# phasefield-accelerator-benchmarks pre-alpha

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# 1 Class Index

## 1.1 Class List

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

Stopwatch 3

# 2 File Index

## 2.1 File List

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

analytic_main.c Analytical solution to semi-infinite diffusion equation	4
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3 Class Documentation			
3.1 Stopwatch Struct Reference			
<pre>#include <type.h></type.h></pre>			
Public Attributes			
double conv			
double step			
• double file			
double soln			
3.1.1 Detailed Description			
Container for timing data			
Definition at line 39 of file type.h.			
3.1.2 Member Data Documentation			

3.1.2.1 conv

double Stopwatch::conv

Definition at line 43 of file type.h.

Cumulative time executing compute\_convolution()

## 3.1.2.2 file

```
double Stopwatch::file
```

Cumulative time executing write\_csv() and write\_png()

Definition at line 53 of file type.h.

#### 3.1.2.3 soln

```
double Stopwatch::soln
```

Cumulative time executing <a href="mailto:check\_solution">check\_solution</a>()

Definition at line 58 of file type.h.

## 3.1.2.4 step

```
double Stopwatch::step
```

Cumulative time executing solve\_diffusion\_equation()

Definition at line 48 of file type.h.

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

• type.h

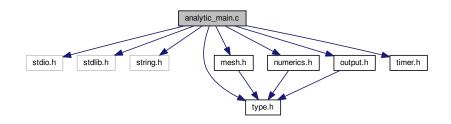
## 4 File Documentation

## 4.1 analytic\_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 dependency graph for analytic\_main.c:



#### **Functions**

- void solve\_diffusion\_equation (fp\_t \*\*conc, int nx, int ny, int nm, fp\_t dx, fp\_t dy, fp\_t D, fp\_t dt, fp\_t elapsed)

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

Find analytical solution at intervals specified in the parameters file.

## 4.1.1 Detailed Description

Analytical solution to semi-infinite diffusion equation.

#### 4.1.2 Function Documentation

#### 4.1.2.1 main()

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

Find analytical solution at intervals specified in the parameters file.

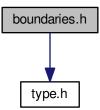
Program will write a series of PNG image files to visualize the scalar composition field, useful for qualitative verification of numerical results.

Definition at line 70 of file analytic\_main.c.

## 4.2 boundaries.h File Reference

Declaration of boundary condition function prototypes.

```
#include "type.h"
Include dependency graph for 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\_old, 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\_old, int nx, int ny, int nm, fp\_t bc[2][2])
 Set fixed value (chi) along left and bottom, zero-flux elsewhere.

## 4.2.1 Detailed Description

Declaration of boundary condition function prototypes.

#### 4.2.2 Function Documentation

## 4.2.2.1 apply\_initial\_conditions()

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 37 of file serial\_boundaries.c.

## 4.2.2.2 set\_boundaries()

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 28 of file serial\_boundaries.c.

## 4.3 cuda\_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 cuda_boundaries.c:
```

math.h omp.h boundaries.h

#### **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.

## 4.3.1 Detailed Description

Implementation of boundary condition functions with OpenMP threading.

## 4.3.2 Function Documentation

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#### 4.3.2.1 apply\_initial\_conditions()

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 38 of file cuda\_boundaries.c.

## 4.3.2.2 set\_boundaries()

Set values to be used along the simulation domain boundaries.

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

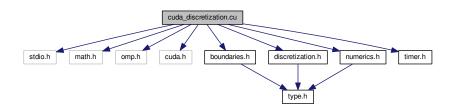
Definition at line 29 of file cuda\_boundaries.c.

## 4.4 cuda\_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 "boundaries.h"
#include "discretization.h"
#include "numerics.h"
#include "timer.h"
```

Include dependency graph for cuda\_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.

#### **Functions**

• \_\_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. Note:

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, fp\_t \*\*mask\_lap, int nx, int ny, int nm, fp\_t bc[2][2], fp\_t D, fp\_t dt, fp\_t \*elapsed, struct Stopwatch \*sw)

Update the scalar composition field using old and Laplacian values.

void check\_solution (fp\_t \*\*conc\_new, fp\_t \*\*conc\_lap, 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 H]

Convolution mask array on the GPU, allocated in protected memory.

## 4.4.1 Detailed Description

Implementation of boundary condition functions with CUDA acceleration.

## 4.4.2 Function Documentation

## 4.4.2.1 check\_solution()

```
void check_solution (
    fp_t ** conc_new,
    fp_t ** conc_lap,
    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.

