phasefield-accelerator-benchmarks

pre-alpha

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4 Module Documentation

4.1 Diffusion equation benchmark

Files

- file common-diffusion/main.c

    Implementation of semi-infinite diffusion equation.
- file mesh.c

    Implemenatation of mesh handling functions for diffusion benchmarks.
- file mesh.h

    Declaration of mesh function prototypes for diffusion benchmarks.
- file numerics.c

    Implementation of boundary condition functions with OpenMP threading.
- file numerics.h

    Declaration of Laplacian operator and analytical solution functions.
- file output.c

    Implementation of file output functions for diffusion benchmarks.
- file output.h

    Declaration of output function prototypes for diffusion benchmarks.
- file timer.c

    High-resolution cross-platform machine time reader.
- file timer.h

    Declaration of timer function prototypes for diffusion benchmarks.
- file type.h

    Definition of scalar data type and Doxygen diffusion group.

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 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.
- fp_t euclidean_distance (fp_t ax, fp_t ay, fp_t bx, fp_t by)

  Compute Euclidean distance between two points, a and b.
- fp_t manhattan_distance (fp_t ax, fp_t ay, fp_t bx, fp_t by)

  Compute Manhattan distance between two points, a and b.
- fp_t distance_point_to_segment (fp_t ax, fp_t ay, fp_t bx, fp_t by, fp_t px, fp_t py)

  Compute minimum distance from point p to a line segment bounded by points a and b.
- 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 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. This choice propagates throughout the code, and may significantly affect runtime on GPU hardware.

Definition at line 40 of file type.h.

4.1.3 Function Documentation

4.1.3.1 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

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

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

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

Definition at line 139 of file numerics.c.

4.1.3.2 distance_point_to_segment()

```
fp_t distance_point_to_segment (
            fp_t ax,
            fp_t ay,
            fp_t bx,
            fp_t by,
            fp_t px,
            fp_t py )
```

Compute minimum distance from point p to a line segment bounded by points a and b.

This function computes the projection of p onto ab, limiting the projected range to [0, 1] to handle projections that fall outside of ab. Implemented after Grumdrig on Stackoverflow, https://stackoverflow.com/a/1501725.

Definition at line 116 of file numerics.c.

4.1.3.3 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 37 of file numerics.c.

4.1.3.4 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 52 of file common-diffusion/main.c.

4.1.3.5 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 mesh.c.

4.1.3.6 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 51 of file numerics.c.

4.1.3.7 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 output.c.

4.1.3.8 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 76 of file numerics.c.

4.1.3.9 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 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 timer.c.

4.2 Analytic

Files

- file cpu-analytic-diffusion/discretization.c

    Implementation of analytical solution functions.
- file cpu-analytic-diffusion/discretization.h

    Declaration of analytical solution prototypes.
- file cpu-analytic-diffusion/main.c

    Analytical solution to semi-infinite diffusion equation.

Functions

- void solve_diffusion_equation (fp_t **conc_old, fp_t **conc_new, fp_t **conc_lap, int nx, int ny, fp_t dx, fp_t dy, int nm, fp_t D, fp_t dt, fp_t elapsed)

    Update the scalar composition field using analytical solution.
- int main (int argc, char *argv[ ])

    Run simulation using input parameters specified on the command line.

4.2.1 Detailed Description

4.2.2 Function Documentation

4.2.2.1 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-analytic-diffusion/main.c.

4.3 Openmp

Files

- file [cpu-openmp-diffusion/boundaries.c](#)

  Implementation of boundary condition functions with OpenMP threading.

- file [cpu-openmp-diffusion/boundaries.h](#)

  Declaration of boundary condition function prototypes for OpenMP benchmarks.

- file [cpu-openmp-diffusion/discretization.c](#)

  Implementation of boundary condition functions with OpenMP threading.

- file [cpu-openmp-diffusion/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 [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 [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 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 56 of file cpu-openmp-diffusion/boundaries.c.

