_t](#) dy, int nm, [fp_t](#) **mask_lap)
Specify which stencil to use for the Laplacian.
- void [compute_convolution](#) ([fp_t](#) **conc_old, [fp_t](#) **conc_lap, [fp_t](#) **mask_lap, int nx, int ny, int nm, int bs)
Perform the convolution of the mask matrix with the composition matrix.
- void [solve_diffusion_equation](#) ([fp_t](#) **conc_old, [fp_t](#) **conc_new, [fp_t](#) **conc_lap, int nx, int ny, int nm, int bs, [fp_t](#) D, [fp_t](#) dt, [fp_t](#) *elapsed)
Update the scalar composition field using old and Laplacian values.
- void [check_solution](#) ([fp_t](#) **conc_new, int nx, int ny, [fp_t](#) dx, [fp_t](#) dy, int nm, int bs, [fp_t](#) elapsed, [fp_t](#) D, [fp_t](#) bc[2][2], [fp_t](#) *rss)
Compare numerical and analytical solutions of the diffusion equation.
- void [analytical_value](#) ([fp_t](#) x, [fp_t](#) t, [fp_t](#) D, [fp_t](#) bc[2][2], [fp_t](#) *c)
Analytical solution of the diffusion equation for a carburizing process.

4.7.1 Detailed Description

4.7.2 Function Documentation

4.7.2.1 analytical_value()

```
void analytical_value (
    fp_t x,
    fp_t t,
    fp_t D,
    fp_t bc[2][2],
    fp_t * c )
```

Analytical solution of the diffusion equation for a carburizing process.

For 1D diffusion through a semi-infinite domain with initial and far-field composition c_∞ and boundary value $c(x = 0, t) = c_0$ with constant diffusivity D , the solution to Fick's second law is

$$c(x, t) = c_0 - (c_0 - c_\infty) \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right)$$

which reduces, when $c_\infty = 0$, to

$$c(x, t) = c_0 \left[1 - \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right) \right].$$

Definition at line 173 of file `cpu/openmp/discretization.c`.

4.7.2.2 apply_initial_conditions()

```
void apply_initial_conditions (
    fp_t ** conc,
    int nx,
    int ny,
    int nm,
    fp_t bc[2][2] )
```

Initialize flat composition field with fixed boundary conditions.

The boundary conditions are fixed values of c_{hi} along the lower-left half and upper-right half walls, no flux everywhere else, with an initial values of c_{lo} everywhere. These conditions represent a carburizing process, with partial exposure (rather than the entire left and right walls) to produce an inhomogeneous workload and highlight numerical errors at the boundaries.

Definition at line 60 of file `gpu/openacc/boundaries.c`.

4.7.2.3 check_solution()

```
void check_solution (
    fp_t ** conc_new,
    int nx,
    int ny,
    fp_t dx,
    fp_t dy,
    int nm,
    int bs,
    fp_t elapsed,
    fp_t D,
    fp_t bc[2][2],
    fp_t * rss )
```

Compare numerical and analytical solutions of the diffusion equation.

Returns the residual sum of squares (RSS), normalized to the domain size.

For 1D diffusion through a semi-infinite domain with initial and far-field composition c_∞ and boundary value $c(x = 0, t) = c_0$ with constant diffusivity D , the solution to Fick's second law is

$$c(x, t) = c_0 - (c_0 - c_\infty) \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right)$$

which reduces, when $c_\infty = 0$, to

$$c(x, t) = c_0 \left[1 - \operatorname{erf} \left(\frac{x}{\sqrt{4Dt}} \right) \right].$$

Definition at line 187 of file gpu/openacc/discretization.c.

4.7.2.4 compute_convolution()

```
void compute_convolution (
    fp_t ** conc_old,
    fp_t ** conc_lap,
    fp_t ** mask_lap,
    int nx,
    int ny,
    int nm,
    int bs )
```

Perform the convolution of the mask matrix with the composition matrix.

If the convolution mask is the Laplacian stencil, the convolution evaluates the discrete Laplacian of the composition field. Other masks are possible, for example the Sobel filters for edge detection. This function is general purpose: as long as the dimensions `nx`, `ny`, and `nm` are properly specified, the convolution will be correctly computed.

Definition at line 123 of file gpu/openacc/discretization.c.

4.7.2.5 five_point_Laplacian_stencil()

```
void five_point_Laplacian_stencil (
    fp_t dx,
    fp_t dy,
    fp_t ** mask_lap )
```

Write 5-point Laplacian stencil into convolution mask.

3×3 mask, 5 values, truncation error $\mathcal{O}(\Delta x^2)$

Definition at line 51 of file `gpu/openacc/discretization.c`.

4.7.2.6 nine_point_Laplacian_stencil()

```
void nine_point_Laplacian_stencil (
    fp_t dx,
    fp_t dy,
    fp_t ** mask_lap )
```

Write 9-point Laplacian stencil into convolution mask.

3×3 mask, 9 values, truncation error $\mathcal{O}(\Delta x^4)$

Definition at line 65 of file `gpu/openacc/discretization.c`.

4.7.2.7 set_boundaries()

```
void set_boundaries (
    fp_t bc[2][2] )
```

Set values to be used along the simulation domain boundaries.

Indexing is row-major, i.e. $A[y][x]$, so `bc` = $[[y_{lo}, y_{hi}], [x_{lo}, x_{hi}]]$.

Definition at line 42 of file `gpu/openacc/boundaries.c`.

4.7.2.8 slow_nine_point_Laplacian_stencil()

```
void slow_nine_point_Laplacian_stencil (
    fp_t dx,
    fp_t dy,
    fp_t ** mask_lap )
```

Write 9-point Laplacian stencil into convolution mask.

4×4 mask, 9 values, truncation error $\mathcal{O}(\Delta x^4)$ Provided for testing and demonstration of scalability, only: as the name indicates, this 9-point stencil is computationally more expensive than the 3×3 version. If your code requires $\mathcal{O}(\Delta x^4)$ accuracy, please use [nine_point_Laplacian_stencil\(\)](#).

Definition at line 89 of file `gpu/openacc/discretization.c`.

5 Class Documentation

5.1 ResidualSumOfSquares2D Class Reference

Comparison algorithm for execution on the block of threads.

5.1.1 Detailed Description

Comparison algorithm for execution on the block of threads.

Definition at line 184 of file discretization.cpp.

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

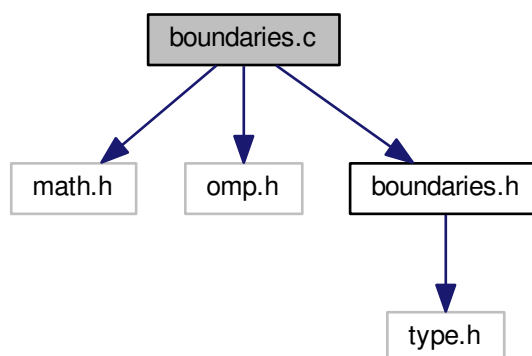
- [discretization.cpp](#)

6 File Documentation

6.1 boundaries.c File Reference

Implementation of boundary condition functions with OpenMP threading.

```
#include <math.h>
#include <omp.h>
#include "boundaries.h"
Include dependency graph for cpu/openmp/boundaries.c:
```



Functions

- void `set_boundaries` (`fp_t` bc[2][2])
Set values to be used along the simulation domain boundaries.
- void `apply_initial_conditions` (`fp_t` **conc, int nx, int ny, int nm, `fp_t` bc[2][2])
Initialize flat composition field with fixed boundary conditions.
- void `apply_boundary_conditions` (`fp_t` **conc, int nx, int ny, int nm, `fp_t` bc[2][2])
Set fixed value (c_{hi}) along left and bottom, zero-flux elsewhere.