Overwrites *conc\_lap*, into which the point-wise RSS is written. Normalized RSS is then computed as the sum of the point-wise values.

Definition at line 203 of file cuda\_discretization.cu.

## 4.4.2.2 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 123 of file cuda discretization.cu.

## 4.4.2.3 convolution\_kernel()

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. Note:

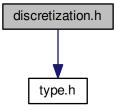
- The source matrix (conc\_old) and destination matrix (conc\_lap) must be identical in size
- One CUDA core operates on one array index: there is no nested loop over matrix elements
- The halo (nm/2 perimeter cells) in conc\_lap are unallocated garbage
- The same cells in conc\_old are boundary values, and contribute to the convolution
- · conc\_tile is the shared tile of input data, accessible by all threads in this block

Definition at line 66 of file cuda\_discretization.cu.

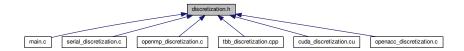
## 4.5 discretization.h File Reference

Declaration of discretized mathematical function prototypes.

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



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



#### **Functions**

- 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, fp\_t \*\*mask\_lap, int nx, int ny, int nm, fp\_t bc[2][2], fp\_t D, fp\_t dt, fp\_t \*elapsed, struct Stopwatch \*sw)

Update the scalar composition field using old and Laplacian values.

void check\_solution (fp\_t \*\*conc\_new, fp\_t \*\*conc\_lap, 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

Declaration of discretized mathematical function prototypes.

#### 4.5.2 Function Documentation

#### 4.5.2.1 check\_solution()

```
void check_solution (
    fp_t ** conc_new,
    fp_t ** conc_lap,
    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.

Overwrites *conc\_lap*, into which the point-wise RSS is written. Normalized RSS is then computed as the sum of the point-wise values.

Definition at line 73 of file serial\_discretization.c.

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## 4.5.2.2 compute\_convolution()

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.

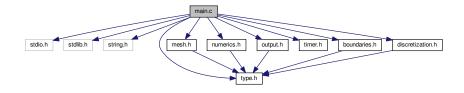
Definition at line 31 of file serial\_discretization.c.

## 4.6 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 main.c:



## **Functions**

• int main (int argc, char \*argv[])

Run simulation using input parameters specified on the command line.

## 4.6.1 Detailed Description

Implementation of semi-infinite diffusion equation.

#### 4.6.2 Function Documentation

#### 4.6.2.1 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*).

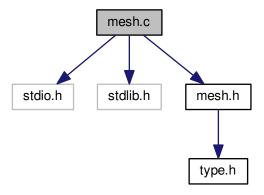
Definition at line 48 of file main.c.

## 4.7 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.

4.7 mesh.c File Reference 15

## 4.7.1 Detailed Description

Implemenatation of mesh handling functions for diffusion benchmarks.

## 4.7.2 Function Documentation

## 4.7.2.1 make\_arrays()

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 29 of file mesh.c.

## 4.7.2.2 swap\_pointers()

Swap pointers to data underlying two arrays.

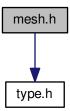
Rather than copy data from *conc\_old* into *conc\_new*, an expensive operation, simply trade the top-most pointers. New becomes old with no data lost and in almost no time.

Definition at line 73 of file mesh.c.

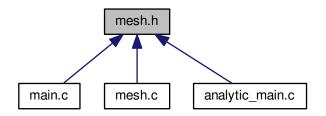
## 4.8 mesh.h File Reference

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.

## 4.8.1 Detailed Description

Declaration of mesh function prototypes for diffusion benchmarks.

#### 4.8.2 Function Documentation

## 4.8.2.1 make\_arrays()

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 29 of file mesh.c.

## 4.8.2.2 swap\_pointers()

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.

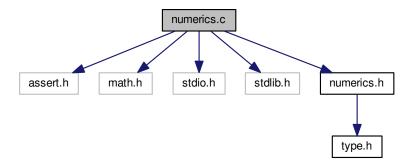
Definition at line 73 of file mesh.c.

## 4.9 numerics.c File Reference

Implementation of Laplacian operator and analytical solution functions.