4.3.2.2 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 106 of file cpu-openmp-diffusion/discretization.c.

4.3.2.3 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 59 of file cpu-openmp-diffusion/discretization.c.

4.3.2.4 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 $\mathrm{bc} = [[y_{lo}, y_{hi}], [x_{lo}, x_{hi}]]$.

Definition at line 38 of file cpu-openmp-diffusion/boundaries.c.

4.4 Serial

Files

- file cpu-serial-diffusion/boundaries.c

    Implementation of boundary condition functions without threading.
- file cpu-serial-diffusion/boundaries.h

    Declaration of boundary condition function prototypes for CPU benchmarks.
- file cpu-serial-diffusion/discretization.c

    Implementation of boundary condition functions without threading.
- file cpu-serial-diffusion/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 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 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.

4.4.1 Detailed Description

4.4.2 Function Documentation

4.4.2.1 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 55 of file cpu-serial-diffusion/boundaries.c.

4.4.2.2 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 98 of file cpu-serial-diffusion/discretization.c.

4.4.2.3 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 60 of file cpu-serial-diffusion/discretization.c.

4.4.2.4 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 $\mathrm{bc} = [[y_{lo}, y_{hi}], [x_{lo}, x_{hi}]]$.

Definition at line 37 of file cpu-serial-diffusion/boundaries.c.

4.4.2.5 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 38 of file cpu-serial-diffusion/discretization.c.

4.5   Tbb

Files

- file boundaries.cpp

    Implementation of boundary condition functions with TBB threading.
- file cpu-tbb-diffusion/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-diffusion/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 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 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.

4.5.1   Detailed Description

4.5.2   Function Documentation

4.5.2.1 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 boundaries.cpp.

4.5.2.2 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 189 of file discretization.cpp.

4.5.2.3 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 65 of file discretization.cpp.

4.5.2.4 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 $\mathrm{bc} = [[y_{lo}, y_{hi}], [x_{lo}, x_{hi}]]$.

Definition at line 41 of file boundaries.cpp.

4.5.2.5 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 43 of file discretization.cpp.

4.6 Cuda

Files

- file gpu-cuda-diffusion/boundaries.c

  Implementation of boundary condition functions with OpenMP threading.
- file gpu-cuda-diffusion/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-diffusion/discretization.h

  Declaration of discretized mathematical function prototypes for CUDA benchmarks.

Macros

- #define MAX_TILE_W 32

  Maximum width of an input tile, including halo cells, for GPU memory allocation.
- #define MAX_TILE_H 32

  Maximum height of an input tile, including halo cells, for GPU memory allocation.
- #define MAX_MASK_W 3

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

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 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
  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.
- 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.
- __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.
- 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 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]

  Allocate constant memory on the GPU for the convolution mask.

4.6.1 Detailed Description

4.6.2 Function Documentation

4.6.2.1 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 56 of file gpu-cuda-diffusion/boundaries.c.

4.6.2.2 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 256 of file discretization.cu.

4.6.2.3 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 158 of file discretization.cu.

4.6.2.4 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 38 of file gpu-cuda-diffusion/boundaries.c.

4.7 Openacc

Files

- file gpu-openacc-diffusion/boundaries.c

  Implementation of boundary condition functions with OpenMP threading.
- file gpu-openacc-diffusion/boundaries.h

  Declaration of boundary condition function prototypes for OpenAcc benchmarks.
- file gpu-openacc-diffusion/discretization.c

  Implementation of boundary condition functions with OpenACC threading.
- file gpu-openacc-diffusion/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 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 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.

4.7.1 Detailed Description

4.7.2 Function Documentation

4.7.2.1 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 56 of file gpu-openacc-diffusion/boundaries.c.

4.7.2.2 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.

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

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

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

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

Definition at line 124 of file gpu-openacc-diffusion/discretization.c.

4.7.2.3 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 60 of file gpu-openacc-diffusion/discretization.c.