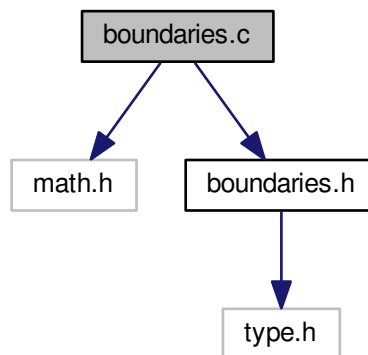
6.1.1 Detailed Description

Implementation of boundary condition functions with OpenMP threading.

6.2 boundaries.c File Reference

Implementation of boundary condition functions without threading.

```
#include <math.h>
#include "boundaries.h"
Include dependency graph for cpu/serial/boundaries.c:
```



Functions

- void `set_boundaries` (`fp_t` bc[2][2])
Set values to be used along the simulation domain boundaries.
- void `apply_initial_conditions` (`fp_t` **conc, int nx, int ny, int nm, `fp_t` bc[2][2])
Initialize flat composition field with fixed boundary conditions.
- void `apply_boundary_conditions` (`fp_t` **conc, int nx, int ny, int nm, `fp_t` bc[2][2])
Set fixed value (c_{hi}) along left and bottom, zero-flux elsewhere.

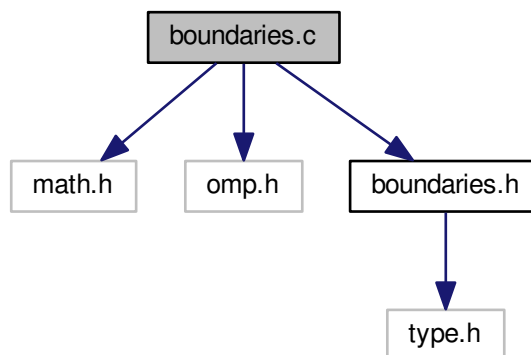
6.2.1 Detailed Description

Implementation of boundary condition functions without threading.

6.3 boundaries.c File Reference

Implementation of boundary condition functions with OpenMP threading.

```
#include <math.h>
#include <omp.h>
#include "boundaries.h"
Include dependency graph for gpu/cuda/boundaries.c:
```



Functions

- void `set_boundaries` (`fp_t` bc[2][2])
Set values to be used along the simulation domain boundaries.
- void `apply_initial_conditions` (`fp_t` **conc, int nx, int ny, int nm, `fp_t` bc[2][2])
Initialize flat composition field with fixed boundary conditions.
- void `apply_boundary_conditions` (`fp_t` **conc, int nx, int ny, int nm, `fp_t` bc[2][2])
Set fixed value (c_{hi}) along left and bottom, zero-flux elsewhere.

6.3.1 Detailed Description

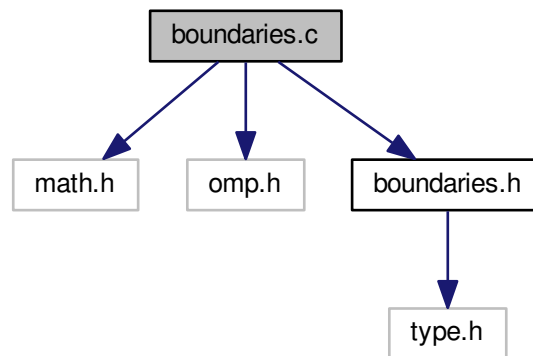
Implementation of boundary condition functions with OpenMP threading.

6.4 boundaries.c File Reference

Implementation of boundary condition functions with OpenMP threading.

```
#include <math.h>
#include <omp.h>
#include "boundaries.h"
```

Include dependency graph for gpu/openacc/boundaries.c:



Functions

- void [set_boundaries](#) ([fp_t](#) bc[2][2])
Set values to be used along the simulation domain boundaries.
- void [apply_initial_conditions](#) ([fp_t](#) **conc, int nx, int ny, int nm, [fp_t](#) bc[2][2])
Initialize flat composition field with fixed boundary conditions.
- void [apply_boundary_conditions](#) ([fp_t](#) **conc, int nx, int ny, int nm, [fp_t](#) bc[2][2])
Set fixed value (c_{hi}) along left and bottom, zero-flux elsewhere.

6.4.1 Detailed Description

Implementation of boundary condition functions with OpenMP threading.

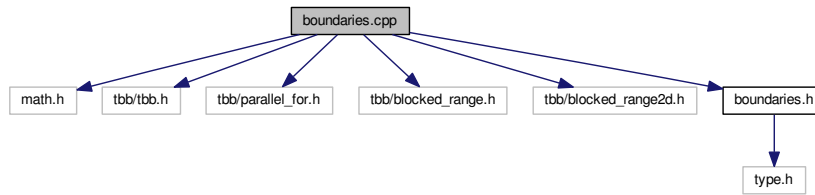
6.5 boundaries.cpp File Reference

Implementation of boundary condition functions with TBB threading.

```
#include <math.h>
#include <tbb/tbb.h>
#include <tbb/parallel_for.h>
#include <tbb/blocked_range.h>
#include <tbb/blocked_range2d.h>
```

```
#include "boundaries.h"
```

Include dependency graph for boundaries.cpp:



Functions

- void `set_boundaries` (`fp_t` bc[2][2])
Set values to be used along the simulation domain boundaries.
- void `apply_initial_conditions` (`fp_t` **conc, int nx, int ny, int nm, `fp_t` bc[2][2])
Initialize flat composition field with fixed boundary conditions.
- void `apply_boundary_conditions` (`fp_t` **conc, int nx, int ny, int nm, `fp_t` bc[2][2])
Set fixed value (c_{hi}) along left and bottom, zero-flux elsewhere.

6.5.1 Detailed Description

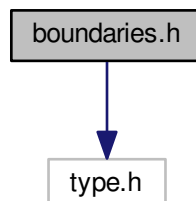
Implementation of boundary condition functions with TBB threading.

6.6 boundaries.h File Reference

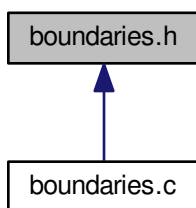
Declaration of boundary condition function prototypes for OpenMP benchmarks.

```
#include "type.h"
```

Include dependency graph for cpu/openmp/boundaries.h:



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



Functions

- void `set_boundaries` (`fp_t` bc[2][2])
Set values to be used along the simulation domain boundaries.
- void `apply_initial_conditions` (`fp_t` **conc, int nx, int ny, int nm, `fp_t` bc[2][2])
Initialize flat composition field with fixed boundary conditions.
- void `apply_boundary_conditions` (`fp_t` **conc, int nx, int ny, int nm, `fp_t` bc[2][2])
Set fixed value (c_{hi}) along left and bottom, zero-flux elsewhere.