```
#include <assert.h>
#include <math.h>
#include <stdio.h>
#include <stdlib.h>
#include "numerics.h"
```

Include dependency graph for numerics.c:



#### **Functions**

void set\_mask (fp\_t dx, fp\_t dy, int code, fp\_t \*\*mask\_lap, int nm)

Specify which stencil (mask) to use for the Laplacian (convolution)

void five\_point\_Laplacian\_stencil (fp\_t dx, fp\_t dy, fp\_t \*\*mask\_lap, int nm)

Write 5-point Laplacian stencil into convolution mask.

• void nine\_point\_Laplacian\_stencil (fp\_t dx, fp\_t dy, fp\_t \*\*mask\_lap, int nm)

Write 9-point Laplacian stencil into convolution mask.

void slow\_nine\_point\_Laplacian\_stencil (fp\_t dx, fp\_t dy, fp\_t \*\*mask\_lap, int nm)

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.

## 4.9.1 Detailed Description

Implementation of Laplacian operator and analytical solution functions.

## 4.9.2 Function Documentation

## 4.9.2.1 analytical\_value()

Analytical solution of the diffusion equation for a carburizing process.

For 1D diffusion through a semi-infinite domain with initial and far-field composition  $c_{\infty}$  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 121 of file numerics.c.

## 4.9.2.2 distance\_point\_to\_segment()

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 108 of file numerics.c.

## 4.9.2.3 five\_point\_Laplacian\_stencil()

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

Write 5-point Laplacian stencil into convolution mask.

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

Definition at line 51 of file numerics.c.

#### 4.9.2.4 nine\_point\_Laplacian\_stencil()

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

Write 9-point Laplacian stencil into convolution mask.

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

Definition at line 62 of file numerics.c.

## 4.9.2.5 set\_mask()

Specify which stencil (mask) to use for the Laplacian (convolution)

The mask corresponding to the numerical code will be applied. The suggested encoding is mask width as the ones digit and value count as the tens digit, *e.g.* 53 specifies five\_point\_Laplacian\_stencil(), while 93 specifies nine\_point\_Laplacian\_stencil().

To add your own mask (stencil), add a case to this function with your chosen numerical encoding, then specify that code in the input parameters file (params.txt by default). Note that, for a Laplacian stencil, the sum of the coefficients must equal zero and *nm* must be an odd integer.

If your stencil is larger than  $5 \times 5$ , you must increase the values defined by MAX\_MASK\_W and MAX\_MASK\_H.

Definition at line 31 of file numerics.c.

## 4.9.2.6 slow\_nine\_point\_Laplacian\_stencil()

Write 9-point Laplacian stencil into convolution mask.

```
5 \times 5 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  $3\times 3$  version. If your code requires  $\mathcal{O}(\Delta x^4)$  accuracy, please use nine\_point\_ $\leftarrow$  Laplacian\_stencil().

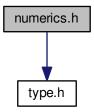
Definition at line 79 of file numerics.c.

## 4.10 numerics.h File Reference

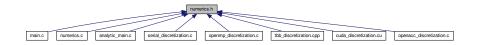
Declaration of Laplacian operator and analytical solution functions.

#include "type.h"

Include dependency graph for numerics.h:



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



## Macros

- #define MAX\_MASK\_W 5
  - Maximum width of the convolution mask (Laplacian stencil) array.
- #define MAX\_MASK\_H 5

Maximum height of the convolution mask (Laplacian stencil) array.

#### **Functions**

- void set\_mask (fp\_t dx, fp\_t dy, int code, fp\_t \*\*mask\_lap, int nm)
  - Specify which stencil (mask) to use for the Laplacian (convolution)
- void five\_point\_Laplacian\_stencil (fp\_t dx, fp\_t dy, fp\_t \*\*mask\_lap, int nm)

Write 5-point Laplacian stencil into convolution mask.

void nine\_point\_Laplacian\_stencil (fp\_t dx, fp\_t dy, fp\_t \*\*mask\_lap, int nm)

Write 9-point Laplacian stencil into convolution mask.

void slow\_nine\_point\_Laplacian\_stencil (fp\_t dx, fp\_t dy, fp\_t \*\*mask\_lap, int nm)

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.

## 4.10.1 Detailed Description

Declaration of Laplacian operator and analytical solution functions.

#### 4.10.2 Function Documentation

## 4.10.2.1 analytical\_value()

Analytical solution of the diffusion equation for a carburizing process.

For 1D diffusion through a semi-infinite domain with initial and far-field composition  $c_{\infty}$  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 121 of file numerics.c.

## 4.10.2.2 distance\_point\_to\_segment()

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 108 of file numerics.c.

## 4.10.2.3 five\_point\_Laplacian\_stencil()

Write 5-point Laplacian stencil into convolution mask.