4.7.2.4 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 $\mathrm{bc} = [[y_{lo}, y_{hi}], [x_{lo}, x_{hi}]]$.

Definition at line 38 of file gpu-openacc-diffusion/boundaries.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 107 of file discretization.cpp.

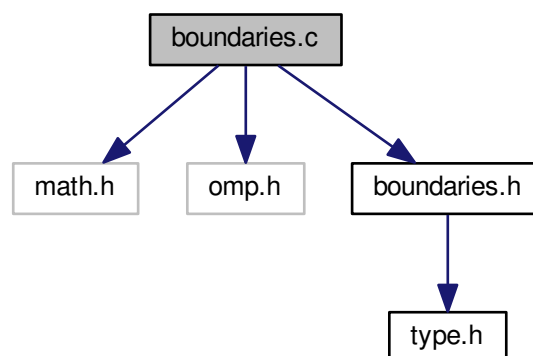The documentation for this class was generated from the following file:

- 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-diffusion/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.
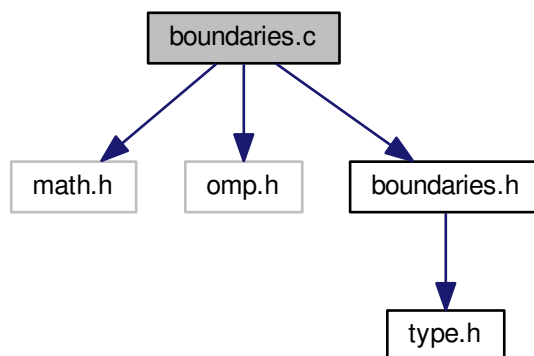
6.1.1 Detailed Description

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-diffusion/boundaries.c:
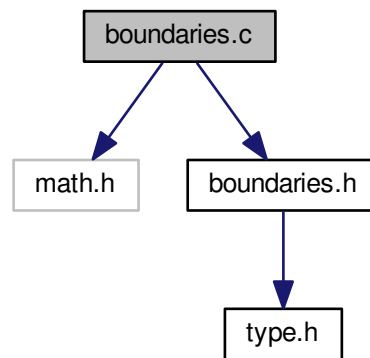
Functions

- 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

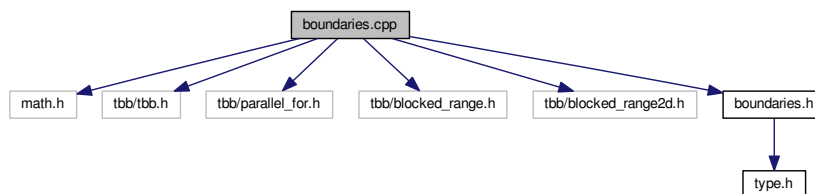Implementation of boundary condition functions without threading.

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-diffusion/boundaries.c:
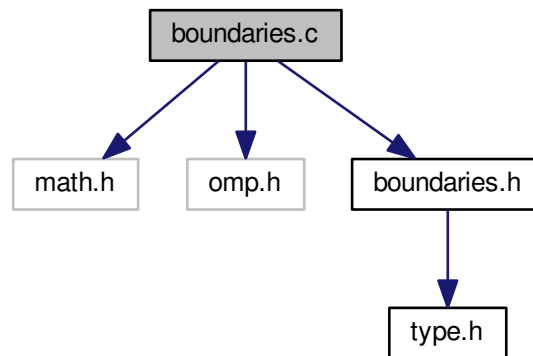
Functions

- 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.
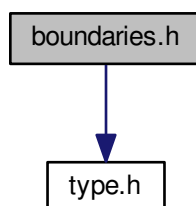
6.3.1 Detailed Description

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-diffusion/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.
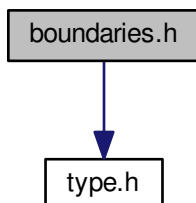
6.4.1 Detailed Description