6.6.1 Detailed Description

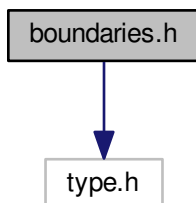
Declaration of boundary condition function prototypes for OpenMP benchmarks.

6.7 boundaries.h File Reference

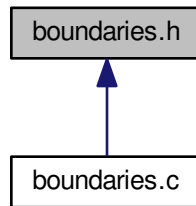
Declaration of boundary condition function prototypes for CPU benchmarks.

```
#include "type.h"
```

Include dependency graph for cpu/serial/boundaries.h:



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



Functions

- void [set_boundaries](#) ([fp_t](#) bc[2][2])
Set values to be used along the simulation domain boundaries.
- void [apply_initial_conditions](#) ([fp_t](#) **conc, int nx, int ny, int nm, [fp_t](#) bc[2][2])
Initialize flat composition field with fixed boundary conditions.
- void [apply_boundary_conditions](#) ([fp_t](#) **conc, int nx, int ny, int nm, [fp_t](#) bc[2][2])
Set fixed value (c_{hi}) along left and bottom, zero-flux elsewhere.

6.7.1 Detailed Description

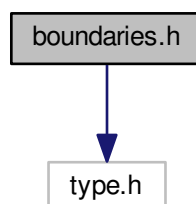
Declaration of boundary condition function prototypes for CPU benchmarks.

6.8 boundaries.h File Reference

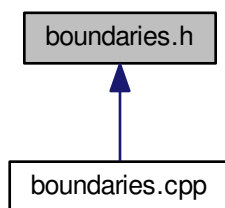
Declaration of boundary condition function prototypes for TBB benchmarks.

```
#include "type.h"
```

Include dependency graph for cpu/tbb/boundaries.h:



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



Functions

- void [set_boundaries](#) ([fp_t](#) bc[2][2])
Set values to be used along the simulation domain boundaries.
- void [apply_initial_conditions](#) ([fp_t](#) **conc, int nx, int ny, int nm, [fp_t](#) bc[2][2])
Initialize flat composition field with fixed boundary conditions.
- void [apply_boundary_conditions](#) ([fp_t](#) **conc, int nx, int ny, int nm, [fp_t](#) bc[2][2])
Set fixed value (c_{hi}) along left and bottom, zero-flux elsewhere.

6.8.1 Detailed Description

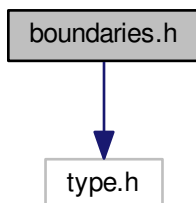
Declaration of boundary condition function prototypes for TBB benchmarks.

6.9 boundaries.h File Reference

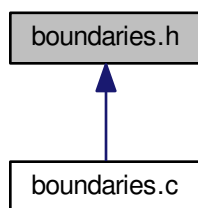
Declaration of boundary condition function prototypes for CUDA benchmarks.

```
#include "type.h"
```

Include dependency graph for gpu/cuda/boundaries.h:



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



Functions

- void [set_boundaries](#) ([fp_t](#) bc[2][2])
Set values to be used along the simulation domain boundaries.
- void [apply_initial_conditions](#) ([fp_t](#) **conc, int nx, int ny, int nm, [fp_t](#) bc[2][2])
Initialize flat composition field with fixed boundary conditions.
- void [apply_boundary_conditions](#) ([fp_t](#) **conc, int nx, int ny, int nm, [fp_t](#) bc[2][2])
Set fixed value (c_{hi}) along left and bottom, zero-flux elsewhere.

6.9.1 Detailed Description

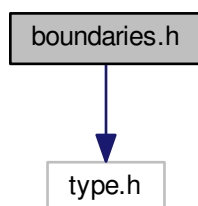
Declaration of boundary condition function prototypes for CUDA benchmarks.

6.10 boundaries.h File Reference

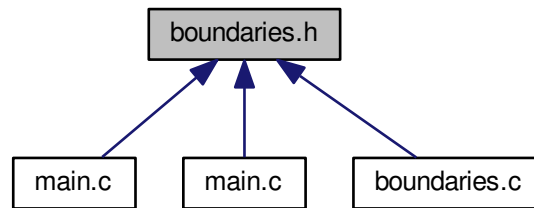
Declaration of boundary condition function prototypes for OpenAcc benchmarks.

```
#include "type.h"
```

Include dependency graph for gpu/openacc/boundaries.h:



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



Functions

- void `set_boundaries` (`fp_t` bc[2][2])
Set values to be used along the simulation domain boundaries.
- void `apply_initial_conditions` (`fp_t` **conc, int nx, int ny, int nm, `fp_t` bc[2][2])
Initialize flat composition field with fixed boundary conditions.
- void `apply_boundary_conditions` (`fp_t` **conc, int nx, int ny, int nm, `fp_t` bc[2][2])
Set fixed value (c_{hi}) along left and bottom, zero-flux elsewhere.

6.10.1 Detailed Description

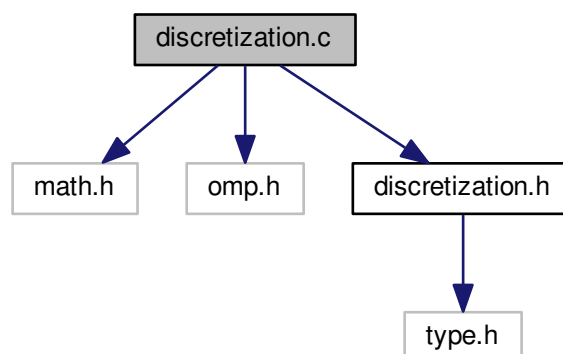
Declaration of boundary condition function prototypes for OpenAcc benchmarks.

6.11 discretization.c File Reference

Implementation of boundary condition functions with OpenMP threading.

```
#include <math.h>
#include <omp.h>
#include "discretization.h"
```

Include dependency graph for `cpu/openmp/discretization.c`:



Functions

- void `set_threads` (int n)
Set number of OpenMP threads to use in parallel code sections.
- void `five_point_Laplacian_stencil` (fp_t dx, fp_t dy, fp_t **mask_lap)
Write 5-point Laplacian stencil into convolution mask.
- void `nine_point_Laplacian_stencil` (fp_t dx, fp_t dy, fp_t **mask_lap)
Write 9-point Laplacian stencil into convolution mask.
- void `slow_nine_point_Laplacian_stencil` (fp_t dx, fp_t dy, fp_t **mask_lap)
Write 9-point Laplacian stencil into convolution mask.
- void `set_mask` (fp_t dx, fp_t dy, int nm, fp_t **mask_lap)
Specify which stencil to use for the Laplacian.
- void `compute_convolution` (fp_t **conc_old, fp_t **conc_lap, fp_t **mask_lap, int nx, int ny, int nm)
Perform the convolution of the mask matrix with the composition matrix.
- void `solve_diffusion_equation` (fp_t **conc_old, fp_t **conc_new, fp_t **conc_lap, int nx, int ny, int nm, fp_t D, fp_t dt, fp_t *elapsed)
Update the scalar composition field using old and Laplacian values.
- void `analytical_value` (fp_t x, fp_t t, fp_t D, fp_t bc[2][2], fp_t *c)
Analytical solution of the diffusion equation for a carburizing process.
- void `check_solution` (fp_t **conc_new, int nx, int ny, fp_t dx, fp_t dy, int nm, fp_t elapsed, fp_t D, fp_t bc[2][2], fp_t *rss)
Compare numerical and analytical solutions of the diffusion equation.