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

Definition at line 51 of file numerics.c.

## 4.10.2.4 nine\_point\_Laplacian\_stencil()

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

Write 9-point Laplacian stencil into convolution mask.

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

Definition at line 62 of file numerics.c.

## 4.10.2.5 set\_mask()

Specify which stencil (mask) to use for the Laplacian (convolution)

The mask corresponding to the numerical code will be applied. The suggested encoding is mask width as the ones digit and value count as the tens digit, *e.g.* 53 specifies five\_point\_Laplacian\_stencil(), while 93 specifies nine\_point\_Laplacian\_stencil().

To add your own mask (stencil), add a case to this function with your chosen numerical encoding, then specify that code in the input parameters file (params.txt by default). Note that, for a Laplacian stencil, the sum of the coefficients must equal zero and nm must be an odd integer.

If your stencil is larger than  $5 \times 5$ , you must increase the values defined by MAX\_MASK\_W and MAX\_MASK\_H.

Definition at line 31 of file numerics.c.

## 4.10.2.6 slow\_nine\_point\_Laplacian\_stencil()

Write 9-point Laplacian stencil into convolution mask.

```
5\times 5 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  $3\times 3$  version. If your code requires  $\mathcal{O}(\Delta x^4)$  accuracy, please use nine\_point\_ $\leftarrow$  Laplacian\_stencil().

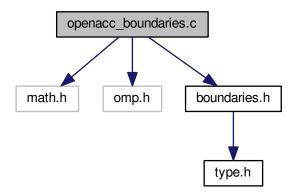
Definition at line 79 of file numerics.c.

## 4.11 openacc\_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 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.

## 4.11.1 Detailed Description

Implementation of boundary condition functions with OpenMP threading.

#### 4.11.2 Function Documentation

## 4.11.2.1 apply\_initial\_conditions()

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 38 of file openacc\_boundaries.c.

## 4.11.2.2 set\_boundaries()

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 29 of file openacc\_boundaries.c.

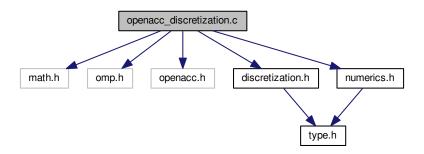
## 4.12 openacc\_discretization.c File Reference

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 openacc\_discretization.c:



#### **Functions**

- 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, fp\_t \*\*mask\_lap, int nx, int ny, int nm, fp\_t bc[2][2], fp\_t D, fp\_t dt, fp\_t \*elapsed, struct Stopwatch \*sw)

Update the scalar composition field using old and Laplacian values.

void check\_solution (fp\_t \*\*conc\_new, fp\_t \*\*conc\_lap, 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.

## 4.12.1 Detailed Description

Implementation of boundary condition functions with OpenACC threading.

## 4.12.2 Function Documentation

#### 4.12.2.1 check\_solution()

```
void check_solution (
    fp_t ** conc_new,
    fp_t ** conc_lap,
    int nx,
    int ny,
    fp_t dx,
    fp_t dy,
    int nm,
    fp_t elapsed,
    fp_t D,
    fp_t * rss )
```

Compare numerical and analytical solutions of the diffusion equation.

#### Returns

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

Overwrites *conc\_lap*, into which the point-wise RSS is written. Normalized RSS is then computed as the sum of the point-wise values.

Definition at line 86 of file openacc discretization.c.

## 4.12.2.2 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.

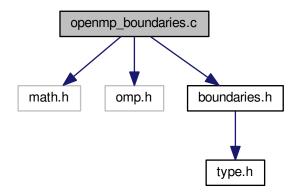
Definition at line 31 of file openacc\_discretization.c.

## 4.13 openmp\_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 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.

## 4.13.1 Detailed Description

Implementation of boundary condition functions with OpenMP threading.

#### 4.13.2 Function Documentation

## 4.13.2.1 apply\_initial\_conditions()

```
void apply_initial_conditions (
    fp_t ** conc_old,
    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 39 of file openmp\_boundaries.c.

## 4.13.2.2 set\_boundaries()

Set values to be used along the simulation domain boundaries.

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

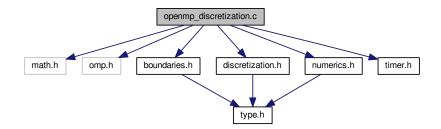
Definition at line 30 of file openmp\_boundaries.c.