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.
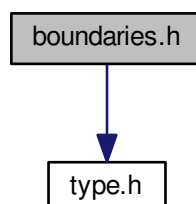
6.5.1   Detailed Description

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-diffusion/boundaries.h:

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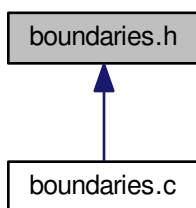
Functions

- 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.
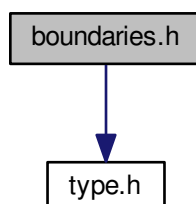
6.6.1 Detailed Description

Declaration of boundary condition function prototypes for OpenMP benchmarks.
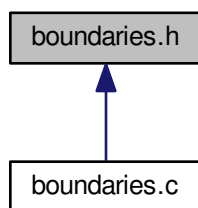
6.7 boundaries.h File Reference

Declaration of boundary condition function prototypes for CPU benchmarks.

```
#include "type.h"
```
Include dependency graph for cpu-serial-diffusion/boundaries.h:

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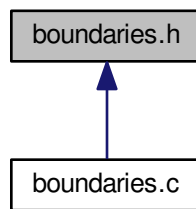
Functions

- 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.
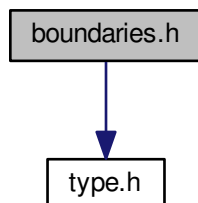
6.7.1 Detailed Description

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-diffusion/boundaries.h:

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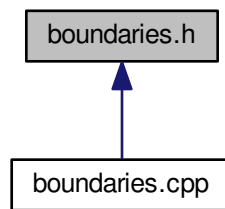
Functions

- 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.
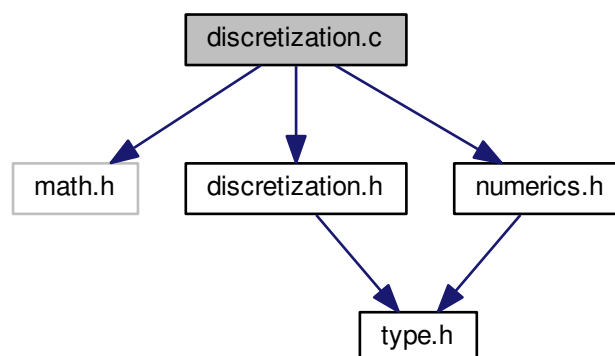
6.8.1 Detailed Description

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-diffusion/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-diffusion/boundaries.h:

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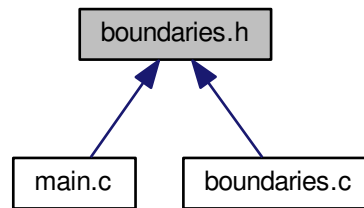
Functions

- 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 analytical solution functions.

```
#include <math.h>
#include "discretization.h"
#include "numerics.h"
```
Include dependency graph for cpu-analytic-diffusion/discretization.c:

Functions

- void solve_diffusion_equation (fp_t ∗∗conc_old, fp_t ∗∗conc_new, fp_t ∗∗conc_lap, int nx, int ny, fp_t dx, fp_t dy, int nm, fp_t D, fp_t dt, fp_t elapsed)

    Update the scalar composition field using analytical solution.

6.11.1 Detailed Description

Implementation of analytical solution functions.

6.12 discretization.c File Reference

Implementation of boundary condition functions with OpenMP threading.

```
#include <math.h>
#include <omp.h>
#include "discretization.h"
#include "numerics.h"
```
Include dependency graph for cpu-openmp-diffusion/discretization.c:

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 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)

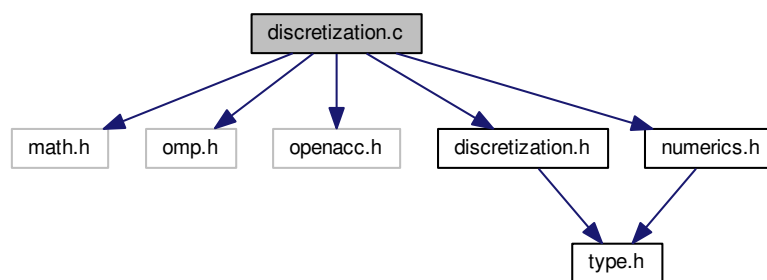   *Compare numerical and analytical solutions of the diffusion equation.*

6.12.1 Detailed Description

Implementation of boundary condition functions with OpenMP threading.