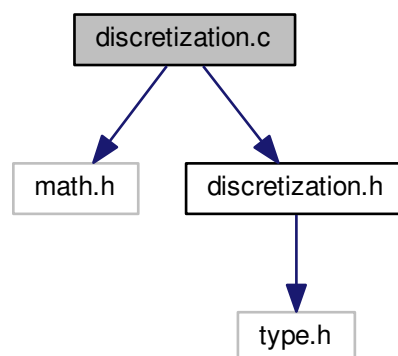
6.11.1 Detailed Description

Implementation of boundary condition functions with OpenMP threading.

6.12 discretization.c File Reference

Implementation of boundary condition functions without threading.

```
#include <math.h>
#include "discretization.h"
Include dependency graph for cpu/serial/discretization.c:
```



Functions

- void `set_threads` (int n)
Set number of OpenMP threads to use in parallel code sections.
- void `five_point_Laplacian_stencil` (fp_t dx, fp_t dy, fp_t **mask_lap)
Write 5-point Laplacian stencil into convolution mask.
- void `nine_point_Laplacian_stencil` (fp_t dx, fp_t dy, fp_t **mask_lap)
Write 9-point Laplacian stencil into convolution mask.
- void `slow_nine_point_Laplacian_stencil` (fp_t dx, fp_t dy, fp_t **mask_lap)
Write 9-point Laplacian stencil into convolution mask.
- void `set_mask` (fp_t dx, fp_t dy, int nm, fp_t **mask_lap)
Specify which stencil to use for the Laplacian.
- void `compute_convolution` (fp_t **conc_old, fp_t **conc_lap, fp_t **mask_lap, int nx, int ny, int nm)
Perform the convolution of the mask matrix with the composition matrix.
- void `solve_diffusion_equation` (fp_t **conc_old, fp_t **conc_new, fp_t **conc_lap, int nx, int ny, int nm, fp_t D, fp_t dt, fp_t *elapsed)
Update the scalar composition field using old and Laplacian values.
- void `analytical_value` (fp_t x, fp_t t, fp_t D, fp_t bc[2][2], fp_t *c)
Analytical solution of the diffusion equation for a carburizing process.
- void `check_solution` (fp_t **conc_new, int nx, int ny, fp_t dx, fp_t dy, int nm, fp_t elapsed, fp_t D, fp_t bc[2][2], fp_t *rss)
Compare numerical and analytical solutions of the diffusion equation.

6.12.1 Detailed Description

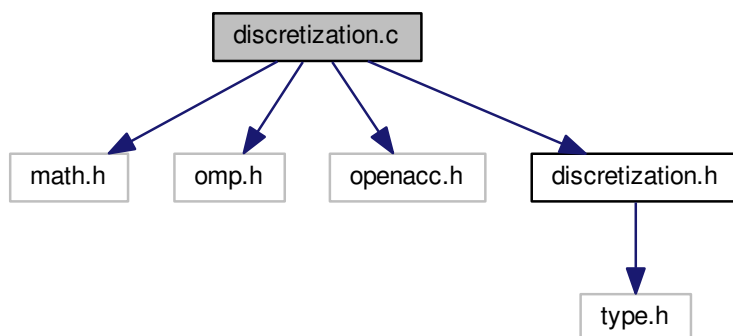
Implementation of boundary condition functions without threading.

6.13 discretization.c File Reference

Implementation of boundary condition functions with OpenACC threading.

```
#include <math.h>
#include <omp.h>
#include <openacc.h>
#include "discretization.h"
```

Include dependency graph for gpu/openacc/discretization.c:



Functions

- void `set_threads` (int n)
Set number of OpenMP threads to use in CPU code sections.
- void `five_point_Laplacian_stencil` (fp_t dx, fp_t dy, fp_t **mask_lap)
Write 5-point Laplacian stencil into convolution mask.
- void `nine_point_Laplacian_stencil` (fp_t dx, fp_t dy, fp_t **mask_lap)
Write 9-point Laplacian stencil into convolution mask.
- void `slow_nine_point_Laplacian_stencil` (fp_t dx, fp_t dy, fp_t **mask_lap)
Write 9-point Laplacian stencil into convolution mask.
- void `set_mask` (fp_t dx, fp_t dy, int nm, fp_t **mask_lap)
Specify which stencil to use for the Laplacian.
- void `compute_convolution` (fp_t **conc_old, fp_t **conc_lap, fp_t **mask_lap, int nx, int ny, int nm, int bs)
Perform the convolution of the mask matrix with the composition matrix.
- void `solve_diffusion_equation` (fp_t **conc_old, fp_t **conc_new, fp_t **conc_lap, int nx, int ny, int nm, int bs, fp_t D, fp_t dt, fp_t *elapsed)
Update the scalar composition field using old and Laplacian values.
- void `check_solution` (fp_t **conc_new, int nx, int ny, fp_t dx, fp_t dy, int nm, int bs, fp_t elapsed, fp_t D, fp_t bc[2][2], fp_t *rss)
Compare numerical and analytical solutions of the diffusion equation.

6.13.1 Detailed Description

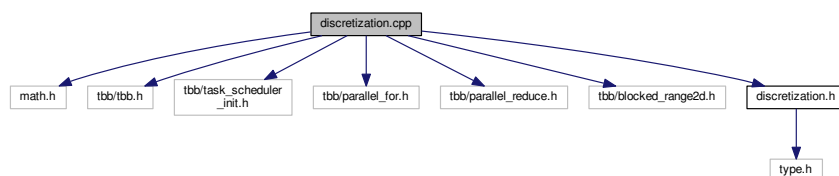
Implementation of boundary condition functions with OpenACC threading.

6.14 discretization.cpp File Reference

Implementation of boundary condition functions with TBB threading.

```
#include <math.h>
#include <tbb/tbb.h>
#include <tbb/task_scheduler_init.h>
#include <tbb/parallel_for.h>
#include <tbb/parallel_reduce.h>
#include <tbb/blocked_range2d.h>
#include "discretization.h"
```

Include dependency graph for discretization.cpp:



Classes

- class `ResidualSumOfSquares2D`
Comparison algorithm for execution on the block of threads.

Functions

- void `set_threads` (int n)
Requested number of TBB threads to use in parallel code sections.
- void `five_point_Laplacian_stencil` (fp_t dx, fp_t dy, fp_t **mask_lap)
Write 5-point Laplacian stencil into convolution mask.
- void `nine_point_Laplacian_stencil` (fp_t dx, fp_t dy, fp_t **mask_lap)
Write 9-point Laplacian stencil into convolution mask.
- void `slow_nine_point_Laplacian_stencil` (fp_t dx, fp_t dy, fp_t **mask_lap)
Write 9-point Laplacian stencil into convolution mask.
- void `set_mask` (fp_t dx, fp_t dy, int nm, fp_t **mask_lap)
Specify which stencil to use for the Laplacian.
- void `compute_convolution` (fp_t **conc_old, fp_t **conc_lap, fp_t **mask_lap, int nx, int ny, int nm)
Perform the convolution of the mask matrix with the composition matrix.
- void `solve_diffusion_equation` (fp_t **conc_old, fp_t **B, fp_t **conc_lap, int nx, int ny, int nm, fp_t D, fp_t dt, fp_t *elapsed)
Update the scalar composition field using old and Laplacian values.
- void `analytical_value` (fp_t x, fp_t t, fp_t D, fp_t chi, fp_t *c)
Analytical solution of the diffusion equation for a carburizing process.
- void `check_solution` (fp_t **conc_new, int nx, int ny, fp_t dx, fp_t dy, int nm, fp_t elapsed, fp_t D, fp_t bc[2][2], fp_t *rss)
Compare numerical and analytical solutions of the diffusion equation.