## 4.14 openmp\_discretization.c File Reference

Implementation of boundary condition functions with OpenMP threading.

```
#include <math.h>
#include <omp.h>
#include "boundaries.h"
#include "discretization.h"
#include "numerics.h"
#include "timer.h"
```

Include dependency graph for openmp\_discretization.c:



## **Functions**

- 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, fp\_t \*\*mask\_lap, int nx, int ny, int nm, fp\_t bc[2][2], fp\_t D, fp\_t dt, fp\_t \*elapsed, struct Stopwatch \*sw)

Update the scalar composition field using old and Laplacian values.

void check\_solution (fp\_t \*\*conc\_new, fp\_t \*\*conc\_lap, 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.

## 4.14.1 Detailed Description

Implementation of boundary condition functions with OpenMP threading.

## 4.14.2 Function Documentation

## 4.14.2.1 check\_solution()

```
void check_solution (
    fp_t ** conc_new,
    fp_t ** conc_lap,
    int nx,
    int ny,
    fp_t dx,
    fp_t dy,
    int nm,
    fp_t elapsed,
    fp_t D,
    fp_t * rss )
```

Compare numerical and analytical solutions of the diffusion equation.

## Returns

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

Overwrites *conc\_lap*, into which the point-wise RSS is written. Normalized RSS is then computed as the sum of the point-wise values.

Definition at line 80 of file openmp\_discretization.c.

## 4.14.2.2 compute\_convolution()

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.

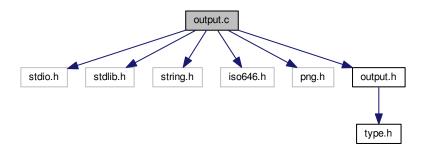
Definition at line 32 of file openmp\_discretization.c.

## 4.15 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 param\_parser (int argc, char \*argv[], int \*nx, int \*ny, int \*nm, int \*code, fp\_t \*dx, fp\_t \*dy, fp\_t \*D, fp\_t \*linStab, int \*steps, int \*checks)

Read parameters from file specified on the command line.

• void <a href="mailto:progress">print\_progress</a> (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.

## 4.15.1 Detailed Description

Implementation of file output functions for diffusion benchmarks.

## 4.15.2 Function Documentation

## 4.15.2.1 print\_progress()

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

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

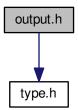
```
for (int step=0; step<steps; step++) {
    print_progress(step, steps);
    take_a_step();
    elapsed += dt;
}</pre>
```

Definition at line 123 of file output.c.

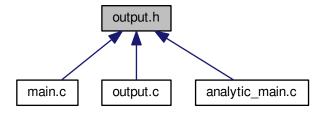
## 4.16 output.h File Reference

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 param\_parser (int argc, char \*argv[], int \*nx, int \*ny, int \*nm, int \*code, fp\_t \*dx, fp\_t \*dy, fp\_t \*D, fp\_t \*linStab, int \*steps, int \*checks)

Read parameters from file specified on the command line.

• void <a href="mailto:progress">print\_progress</a> (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.

## 4.16.1 Detailed Description

Declaration of output function prototypes for diffusion benchmarks.

## 4.16.2 Function Documentation

## 4.16.2.1 print\_progress()

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

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

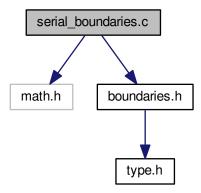
```
for (int step=0; step<steps; step++) {
    print_progress(step, steps);
    take_a_step();
    elapsed += dt;
}</pre>
```

Definition at line 123 of file output.c.

## 4.17 serial\_boundaries.c File Reference

Implementation of boundary condition functions without threading.

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



## **Functions**

- void set\_boundaries (fp\_t bc[2][2])
  - Set values to be used along the simulation domain boundaries.
- $\bullet \ \ void\ apply\_initial\_conditions\ (fp\_t\ **conc,\ int\ nx,\ int\ ny,\ int\ nm,\ fp\_t\ bc[2][2])\\$

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.

## 4.17.1 Detailed Description

Implementation of boundary condition functions without threading.

## 4.17.2 Function Documentation

## 4.17.2.1 apply\_initial\_conditions()

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 37 of file serial boundaries.c.

## 4.17.2.2 set\_boundaries()

Set values to be used along the simulation domain boundaries.

