# HiPerC alpha

Generated by Doxygen 1.9.1

1 Class Index		1
1.1 Class List	 	1
2 File Index		1
2.1 File List	 	1
3 Class Documentation		3
3.1 CudaData Struct Reference	 	3
3.1.1 Detailed Description	 	4
3.1.2 Member Data Documentation	 	4
3.2 OpenCLData Struct Reference	 	4
3.2.1 Detailed Description	 	5
3.2.2 Member Data Documentation	 	5
3.3 Stopwatch Struct Reference	 	7
3.3.1 Detailed Description	 	8
3.3.2 Member Data Documentation	 	8
4 File Documentation		9
4.1 boundaries.h File Reference	 	9
4.1.1 Detailed Description	 	10
4.1.2 Function Documentation	 	10
4.2 cuda_boundaries.cu File Reference	 	11
4.2.1 Detailed Description	 	12
4.2.2 Function Documentation	 	12
4.3 cuda_data.cu File Reference	 	14
4.3.1 Detailed Description	 	14
4.3.2 Function Documentation	 	14
4.4 cuda_data.h File Reference	 	16
4.4.1 Detailed Description	 	17
4.4.2 Function Documentation	 	17
4.5 cuda_discretization.cu File Reference	 	21
4.5.1 Detailed Description	 	22
4.5.2 Function Documentation	 	22
4.5.3 Variable Documentation	 	27
4.6 cuda_kernels.cuh File Reference	 	27
4.6.1 Detailed Description	 	29
4.6.2 Function Documentation	 	29
4.6.3 Variable Documentation	 	31
4.7 cuda_main.c File Reference	 	31
4.7.1 Detailed Description	 	32

4.7.2 Function Documentation	 . 32
4.8 kernel_boundary.cl File Reference	 . 33
4.8.1 Function Documentation	 . 34
4.9 kernel_convolution.cl File Reference	 . 34
4.9.1 Function Documentation	 . 35
4.10 kernel_diffusion.cl File Reference	 . 36
4.10.1 Function Documentation	 . 36
4.11 mesh.c File Reference	 . 37
4.11.1 Detailed Description	 . 38
4.11.2 Function Documentation	 . 38
4.12 mesh.h File Reference	 . 40
4.12.1 Detailed Description	 . 41
4.12.2 Function Documentation	 . 41
4.13 numerics.c File Reference	 . 43
4.13.1 Detailed Description	 . 44
4.13.2 Function Documentation	 . 44
4.14 numerics.h File Reference	 . 50
4.14.1 Detailed Description	 . 51
4.14.2 Macro Definition Documentation	 . 51
4.14.3 Function Documentation	 . 52
4.15 openacc_boundaries.c File Reference	 . 59
4.15.1 Detailed Description	 . 59
4.15.2 Function Documentation	 . 59
4.16 openacc_discretization.c File Reference	 . 61
4.16.1 Detailed Description	 . 62
4.16.2 Function Documentation	 . 62
4.17 openacc_kernels.h File Reference	 . 63
4.17.1 Detailed Description	 . 64
4.17.2 Function Documentation	 . 64
4.18 openacc_main.c File Reference	 . 65
4.18.1 Detailed Description	 . 65
4.18.2 Function Documentation	 . 65
4.19 opencl_boundaries.c File Reference	 . 66
4.19.1 Detailed Description	 . 67
4.19.2 Function Documentation	 . 67
4.20 opencl_data.c File Reference	 . 68
4.20.1 Detailed Description	 . 69
4.20.2 Function Documentation	 . 69
4.21 opencl_data.h File Reference	 . 71