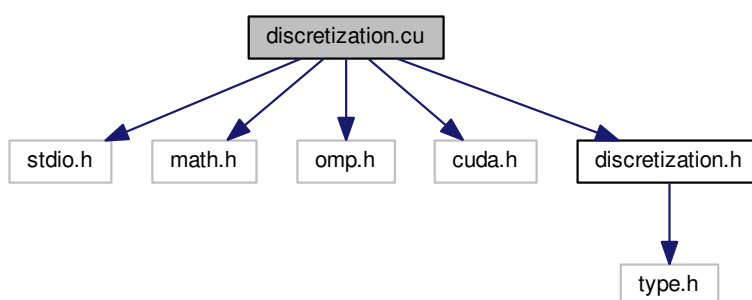
6.14.1 Detailed Description

Implementation of boundary condition functions with TBB threading.

6.15 discretization.cu File Reference

Implementation of boundary condition functions with CUDA acceleration.

```
#include <stdio.h>
#include <math.h>
#include <omp.h>
#include <cuda.h>
#include "discretization.h"
Include dependency graph for discretization.cu:
```



Macros

- #define `MAX_TILE_W` 32
- #define `MAX_TILE_H` 32
- #define `MAX_MASK_W` 3

Functions

- void `set_threads` (int n)
Set number of OpenMP threads to use in CPU code sections.
- void `five_point_Laplacian_stencil` (fp_t dx, fp_t dy, fp_t **mask_lap)
Write 5-point Laplacian stencil into convolution mask.
- void `nine_point_Laplacian_stencil` (fp_t dx, fp_t dy, fp_t **mask_lap)
Write 9-point Laplacian stencil into convolution mask.
- void `slow_nine_point_Laplacian_stencil` (fp_t dx, fp_t dy, fp_t **mask_lap)
Write 9-point Laplacian stencil into convolution mask.
- void `set_mask` (fp_t dx, fp_t dy, int nm, fp_t **mask_lap)
Specify which stencil to use for the Laplacian.
- __global__ void `convolution_kernel` (fp_t *conc_old, fp_t *conc_lap, int nx, int ny, int nm)
Tiled convolution algorithm for execution on the GPU.
- void `compute_convolution` (fp_t **conc_old, fp_t **conc_lap, fp_t **mask_lap, int nx, int ny, int nm, int bs)
Perform the convolution of the mask matrix with the composition matrix.
- __global__ void `diffusion_kernel` (fp_t *conc_old, fp_t *conc_new, fp_t *conc_lap, int nx, int ny, int nm, fp_t D, fp_t dt)
Vector addition algorithm for execution on the GPU.
- void `solve_diffusion_equation` (fp_t **conc_old, fp_t **conc_new, fp_t **conc_lap, int nx, int ny, int nm, int bs, fp_t D, fp_t dt, fp_t *elapsed)
Update the scalar composition field using old and Laplacian values.
- void `analytical_value` (fp_t x, fp_t t, fp_t D, fp_t bc[2][2], fp_t *c)
Analytical solution of the diffusion equation for a carburizing process.
- void `check_solution` (fp_t **conc_new, int nx, int ny, fp_t dx, fp_t dy, int nm, int bs, fp_t elapsed, fp_t D, fp_t bc[2][2], fp_t *rss)
Compare numerical and analytical solutions of the diffusion equation.

Variables

- __constant__ fp_t `Mc` [MAX_MASK_W * MAX_MASK_W]

6.15.1 Detailed Description

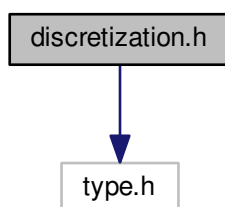
Implementation of boundary condition functions with CUDA acceleration.

6.16 discretization.h File Reference

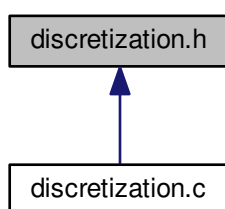
Declaration of discretized mathematical function prototypes for OpenMP benchmarks.

```
#include "type.h"
```

Include dependency graph for `cpu/openmp/discretization.h`:



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



Functions

- void `set_threads` (int n)
Set number of OpenMP threads to use in parallel code sections.
- void `set_mask` (fp_t dx, fp_t dy, int nm, fp_t **mask_lap)
Specify which stencil to use for the Laplacian.
- void `compute_convolution` (fp_t **conc_old, fp_t **conc_lap, fp_t **mask_lap, int nx, int ny, int nm)
Perform the convolution of the mask matrix with the composition matrix.
- void `solve_diffusion_equation` (fp_t **conc_old, fp_t **conc_new, fp_t **conc_lap, int nx, int ny, int nm, fp_t D, fp_t dt, fp_t *elapsed)
Update the scalar composition field using old and Laplacian values.
- void `analytical_value` (fp_t x, fp_t t, fp_t D, fp_t bc[2][2], fp_t *c)
Analytical solution of the diffusion equation for a carburizing process.
- void `check_solution` (fp_t **conc_new, int nx, int ny, fp_t dx, fp_t dy, int nm, fp_t elapsed, fp_t D, fp_t bc[2][2], fp_t *rss)
Compare numerical and analytical solutions of the diffusion equation.

6.16.1 Detailed Description

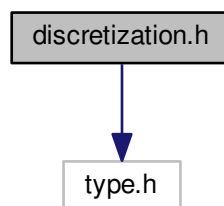
Declaration of discretized mathematical function prototypes for OpenMP benchmarks.

6.17 discretization.h File Reference

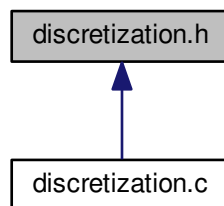
Declaration of discretized mathematical function prototypes for CPU benchmarks.

```
#include "type.h"
```

Include dependency graph for cpu/serial/discretization.h:



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



Functions

- void [set_threads](#) (int n)
Set number of OpenMP threads to use in parallel code sections.
- void [set_mask](#) (fp_t dx, fp_t dy, int nm, fp_t **mask_lap)
Specify which stencil to use for the Laplacian.
- void [compute_convolution](#) (fp_t **conc_old, fp_t **conc_lap, fp_t **mask_lap, int nx, int ny, int nm)
Perform the convolution of the mask matrix with the composition matrix.
- void [solve_diffusion_equation](#) (fp_t **conc_old, fp_t **conc_new, fp_t **conc_lap, int nx, int ny, int nm, fp_t D, fp_t dt, fp_t *elapsed)

Update the scalar composition field using old and Laplacian values.

- void `analytical_value` (`fp_t` x, `fp_t` t, `fp_t` D, `fp_t` bc[2][2], `fp_t` *c)

Analytical solution of the diffusion equation for a carburizing process.