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

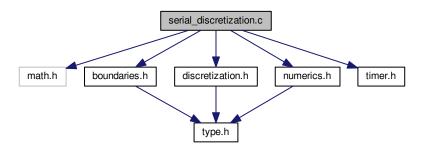
Definition at line 28 of file serial\_boundaries.c.

## 4.18 serial\_discretization.c File Reference

Implementation of boundary condition functions without threading.

```
#include <math.h>
#include "boundaries.h"
#include "discretization.h"
#include "numerics.h"
#include "timer.h"
```

Include dependency graph for serial\_discretization.c:



#### **Functions**

• 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, fp\_t \*\*mask\_lap, int nx, int ny, int nm, fp\_t bc[2][2], fp\_t D, fp\_t dt, fp\_t \*elapsed, struct Stopwatch \*sw)

Update the scalar composition field using old and Laplacian values.

void check\_solution (fp\_t \*\*conc\_new, fp\_t \*\*conc\_lap, 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.

#### 4.18.1 Detailed Description

Implementation of boundary condition functions without threading.

#### 4.18.2 Function Documentation

#### 4.18.2.1 check\_solution()

```
void check_solution (
    fp_t ** conc_new,
    fp_t ** conc_lap,
    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.

Overwrites *conc\_lap*, into which the point-wise RSS is written. Normalized RSS is then computed as the sum of the point-wise values.

Definition at line 73 of file serial\_discretization.c.

## 4.18.2.2 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.

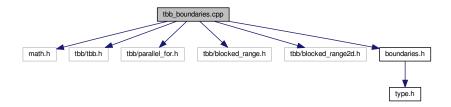
Definition at line 31 of file serial discretization.c.

## 4.19 tbb 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 tbb 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.

## 4.19.1 Detailed Description

Implementation of boundary condition functions with TBB threading.

#### 4.19.2 Function Documentation

## 4.19.2.1 apply\_initial\_conditions()

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 41 of file tbb boundaries.cpp.

#### 4.19.2.2 set\_boundaries()

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 32 of file tbb\_boundaries.cpp.

## 4.20 tbb\_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 "boundaries.h"
#include "discretization.h"
#include "numerics.h"
#include "timer.h"
```

Include dependency graph for tbb\_discretization.cpp:



#### **Functions**

- 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, fp\_t \*\*mask\_lap, int nx, int ny, int nm, fp\_t bc[2][2], fp\_t D, fp\_t dt, fp\_t \*elapsed, struct Stopwatch \*sw)

Update the scalar composition field using old and Laplacian values.

void check\_solution (fp\_t \*\*conc\_new, fp\_t \*\*conc\_lap, 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.

#### 4.20.1 Detailed Description

Implementation of boundary condition functions with TBB threading.

#### 4.20.2 Function Documentation

#### 4.20.2.1 check\_solution()

```
void check_solution (
    fp_t ** conc_new,
    fp_t ** conc_lap,
    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.

Overwrites *conc\_lap*, into which the point-wise RSS is written. Normalized RSS is then computed as the sum of the point-wise values.

Definition at line 132 of file tbb\_discretization.cpp.

## 4.20.2.2 compute\_convolution()

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

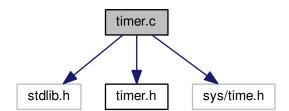
If the convolution mask is the Laplacian stencil, the convolution evaluates the discrete Laplacian of the composition field. Other masks are possible, for example the Sobel filters for edge detection. This function is general purpose: as long as the dimensions nx, ny, and nm are properly specified, the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

Definition at line 36 of file tbb\_discretization.cpp.

#### 4.21 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

## 4.21.1 Detailed Description

High-resolution cross-platform machine time reader.

Author

**NVIDIA** 

## 4.21.2 Variable Documentation

## 4.21.2.1 timerStart

struct timeval timerStart

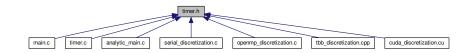
Platform-dependent data type of hardware time value

Definition at line 45 of file timer.c.

## 4.22 timer.h File Reference

Declaration of timer function prototypes for diffusion benchmarks.

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.

## 4.22.1 Detailed Description

Declaration of timer function prototypes for diffusion benchmarks.

## 4.23 type.h File Reference

Definition of scalar data type and Doxygen diffusion group.

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



## Classes

struct Stopwatch

## **Typedefs**

typedef double fp\_t

## 4.23.1 Detailed Description

Definition of scalar data type and Doxygen diffusion group.

## 4.23.2 Typedef Documentation

## 4.23.2.1 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 34 of file type.h.

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