	4.21.1 Detailed Description	73
	4.21.2 Function Documentation	73
4.22	opencl_discretization.c File Reference	78
	4.22.1 Detailed Description	78
	4.22.2 Function Documentation	78
4.23	opencl_main.c File Reference	80
	4.23.1 Detailed Description	81
	4.23.2 Function Documentation	81
4.24	openmp_boundaries.c File Reference	82
	4.24.1 Detailed Description	83
	4.24.2 Function Documentation	83
4.25	openmp_discretization.c File Reference	84
	4.25.1 Detailed Description	85
	4.25.2 Function Documentation	85
4.26	openmp_main.c File Reference	86
	4.26.1 Detailed Description	86
	4.26.2 Function Documentation	86
4.27	output.c File Reference	87
	4.27.1 Detailed Description	88
	4.27.2 Function Documentation	88
4.28	output.h File Reference	91
	4.28.1 Detailed Description	91
	4.28.2 Function Documentation	92
4.29	serial_boundaries.c File Reference	94
	4.29.1 Detailed Description	94
	4.29.2 Function Documentation	95
4.30	serial_discretization.c File Reference	95
	4.30.1 Detailed Description	96
	4.30.2 Function Documentation	96
4.31	serial_main.c File Reference	97
	4.31.1 Detailed Description	97
	4.31.2 Function Documentation	98
4.32	tbb_boundaries.cpp File Reference	99
	4.32.1 Detailed Description	99
	4.32.2 Function Documentation	99
4.33	tbb_discretization.cpp File Reference	100
	4.33.1 Detailed Description	101
	4.33.2 Function Documentation	101
4.34	tbb main.c File Reference	102

1 Class Index

4.34.1 Detailed Description	103
4.34.2 Function Documentation	103
4.35 timer.c File Reference	105
4.35.1 Detailed Description	106
4.35.2 Macro Definition Documentation	106
4.35.3 Function Documentation	107
4.35.4 Variable Documentation	108
4.36 timer.h File Reference	108
4.36.1 Detailed Description	108
4.36.2 Function Documentation	108
4.37 type.h File Reference	109
4.37.1 Detailed Description	110
4.37.2 Typedef Documentation	110
Index	111
1.1 Class List  Here are the classes, structs, unions and interfaces with brief descriptions:  CudoDate	
CudaData Container for pointers to arrays on the GPU	3
OpenCLData Container for GPU array pointers and parameters	4
Stopwatch	7
2 File Index	
2.1 File List	
Here is a list of all files with brief descriptions:	
boundaries.h	9
Declaration of boundary condition function prototypes	9
cuda_boundaries.cu Implementation of boundary condition functions with OpenMP threading	11

cuda_data.cu Implementation of functions to create and destroy CudaData struct	14
cuda_data.h  Declaration of CUDA data container	16
cuda_discretization.cu Implementation of boundary condition functions with CUDA acceleration	21
cuda_kernels.cuh Declaration of functions to execute on the GPU (CUDA kernels)	27
cuda_main.c CUDA implementation of semi-infinite diffusion equation	31
kernel_boundary.cl	33
kernel_convolution.cl	34
kernel_diffusion.cl	36
mesh.c Implemenatation of mesh handling functions for diffusion benchmarks	37
mesh.h  Declaration of mesh function prototypes for diffusion benchmarks	40
numerics.c Implementation of Laplacian operator and analytical solution functions	43
numerics.h  Declaration of Laplacian operator and analytical solution functions	50
openacc_boundaries.c Implementation of boundary condition functions with OpenMP threading	59
openacc_discretization.c Implementation of boundary condition functions with OpenACC threading	61
openacc_kernels.h  Declaration of functions to execute on the GPU (OpenACC kernels)	63
openacc_main.c OpenACC implementation of semi-infinite diffusion equation	65
opencl_boundaries.c Implementation of boundary condition functions with OpenCL acceleration	66
opencl_data.c Implementation of functions to create and destroy OpenCLData struct	68
opencl_data.h  Declaration of OpenCL data container	71
opencl_discretization.c Implementation of boundary condition functions with OpenCL acceleration	78

3 Class Documentation 3

opencl_main.c OpenCL implementation of semi-infinite diffusion equation	80
openmp_boundaries.c Implementation of boundary condition functions with OpenMP threading	82
openmp_discretization.c Implementation of boundary condition functions with OpenMP threading	84
openmp_main.c OpenMP implementation of semi-infinite diffusion equation	86
output.c Implementation of file output functions for diffusion benchmarks	87
output.h  Declaration of output function prototypes for diffusion benchmarks	91
serial_boundaries.c Implementation of boundary condition functions without threading	94
serial_discretization.c Implementation of boundary condition functions without threading	95
serial_main.c Serial implementation of semi-infinite diffusion equation	97
tbb_boundaries.cpp Implementation of boundary condition functions with TBB threading	99
tbb_discretization.cpp Implementation of boundary condition functions with TBB threading	100
tbb_main.c Threading Building Blocks implementation of semi-infinite diffusion equation	102
timer.c High-resolution cross-platform machine time reader	105
timer.h  Declaration of timer function prototypes for diffusion benchmarks	108
type.h Definition of scalar data type and Doxygen diffusion group	109

# 3 Class Documentation

# 3.1 CudaData Struct Reference

Container for pointers to arrays on the GPU.