- void `check_solution` (`fp_t` **conc_new, int nx, int ny, `fp_t` dx, `fp_t` dy, int nm, `fp_t` elapsed, `fp_t` D, `fp_t` bc[2][2], `fp_t` *rss)

Compare numerical and analytical solutions of the diffusion equation.

6.17.1 Detailed Description

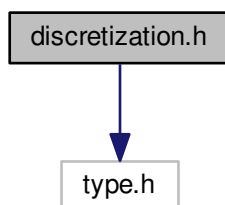
Declaration of discretized mathematical function prototypes for CPU benchmarks.

6.18 discretization.h File Reference

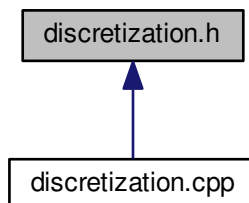
Declaration of discretized mathematical function prototypes for TBB benchmarks.

```
#include "type.h"
```

Include dependency graph for `cpu/tbb/discretization.h`:



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



Functions

- void `set_threads` (int n)
Requested number of TBB threads to use in parallel code sections.
- void `set_mask` (fp_t dx, fp_t dy, int nm, fp_t **mask_lap)
Specify which stencil to use for the Laplacian.
- void `compute_convolution` (fp_t **conc_old, fp_t **conc_lap, fp_t **mask_lap, int nx, int ny, int nm)
Perform the convolution of the mask matrix with the composition matrix.
- void `solve_diffusion_equation` (fp_t **conc_old, fp_t **B, fp_t **conc_lap, int nx, int ny, int nm, fp_t D, fp_t dt, fp_t *elapsed)
Update the scalar composition field using old and Laplacian values.
- void `analytical_value` (fp_t x, fp_t t, fp_t D, fp_t bc[2][2], fp_t *c)
Analytical solution of the diffusion equation for a carburizing process.
- void `check_solution` (fp_t **conc_new, int nx, int ny, fp_t dx, fp_t dy, int nm, fp_t elapsed, fp_t D, fp_t bc[2][2], fp_t *rss)
Compare numerical and analytical solutions of the diffusion equation.

6.18.1 Detailed Description

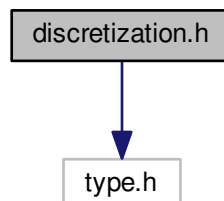
Declaration of discretized mathematical function prototypes for TBB benchmarks.

6.19 discretization.h File Reference

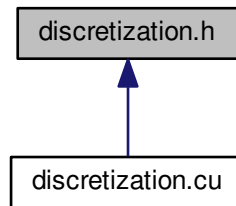
Declaration of discretized mathematical function prototypes for CUDA benchmarks.

```
#include "type.h"
```

Include dependency graph for gpu/cuda/discretization.h:



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



Functions

- void `set_threads` (int n)
Set number of OpenMP threads to use in CPU code sections.
- void `set_mask` (fp_t dx, fp_t dy, int nm, fp_t **mask_lap)
Specify which stencil to use for the Laplacian.
- void `compute_convolution` (fp_t **conc_old, fp_t **conc_lap, fp_t **mask_lap, int nx, int ny, int nm, int bs)
Perform the convolution of the mask matrix with the composition matrix.
- void `solve_diffusion_equation` (fp_t **conc_old, fp_t **conc_new, fp_t **conc_lap, int nx, int ny, int nm, int bs, fp_t D, fp_t dt, fp_t *elapsed)
Update the scalar composition field using old and Laplacian values.
- void `analytical_value` (fp_t x, fp_t t, fp_t D, fp_t bc[2][2], fp_t *c)
Analytical solution of the diffusion equation for a carburizing process.
- void `check_solution` (fp_t **conc_new, int nx, int ny, fp_t dx, fp_t dy, int nm, fp_t elapsed, fp_t D, fp_t bc[2][2], fp_t *rss)
Compare numerical and analytical solutions of the diffusion equation.

6.19.1 Detailed Description

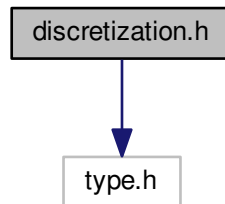
Declaration of discretized mathematical function prototypes for CUDA benchmarks.

6.20 discretization.h File Reference

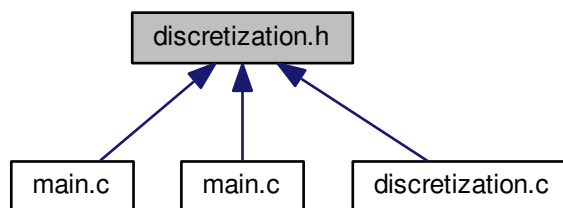
Declaration of discretized mathematical function prototypes for OpenAcc benchmarks.

```
#include "type.h"
```

Include dependency graph for gpu/openacc/discretization.h:



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



Functions

- void [set_threads](#) (int n)
Set number of OpenMP threads to use in CPU code sections.
- void [set_mask](#) (fp_t dx, fp_t dy, int nm, fp_t **mask_lap)
Specify which stencil to use for the Laplacian.
- void [compute_convolution](#) (fp_t **conc_old, fp_t **conc_lap, fp_t **mask_lap, int nx, int ny, int nm, int bs)
Perform the convolution of the mask matrix with the composition matrix.
- void [solve_diffusion_equation](#) (fp_t **conc_old, fp_t **conc_new, fp_t **conc_lap, int nx, int ny, int nm, int bs, fp_t D, fp_t dt, fp_t *elapsed)
Update the scalar composition field using old and Laplacian values.
- void [analytical_value](#) (fp_t x, fp_t t, fp_t D, fp_t bc[2][2], fp_t *c)
Analytical solution of the diffusion equation for a carburizing process.
- void [check_solution](#) (fp_t **conc_new, int nx, int ny, fp_t dx, fp_t dy, int nm, int bs, fp_t elapsed, fp_t D, fp_t bc[2][2], fp_t *rss)
Compare numerical and analytical solutions of the diffusion equation.

6.20.1 Detailed Description

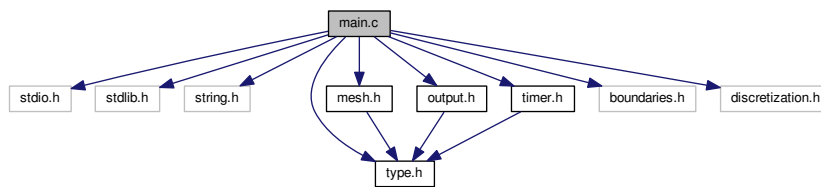
Declaration of discretized mathematical function prototypes for OpenAcc benchmarks.

6.21 main.c File Reference

Implementation of semi-infinite diffusion equation.