6.13 discretization.c File Reference

Implementation of boundary condition functions without threading.

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

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 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.
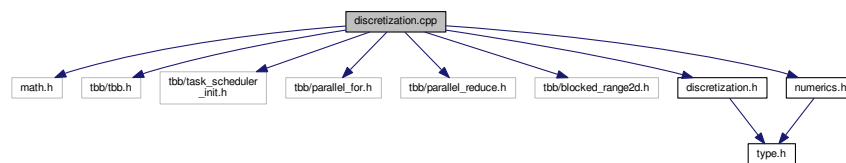
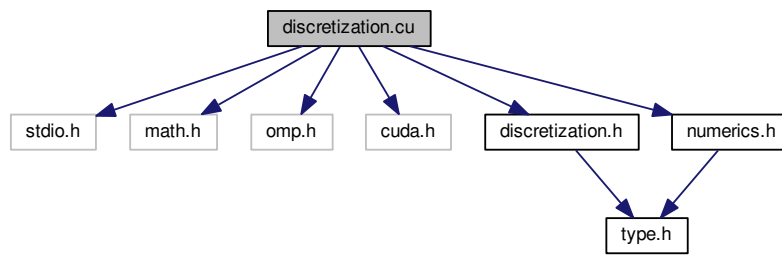**6.13.1 Detailed Description**

Implementation of boundary condition functions without threading.

6.14   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 "numerics.h"
```
Include dependency graph for gpu-openacc-diffusion/discretization.c:

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)

    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 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 OpenACC threading.

6.15 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 "numerics.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 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 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.

6.15.1 Detailed Description

Implementation of boundary condition functions with TBB threading.

6.16 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 "numerics.h"
```
Include dependency graph for discretization.cu:

Macros

- #define MAX_TILE_W 32

    Maximum width of an input tile, including halo cells, for GPU memory allocation.
- #define MAX_TILE_H 32

    Maximum height of an input tile, including halo cells, for GPU memory allocation.
- #define MAX_MASK_W 3

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

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.
- __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.
- 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.
- __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.
- 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 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](#)]

  Allocate constant memory on the GPU for the convolution mask.

6.16.1 Detailed Description

Implementation of boundary condition functions with CUDA acceleration.
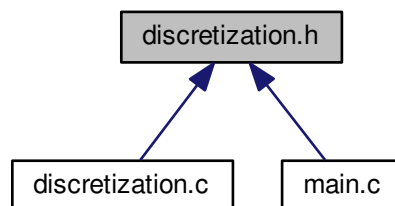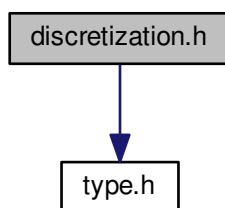
6.17 discretization.h File Reference

Declaration of analytical solution prototypes.

```
#include "type.h"
```
Include dependency graph for cpu-analytic-diffusion/discretization.h:
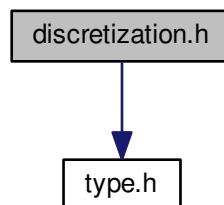
This graph shows which files directly or indirectly include this file:

Functions

- void [solve_diffusion_equation](#) ([fp_t](#) ∗∗conc_old, [fp_t](#) ∗∗conc_new, [fp_t](#) ∗∗conc_lap, int nx, int ny, [fp_t](#) dx, [fp_t](#) dy, int nm, [fp_t](#) D, [fp_t](#) dt, [fp_t](#) elapsed)

  Update the scalar composition field using analytical solution.