#include <cuda\_data.h>

## **Public Attributes**

```
• fp t * conc old
```

```
• fp_t * conc_new
```

• fp t \* conc lap

#### 3.1.1 Detailed Description

Container for pointers to arrays on the GPU.

Definition at line 21 of file cuda\_data.h.

## 3.1.2 Member Data Documentation

```
3.1.2.1 conc_lap fp_t* CudaData::conc_lap
```

Definition at line 24 of file cuda\_data.h.

```
3.1.2.2 conc_new fp_t* CudaData::conc_new
```

Definition at line 23 of file cuda\_data.h.

```
3.1.2.3 conc_old fp_t* CudaData::conc_old
```

Definition at line 22 of file cuda\_data.h.

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

• cuda\_data.h

# 3.2 OpenCLData Struct Reference

Container for GPU array pointers and parameters.

```
#include <opencl_data.h>
```

#### **Public Attributes**

- · cl context context
- · cl\_mem conc\_old
- cl\_mem conc\_new
- cl\_mem conc\_lap
- cl mem mask
- cl program boundary program
- cl\_program convolution\_program
- cl\_program diffusion\_program
- · cl kernel boundary kernel
- · cl kernel convolution kernel
- cl\_kernel diffusion\_kernel
- cl command queue commandQueue

## 3.2.1 Detailed Description

Container for GPU array pointers and parameters.

From the OpenCL v1.2 spec:

- A Context is the environment within which the kernels execute and the domain in which synchronization and memory management is defined. The context includes a set of devices, the memory accessible to those devices, the corresponding memory properties and one or more command-queues used to schedule execution of a kernel(s) or operations on memory objects.
- A Program Object encapsulates the following information:
  - A reference to an associated context.
  - A program source or binary.
  - The latest successfully built program executable, the list of devices for which the program executable is built, the build options used and a build log.
  - The number of kernel objects currently attached.
- A *Kernel Object* encapsulates a specific <u>kernel</u> function declared in a program and the argument values to be used when executing this <u>kernel</u> function.

Definition at line 37 of file opencl\_data.h.

#### 3.2.2 Member Data Documentation

## 3.2.2.1 boundary\_kernel cl\_kernel OpenCLData::boundary\_kernel

Boundary program executable for the GPU

Definition at line 59 of file opencl\_data.h.

**3.2.2.2 boundary\_program** cl\_program OpenCLData::boundary\_program

Boundary program source for JIT compilation on the GPU

Definition at line 52 of file opencl\_data.h.

3.2.2.3 commandQueue cl\_command\_queue OpenCLData::commandQueue

Queue for submitting OpenCL jobs to the GPU

Definition at line 66 of file opencl\_data.h.

3.2.2.4 conc\_lap cl\_mem OpenCLData::conc\_lap

Copy of Laplacian field on the GPU

Definition at line 46 of file opencl data.h.

3.2.2.5 conc\_new cl\_mem OpenCLData::conc\_new

Copy of new composition field on the GPU

Definition at line 44 of file opencl\_data.h.

3.2.2.6 conc\_old cl\_mem OpenCLData::conc\_old

Copy of old composition field on the GPU

Definition at line 42 of file opencl\_data.h.

3.2.2.7 context cl\_context OpenCLData::context

OpenCL interface to the GPU, hardware and software

Definition at line 39 of file opencl\_data.h.

3.2.2.8 convolution\_kernel cl\_kernel OpenCLData::convolution\_kernel

Convolution program executable for the GPU

Definition at line 61 of file opencl\_data.h.

**3.2.2.9 convolution\_program** cl\_program OpenCLData::convolution\_program

Convolution program source for JIT compilation on the GPU

Definition at line 54 of file opencl\_data.h.

3.2.2.10 diffusion\_kernel cl\_kernel OpenCLData::diffusion\_kernel

Timestepping program executable for the GPU

Definition at line 63 of file opencl\_data.h.