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include "type.h"
#include "mesh.h"
#include "output.h"
#include "timer.h"
#include "boundaries.h"
#include "discretization.h"
```

Include dependency graph for cpu/main.c:



Functions

- int [main](#) (int argc, char *argv[])

Run simulation using input parameters specified on the command line.

6.21.1 Detailed Description

Implementation of semi-infinite diffusion equation.

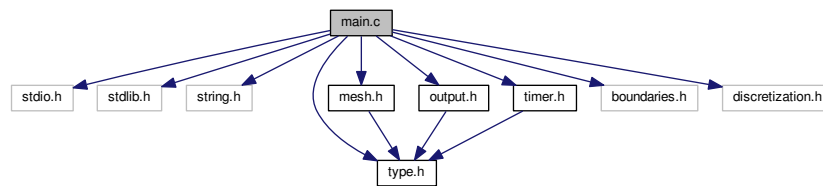
6.22 main.c File Reference

Implementation of semi-infinite diffusion equation.

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include "type.h"
#include "mesh.h"
#include "output.h"
#include "timer.h"
#include "boundaries.h"
```

```
#include "discretization.h"
```

Include dependency graph for gpu/main.c:



Functions

- `int main (int argc, char *argv[])`

Run simulation using input parameters specified on the command line.

6.22.1 Detailed Description

Implementation of semi-infinite diffusion equation.

6.23 mesh.c File Reference

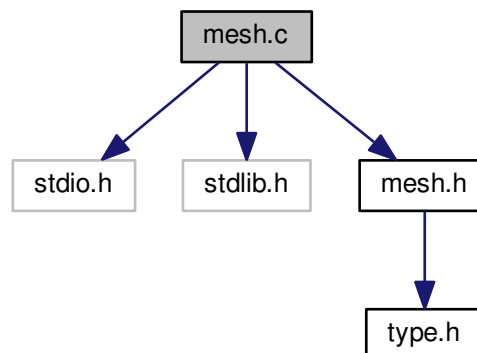
Implemenatation of mesh handling functions.

```
#include <stdio.h>
```

```
#include <stdlib.h>
```

```
#include "mesh.h"
```

Include dependency graph for cpu/mesh.c:



Functions

- void `make_arrays` (`fp_t ***conc_old`, `fp_t ***conc_new`, `fp_t ***conc_lap`, `fp_t ***mask_lap`, `int nx`, `int ny`, `int nm`)
Allocate 2D arrays to store scalar composition values.
- void `free_arrays` (`fp_t **conc_old`, `fp_t **conc_new`, `fp_t **conc_lap`, `fp_t **mask_lap`)
Free dynamically allocated memory.
- void `swap_pointers` (`fp_t ***conc_old`, `fp_t ***conc_new`)
Swap pointers to data underlying two arrays.

6.23.1 Detailed Description

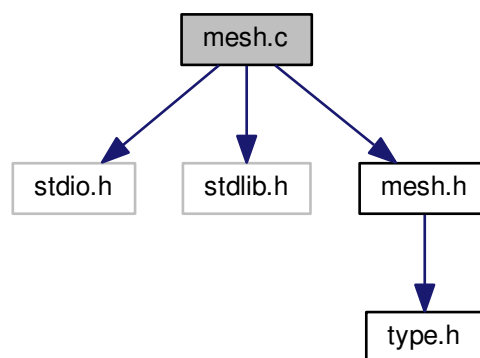
Implementation of mesh handling functions.

6.24 mesh.c File Reference

Implementation of mesh handling functions.

```
#include <stdio.h>
#include <stdlib.h>
#include "mesh.h"
```

Include dependency graph for gpu/mesh.c:



Functions

- void `make_arrays` (`fp_t ***conc_old`, `fp_t ***conc_new`, `fp_t ***conc_lap`, `fp_t ***mask_lap`, `int nx`, `int ny`, `int nm`)
Allocate 2D arrays to store scalar composition values.
- void `free_arrays` (`fp_t **conc_old`, `fp_t **conc_new`, `fp_t **conc_lap`, `fp_t **mask_lap`)
Free dynamically allocated memory.
- void `swap_pointers` (`fp_t ***conc_old`, `fp_t ***conc_new`)
Swap pointers to data underlying two arrays.

6.24.1 Detailed Description

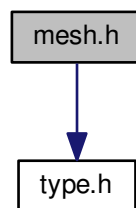
Implementation of mesh handling functions.

6.25 mesh.h File Reference

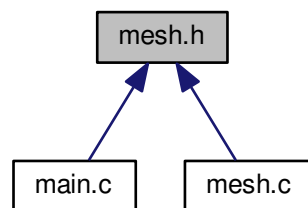
Declaration of mesh function prototypes for CPU benchmarks.

```
#include "type.h"
```

Include dependency graph for cpu/mesh.h:



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



Functions

- void [make_arrays](#) ([fp_t](#) ***conc_old, [fp_t](#) ***conc_new, [fp_t](#) ***conc_lap, [fp_t](#) ***mask_lap, int nx, int ny, int nm)
Allocate 2D arrays to store scalar composition values.
- void [free_arrays](#) ([fp_t](#) **conc_old, [fp_t](#) **conc_new, [fp_t](#) **conc_lap, [fp_t](#) **mask_lap)
Free dynamically allocated memory.
- void [swap_pointers](#) ([fp_t](#) ***conc_old, [fp_t](#) ***conc_new)
Swap pointers to data underlying two arrays.

6.25.1 Detailed Description

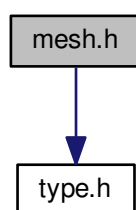
Declaration of mesh function prototypes for CPU benchmarks.

6.26 mesh.h File Reference

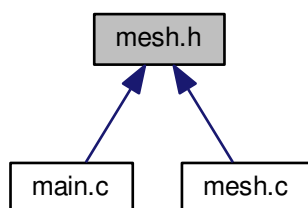
Declaration of mesh function prototypes for GPU benchmarks.

```
#include "type.h"
```

Include dependency graph for gpu/mesh.h:



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



Functions

- void [make_arrays](#) ([fp_t](#) ***conc_old, [fp_t](#) ***conc_new, [fp_t](#) ***conc_lap, [fp_t](#) ***mask_lap, int nx, int ny, int nm)
Allocate 2D arrays to store scalar composition values.
- void [free_arrays](#) ([fp_t](#) **conc_old, [fp_t](#) **conc_new, [fp_t](#) **conc_lap, [fp_t](#) **mask_lap)
Free dynamically allocated memory.
- void [swap_pointers](#) ([fp_t](#) ***conc_old, [fp_t](#) ***conc_new)
Swap pointers to data underlying two arrays.

6.26.1 Detailed Description

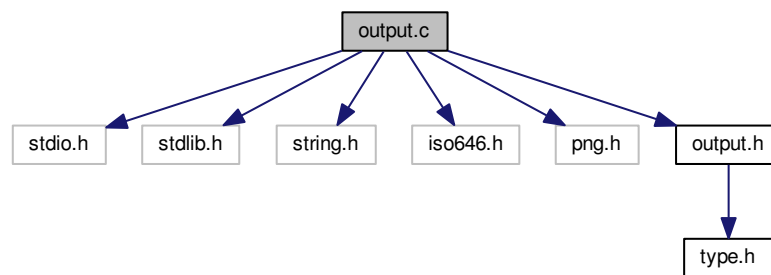
Declaration of mesh function prototypes for GPU benchmarks.

6.27 output.c File Reference

Implementation of file output functions.