6.17.1   Detailed Description

Declaration of analytical solution prototypes.
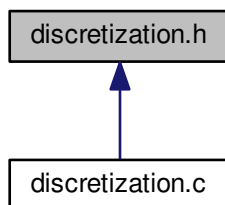
6.18   discretization.h File Reference

Declaration of discretized mathematical function prototypes for OpenMP benchmarks.

```
#include "type.h"
```
Include dependency graph for cpu-openmp-diffusion/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 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.
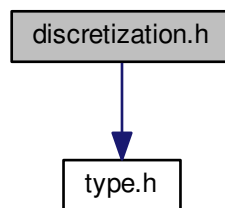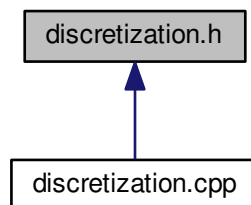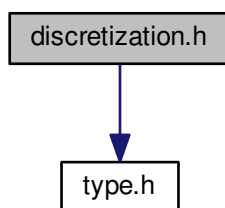
6.18.1 Detailed Description

Declaration of discretized mathematical function prototypes for OpenMP benchmarks.
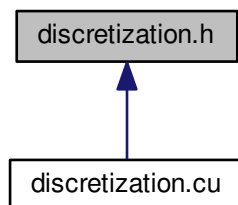
6.19 discretization.h File Reference

Declaration of discretized mathematical function prototypes for CPU benchmarks.

```
#include "type.h"
```
Include dependency graph for cpu-serial-diffusion/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 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.
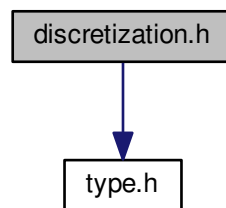
6.19.1 Detailed Description

Declaration of discretized mathematical function prototypes for CPU benchmarks.
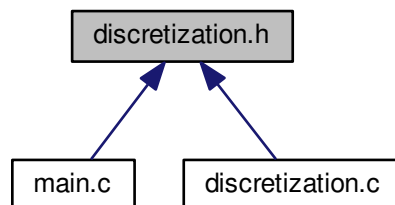
6.20 discretization.h File Reference

Declaration of discretized mathematical function prototypes for TBB benchmarks.

```
#include "type.h"
```
Include dependency graph for cpu-tbb-diffusion/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 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.
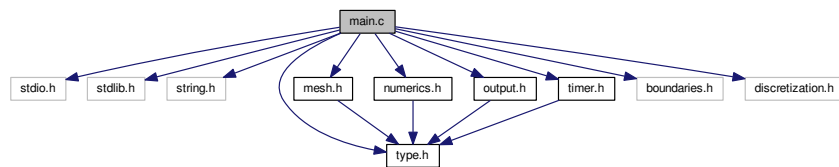
6.20.1 Detailed Description

Declaration of discretized mathematical function prototypes for TBB benchmarks.

6.21 discretization.h File Reference

Declaration of discretized mathematical function prototypes for CUDA benchmarks.

```
#include "type.h"
```
Include dependency graph for gpu-cuda-diffusion/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)

    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 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.

6.21.1 Detailed Description

Declaration of discretized mathematical function prototypes for CUDA benchmarks.

6.22 discretization.h File Reference

Declaration of discretized mathematical function prototypes for OpenAcc benchmarks.

```
#include "type.h"
```
Include dependency graph for gpu-openacc-diffusion/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)

    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 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.

6.22.1 Detailed Description

Declaration of discretized mathematical function prototypes for OpenAcc benchmarks.