3.2.2.11 diffusion\_program cl\_program OpenCLData::diffusion\_program

Timestepping program source for JIT compilation on the GPU

Definition at line 56 of file opencl\_data.h.

3.2.2.12 mask cl\_mem OpenCLData::mask

Copy of Laplacian mask on the GPU

Definition at line 49 of file opencl\_data.h.

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

· opencl\_data.h

## 3.3 Stopwatch Struct Reference

#include <type.h>

## **Public Attributes**

- fp\_t conv
- fp\_t step
- fp\_t file
- fp\_t soln

# 3.3.1 Detailed Description

Container for timing data

Definition at line 27 of file type.h.

#### 3.3.2 Member Data Documentation

```
3.3.2.1 conv fp_t Stopwatch::conv
```

Cumulative time executing compute\_convolution()

Definition at line 31 of file type.h.

```
3.3.2.2 file fp_t Stopwatch::file
```

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

Definition at line 41 of file type.h.

3.3.2.3 soln fp\_t Stopwatch::soln

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

Definition at line 46 of file type.h.

4 File Documentation 9

```
3.3.2.4 step fp_t Stopwatch::step
```

Cumulative time executing solve\_diffusion\_equation()

Definition at line 36 of file type.h.

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

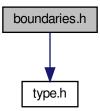
• type.h

## 4 File Documentation

## 4.1 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 apply\_initial\_conditions (fp\_t \*\*conc\_old, const int nx, const int ny, const int nm)

  Initialize flat composition field with fixed boundary conditions.
- void apply\_boundary\_conditions (fp\_t \*\*conc\_old, const int nx, const int ny, const int nm) Set fixed value  $(c_{hi})$  along left and bottom, zero-flux elsewhere.

## 4.1.1 Detailed Description

Declaration of boundary condition function prototypes.

## 4.1.2 Function Documentation

```
4.1.2.1 apply_boundary_conditions() void apply_boundary_conditions ( fp_t ** conc_old,
```

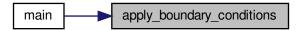
```
const int nx,
const int ny,
const int nm)
```

Set fixed value  $(c_{hi})$  along left and bottom, zero-flux elsewhere.

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

Here is the call graph for this function:





## 4.1.2.2 apply\_initial\_conditions() void apply\_initial\_conditions (

```
fp_t ** conc_old,
const int nx,
const int ny,
const int nm )
```

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 14 of file serial\_boundaries.c.

Here is the caller graph for this function:

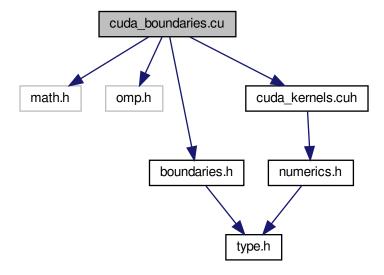


## 4.2 cuda\_boundaries.cu File Reference

Implementation of boundary condition functions with OpenMP threading.

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

Include dependency graph for cuda\_boundaries.cu:



#### **Functions**

- void apply\_initial\_conditions (fp\_t \*\*conc, const int nx, const int ny, const int nm)

  Initialize flat composition field with fixed boundary conditions.
- void boundary\_kernel (fp\_t \*d\_conc, const int nx, const int ny, const int nm) Enable double-precision floats.

## 4.2.1 Detailed Description

Implementation of boundary condition functions with OpenMP threading.

#### 4.2.2 Function Documentation

## 4.2.2.1 apply\_initial\_conditions() void apply\_initial\_conditions (

```
fp_t ** conc_old,
const int nx,
const int ny,
const int nm )
```

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 20 of file cuda\_boundaries.cu.

#### 4.2.2.2 boundary\_kernel() void boundary\_kernel (

```
fp_t * d_conc,
const int nx,
const int ny,
const int nm )
```

Enable double-precision floats.

Boundary condition kernel for execution on the GPU.

Boundary condition kernel for execution on the GPU

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

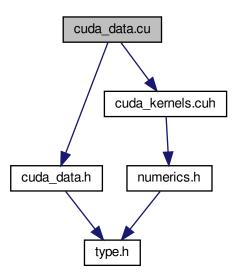
Definition at line 41 of file cuda\_boundaries.cu.