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <iso646.h>
#include <png.h>
#include "output.h"
```

Include dependency graph for cpu/output.c:



Functions

- void [print_progress](#) (const int step, const int steps)
Prints timestamps and a 20-point progress bar to stdout.
- void [write_csv](#) (fp_t **conc, int nx, int ny, fp_t dx, fp_t dy, int step)
Writes scalar composition field to diffusion.?????.csv.
- void [write_png](#) (fp_t **conc, int nx, int ny, int step)
Writes scalar composition field to diffusion.?????.png.

6.27.1 Detailed Description

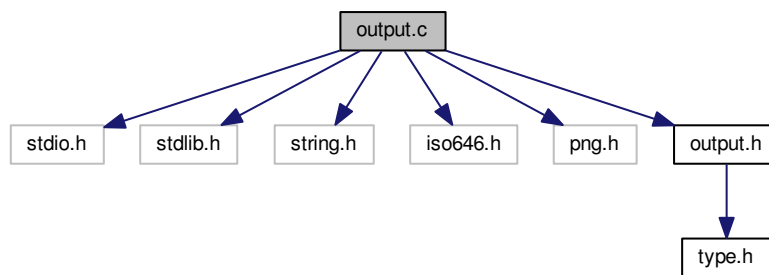
Implementation of file output functions.

6.28 output.c File Reference

Implementation of file output functions.

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <iso646.h>
#include <png.h>
#include "output.h"
```

Include dependency graph for gpu/output.c:



Functions

- void `print_progress` (const int step, const int steps)
Prints timestamps and a 20-point progress bar to stdout.
- void `write_csv` (fp_t **conc, int nx, int ny, fp_t dx, fp_t dy, int step)
Writes scalar composition field to diffusion.?????.csv.
- void `write_png` (fp_t **conc, int nx, int ny, int step)
Writes scalar composition field to diffusion.?????.png.

6.28.1 Detailed Description

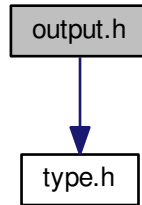
Implementation of file output functions.

6.29 output.h File Reference

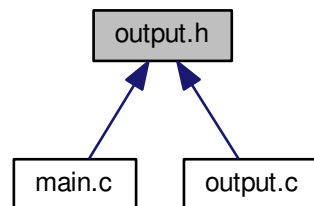
Declaration of output function prototypes for CPU benchmarks.

```
#include "type.h"
```

Include dependency graph for cpu/output.h:



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



Functions

- void [print_progress](#) (const int step, const int steps)
Prints timestamps and a 20-point progress bar to stdout.
- void [write_csv](#) (fp_t **conc, int nx, int ny, fp_t dx, fp_t dy, int step)
Writes scalar composition field to diffusion.???????.csv.
- void [write_png](#) (fp_t **conc, int nx, int ny, int step)
Writes scalar composition field to diffusion.???????.png.

6.29.1 Detailed Description

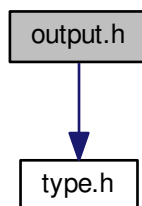
Declaration of output function prototypes for CPU benchmarks.

6.30 output.h File Reference

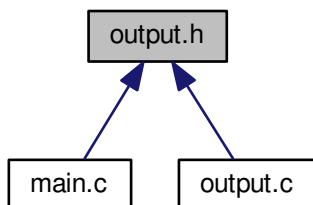
Declaration of output function prototypes for GPU benchmarks.

```
#include "type.h"
```

Include dependency graph for gpu/output.h:



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



Functions

- void `print_progress` (const int step, const int steps)
Prints timestamps and a 20-point progress bar to stdout.
- void `write_csv` (fp_t **conc, int nx, int ny, fp_t dx, fp_t dy, int step)
Writes scalar composition field to diffusion.???????.csv.
- void `write_png` (fp_t **conc, int nx, int ny, int step)
Writes scalar composition field to diffusion.???????.png.

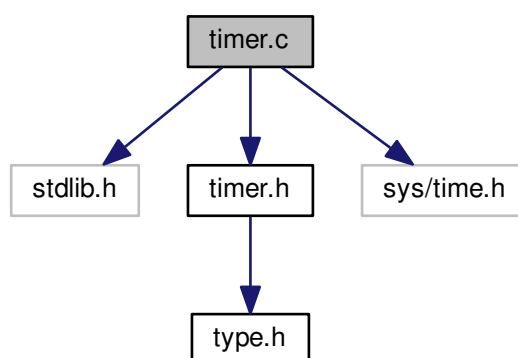
6.30.1 Detailed Description

Declaration of output function prototypes for GPU benchmarks.

6.31 timer.c File Reference

High-resolution cross-platform machine time reader.

```
#include <stdlib.h>
#include "timer.h"
#include <sys/time.h>
Include dependency graph for cpu/timer.c:
```



Functions

- void [StartTimer](#) ()
Set CPU frequency and begin timing.
- double [GetTimer](#) ()
Return elapsed time in seconds.

Variables

- struct timeval [timerStart](#)

6.31.1 Detailed Description

High-resolution cross-platform machine time reader.

Author

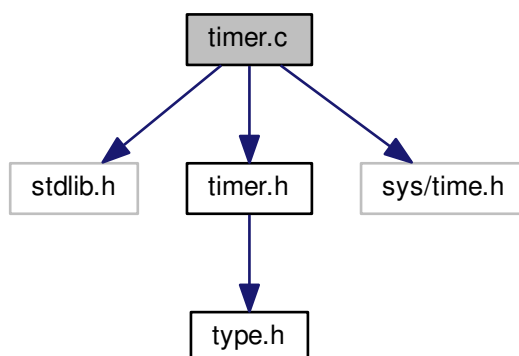
NVIDIA

6.32 timer.c File Reference

High-resolution cross-platform machine time reader.

```
#include <stdlib.h>
#include "timer.h"
#include <sys/time.h>
```

Include dependency graph for gpu/timer.c:



Functions

- void [StartTimer](#) ()
Set CPU frequency and begin timing.
- double [GetTimer](#) ()
Return elapsed time in seconds.

Variables

- struct timeval [timerStart](#)

6.32.1 Detailed Description

High-resolution cross-platform machine time reader.

Author

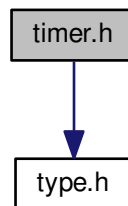
NVIDIA

6.33 timer.h File Reference

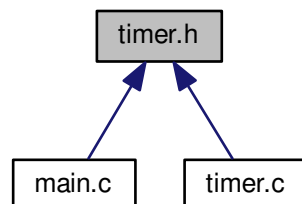
Declaration of timer function prototypes for CPU benchmarks.

```
#include "type.h"
```

Include dependency graph for cpu/timer.h:



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



Functions

- void [StartTimer](#) ()
Set CPU frequency and begin timing.
- double [GetTimer](#) ()
Return elapsed time in seconds.

6.33.1 Detailed Description

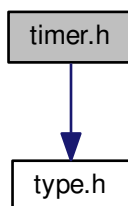
Declaration of timer function prototypes for CPU benchmarks.

6.34 timer.h File Reference

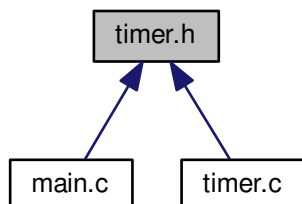
Declaration of timer function prototypes for GPU benchmarks.

```
#include "type.h"
```

Include dependency graph for gpu/timer.h:



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



Functions

- void [StartTimer](#) ()
Set CPU frequency and begin timing.
- double [GetTimer](#) ()
Return elapsed time in seconds.

6.34.1 Detailed Description

Declaration of timer function prototypes for GPU benchmarks.

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