6.23 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 "numerics.h"
#include "output.h"
#include "timer.h"
#include "boundaries.h"
#include "discretization.h"
```
Include dependency graph for common-diffusion/main.c:

Functions

- int main (int argc, char ∗argv[ ])

    Run simulation using input parameters specified on the command line.

6.23.1 Detailed Description

Implementation of semi-infinite diffusion equation.

6.24 main.c File Reference

Analytical solution to semi-infinite diffusion equation.

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

`#include "discretization.h"`
Include dependency graph for cpu-analytic-diffusion/main.c:
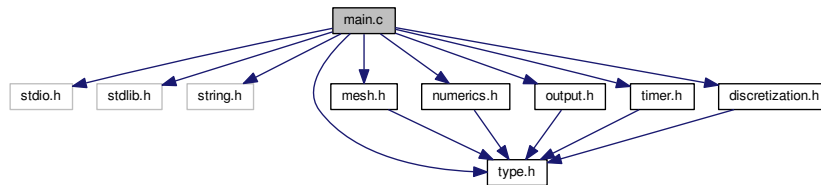
Functions

- int main (int argc, char ∗argv[ ])

  Run simulation using input parameters specified on the command line.

6.24.1   Detailed Description

Analytical solution to semi-infinite diffusion equation.

6.25   mesh.c File Reference

Implemenatation of mesh handling functions for diffusion benchmarks.

`#include <stdio.h>`
`#include <stdlib.h>`
`#include "mesh.h"`
Include dependency graph for mesh.c:
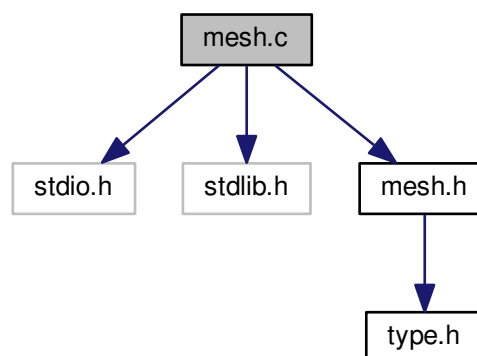
Functions

- 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.

6.25.1 Detailed Description

Implemenatation of mesh handling functions for diffusion benchmarks.

6.26 mesh.h File Reference

Declaration of mesh function prototypes for diffusion benchmarks.

```
#include "type.h"
```
Include dependency graph for mesh.h:
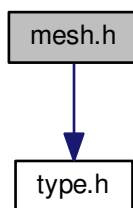
This graph shows which files directly or indirectly include this file:
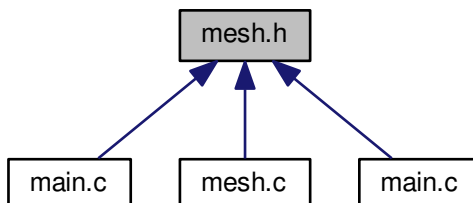
Functions

- 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 diffusion benchmarks.

6.27   numerics.c File Reference

Implementation of boundary condition functions with OpenMP threading.

```
#include <math.h>
#include "numerics.h"
```
Include dependency graph for numerics.c:

Functions

- 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.
- fp_t euclidean_distance (fp_t ax, fp_t ay, fp_t bx, fp_t by)

     Compute Euclidean distance between two points, a and b.

- fp_t manhattan_distance (fp_t ax, fp_t ay, fp_t bx, fp_t by)

  Compute Manhattan distance between two points, a and b.
- fp_t distance_point_to_segment (fp_t ax, fp_t ay, fp_t bx, fp_t by, fp_t px, fp_t py)

  Compute minimum distance from point p to a line segment bounded by points a and b.
- 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.*

6.27.1 Detailed Description

Implementation of boundary condition functions with OpenMP threading.

6.28 numerics.h File Reference

Declaration of Laplacian operator and analytical solution functions.