## 4.3 cuda\_data.cu File Reference

Implementation of functions to create and destroy CudaData struct.

```
#include "cuda_data.h"
#include "cuda_kernels.cuh"
Include dependency graph for cuda_data.cu:
```



## **Functions**

- void init\_cuda (fp\_t \*\*conc\_old, fp\_t \*\*mask\_lap, const int nx, const int ny, const int nm, struct CudaData \*dev)

  \*Initialize CUDA device memory before marching.
- void free\_cuda (struct CudaData \*dev)

Free CUDA device memory after marching.

## 4.3.1 Detailed Description

Implementation of functions to create and destroy CudaData struct.

## 4.3.2 Function Documentation

```
4.3.2.1 free_cuda() void free_cuda ( struct CudaData * dev )
```

Free CUDA device memory after marching.

Definition at line 33 of file cuda\_data.cu.

Here is the caller graph for this function:



Initialize CUDA device memory before marching.

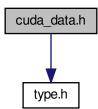
Definition at line 17 of file cuda\_data.cu.



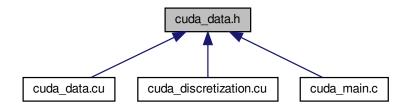
## 4.4 cuda\_data.h File Reference

Declaration of CUDA data container.

#include "type.h"
Include dependency graph for cuda\_data.h:



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



#### Classes

• struct CudaData

Container for pointers to arrays on the GPU.

## **Functions**

- void init\_cuda (fp\_t \*\*conc\_old, fp\_t \*\*mask\_lap, const int nx, const int ny, const int nm, struct CudaData \*dev)

  Initialize CUDA device memory before marching.
- void free\_cuda (struct CudaData \*dev)

Free CUDA device memory after marching.

- void device\_boundaries (fp\_t \*conc, const int nx, const int ny, const int nm, const int bx, const int by)

  Apply boundary conditions on device.
- void device\_convolution (fp\_t \*conc\_old, fp\_t \*conc\_lap, const int nx, const int ny, const int nm, const int bx, const int by)

Compute convolution on device.

• void device\_composition (fp\_t \*conc\_old, fp\_t \*conc\_new, fp\_t \*conc\_lap, const int nx, const int ny, const int nm, const int bx, const int by, const fp\_t D, const fp\_t dt)

Step diffusion equation on device.

void cuda\_diffusion\_solver (struct CudaData \*dev, fp\_t \*\*conc\_new, const int bx, const int by, const int nm, const int nx, const int ny, const fp\_t D, const fp\_t dt, struct Stopwatch \*sw)

Solve diffusion equation on the GPU.

void read\_out\_result (fp\_t \*\*conc, fp\_t \*d\_conc, const int nx, const int ny)

Read data from device.

#### 4.4.1 Detailed Description

Declaration of CUDA data container.

#### 4.4.2 Function Documentation

```
4.4.2.1 cuda_diffusion_solver() void cuda_diffusion_solver ( struct CudaData * dev,
```

```
fp_t ** conc_new,
const int bx,
const int by,
const int nm,
const int nx,
const int ny,
const fp_t D,
const fp_t dt,
struct Stopwatch * sw )
```

Solve diffusion equation on the GPU.

Solve diffusion equation on the GPU.

Compare cuda\_diffusion\_solver(): it accomplishes the same result, but without the memory allocation, data transfer, and array release. These are handled in cuda\_init(), with arrays on the host and device managed through CudaData, which is a struct passed by reference into the function. In this way, device kernels can be called in isolation without incurring the cost of data transfers and with reduced risk of memory leaks.

Definition at line 219 of file cuda discretization.cu.

Here is the call graph for this function:



Apply boundary conditions on device.

Definition at line 108 of file cuda\_discretization.cu.



```
const fp_t D,
const fp_t dt )
```

Step diffusion equation on device.

Definition at line 140 of file cuda\_discretization.cu.

Here is the caller graph for this function:



## 4.4.2.4 device\_convolution() void device\_convolution (

```
fp_t * conc_old,
fp_t * conc_lap,
const int nx,
const int ny,
const int nm,
const int bx,
const int by)
```

Compute convolution on device.

Definition at line 123 of file cuda\_discretization.cu.



```
4.4.2.5 free_cuda() void free_cuda ( struct CudaData * dev )
```

Free CUDA device memory after marching.

Definition at line 33 of file cuda\_data.cu.

Here is the caller graph for this function:



Initialize CUDA device memory before marching.

Definition at line 17 of file cuda\_data.cu.



Read data from device.

Definition at line 155 of file cuda\_discretization.cu.

Here is the caller graph for this function:

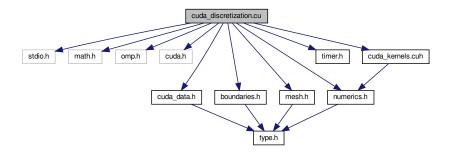


## 4.5 cuda\_discretization.cu File Reference

Implementation of boundary condition functions with CUDA acceleration.

```
#include <stdio.h>
#include <math.h>
#include <omp.h>
#include <cuda.h>
#include "cuda_data.h"
#include "boundaries.h"
#include "numerics.h"
#include "mesh.h"
#include "timer.h"
#include "cuda_kernels.cuh"
```

Include dependency graph for cuda\_discretization.cu:



#### **Functions**

void convolution\_kernel (fp\_t \*d\_conc\_old, fp\_t \*d\_conc\_lap, const int nx, const int ny, const int nm)

Tiled convolution algorithm for execution on the GPU.

void diffusion\_kernel (fp\_t \*d\_conc\_old, fp\_t \*d\_conc\_new, fp\_t \*d\_conc\_lap, const int nx, const int

Vector addition algorithm for execution on the GPU.

• void device\_boundaries (fp\_t \*conc, const int nx, const int ny, const int nm, const int bx, const int by)

Apply boundary conditions on device.

• void device\_convolution (fp\_t \*conc\_old, fp\_t \*conc\_lap, const int nx, const int ny, const int nm, const int bx, const int by)

Compute convolution on device.

• void device\_composition (fp\_t \*conc\_old, fp\_t \*conc\_new, fp\_t \*conc\_lap, const int nx, const int ny, const int nm, const int bx, const int by, const fp\_t D, const fp\_t dt)

Step diffusion equation on device.

void read\_out\_result (fp\_t \*\*conc, fp\_t \*d\_conc, const int nx, const int ny)

Read data from device.

void compute\_convolution (fp\_t \*\*conc\_old, fp\_t \*\*conc\_lap, fp\_t \*\*mask\_lap, const int bx, const int by, const int nm, const int nx, const int ny)

Reference showing how to invoke the convolution kernel.

• void cuda\_diffusion\_solver (struct CudaData \*dev, fp\_t \*\*conc\_new, const int bx, const int by, const int nm, const int nx, const int ny, const fp\_t D, const fp\_t dt, struct Stopwatch \*sw)

Reference optimized code for solving the diffusion equation.

#### **Variables**

• fp t d mask [5 \*5]

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

#### 4.5.1 Detailed Description

Implementation of boundary condition functions with CUDA acceleration.

#### 4.5.2 Function Documentation

#### 4.5.2.1 compute\_convolution() void compute\_convolution (

```
fp_t ** conc_old,
fp_t ** conc_lap,
fp_t ** mask_lap,
const int bx,
const int by,
const int nm,
const int nx,
const int ny)
```

Reference showing how to invoke the convolution kernel.

A stand-alone function like this incurs the cost of host-to-device data transfer each time it is called: it is a teaching tool, not reusable code. It is the basis for cuda\_diffusion\_solver(), which achieves much better performance by bundling CUDA kernels together and intelligently managing data transfers between the host (CPU) and device (GPU).

Definition at line 170 of file cuda\_discretization.cu.