```
#include "type.h"
```
Include dependency graph for numerics.h:

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

Functions

- 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.
- fp_t euclidean_distance (fp_t ax, fp_t ay, fp_t bx, fp_t by)

Compute Euclidean distance between two points, `a` *and* `b`.

- fp_t manhattan_distance (fp_t ax, fp_t ay, fp_t bx, fp_t by)

    Compute Manhattan distance between two points, `a` *and* `b`.

- fp_t distance_point_to_segment (fp_t ax, fp_t ay, fp_t bx, fp_t by, fp_t px, fp_t py)

    Compute minimum distance from point `p` *to a line segment bounded by points* `a` *and* `b`.

- 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.

6.28.1 Detailed Description

Declaration of Laplacian operator and analytical solution functions.

6.29 output.c File Reference

Implementation of file output functions for diffusion benchmarks.

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <iso646.h>
#include <png.h>
#include "output.h"
```
Include dependency graph for output.c:
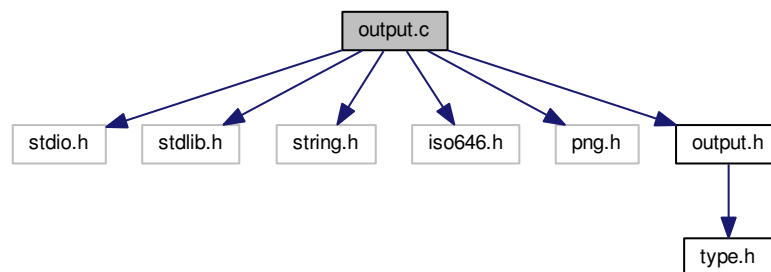
Functions

- 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.*

6.29.1 Detailed Description

Implementation of file output functions for diffusion benchmarks.

6.30 output.h File Reference

Declaration of output function prototypes for diffusion benchmarks.

```
#include "type.h"
```
Include dependency graph for output.h:
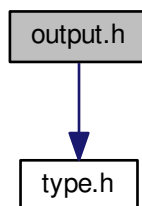
This graph shows which files directly or indirectly include this file:
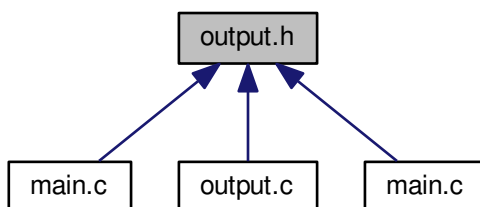
Functions

- 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 diffusion 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 timer.c:
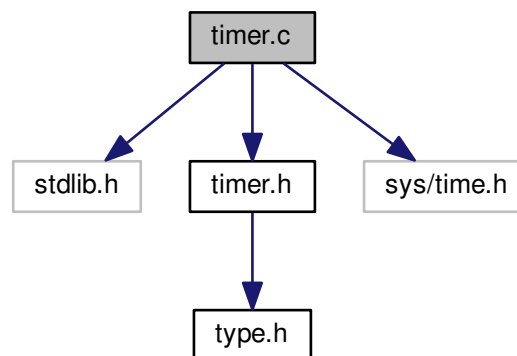
Functions

- 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.h File Reference

Declaration of timer function prototypes for diffusion benchmarks.

```
#include "type.h"
```
Include dependency graph for timer.h:
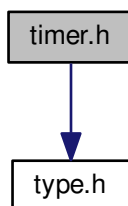
This graph shows which files directly or indirectly include this file:
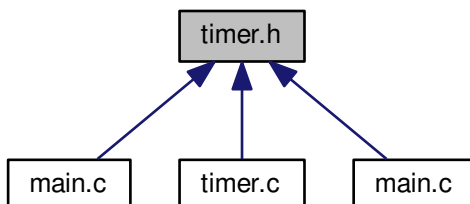
Functions

- void StartTimer ()

    Set CPU frequency and begin timing.
- double GetTimer ()

    Return elapsed time in seconds.

6.32.1 Detailed Description

Declaration of timer function prototypes for diffusion benchmarks.

6.33 type.h File Reference

Definition of scalar data type and Doxygen diffusion group.

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

Typedefs

- typedef double fp_t

6.33.1 Detailed Description

Definition of scalar data type and Doxygen diffusion group.

Index