#### 4.5.2.2 convolution\_kernel() void convolution\_kernel (

```
fp_t * conc_old,
fp_t * conc_lap,
const int nx,
const int ny,
const 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:

- 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 28 of file cuda\_discretization.cu.



# **4.5.2.3 cuda\_diffusion\_solver()** void cuda\_diffusion\_solver ( struct CudaData \* dev,

```
fp_t ** conc_new,
const int bx,
const int by,
const int nm,
const int nx,
const int ny,
const fp_t D,
const fp_t dt,
struct Stopwatch * sw )
```

Reference optimized code for solving the diffusion equation.

Solve diffusion equation on the GPU.

Compare cuda\_diffusion\_solver(): it accomplishes the same result, but without the memory allocation, data transfer, and array release. These are handled in cuda\_init(), with arrays on the host and device managed through CudaData, which is a struct passed by reference into the function. In this way, device kernels can be called in isolation without incurring the cost of data transfers and with reduced risk of memory leaks.

Definition at line 219 of file cuda discretization.cu.

Here is the call graph for this function:



# $\textbf{4.5.2.4} \quad \textbf{device\_boundaries()} \quad \texttt{void device\_boundaries} \quad ($

```
fp_t * conc,
const int nx,
const int ny,
const int nm,
const int bx,
const int by )
```

Apply boundary conditions on device.

Definition at line 108 of file cuda\_discretization.cu.

Here is the caller graph for this function:

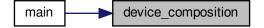


## 

Step diffusion equation on device.

Definition at line 140 of file cuda\_discretization.cu.

const fp\_t dt )



#### 4.5.2.6 device\_convolution() void device\_convolution (

```
fp_t * conc_old,
fp_t * conc_lap,
const int nx,
const int ny,
const int nm,
const int bx,
const int by)
```

Compute convolution on device.

Definition at line 123 of file cuda\_discretization.cu.

Here is the caller graph for this function:



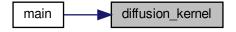
#### 4.5.2.7 diffusion\_kernel() void diffusion\_kernel (

```
fp_t * conc_old,
fp_t * conc_new,
fp_t * conc_lap,
const int nx,
const int ny,
const int nm,
const fp_t D,
const 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. Memory allocation, data transfer, and array release are handled in cuda\_init(), with arrays on the host and device managed through CudaData, which is a struct passed by reference into the function. In this way, device kernels can be called in isolation without incurring the cost of data transfers and with reduced risk of memory leaks.

Definition at line 85 of file cuda\_discretization.cu.



Read data from device.

Definition at line 155 of file cuda\_discretization.cu.

Here is the caller graph for this function:



#### 4.5.3 Variable Documentation

```
4.5.3.1 d_mask fp_t d_mask[5 * 5]
```

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

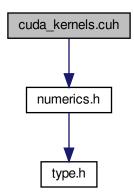
Definition at line 26 of file cuda\_discretization.cu.

# 4.6 cuda\_kernels.cuh File Reference

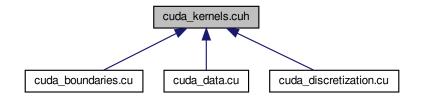
Declaration of functions to execute on the GPU (CUDA kernels)

```
#include "numerics.h"
```

Include dependency graph for cuda kernels.cuh:



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



#### **Functions**

- void boundary\_kernel (fp\_t \*conc, const int nx, const int ny, const int nm)
  - Boundary condition kernel for execution on the GPU.
- void convolution\_kernel (fp\_t \*conc\_old, fp\_t \*conc\_lap, const int nx, const int ny, const int nm)
  - Tiled convolution algorithm for execution on the GPU.
- void diffusion\_kernel (fp\_t \*conc\_old, fp\_t \*conc\_new, fp\_t \*conc\_lap, const int nx, const int ny, const int nm, const fp\_t D, const fp\_t dt)

Vector addition algorithm for execution on the GPU.

## **Variables**

• fp\_t d\_mask [5 \*5]

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

## 4.6.1 Detailed Description

Declaration of functions to execute on the GPU (CUDA kernels)

## 4.6.2 Function Documentation

# 

Boundary condition kernel for execution on the GPU.

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

Boundary condition kernel for execution on the GPU.

Boundary condition kernel for execution on the GPU

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

Definition at line 41 of file cuda\_boundaries.cu.



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 28 of file cuda discretization.cu.

Here is the caller graph for this function:



Vector addition algorithm for execution on the GPU.

This function accesses 1D data rather than the 2D array representation of the scalar composition field. Memory allocation, data transfer, and array release are handled in cuda\_init(), with arrays on the host and device managed through CudaData, which is a struct passed by reference into the function. In this way, device kernels can be called in isolation without incurring the cost of data transfers and with reduced risk of memory leaks.

Definition at line 85 of file cuda\_discretization.cu.

Here is the caller graph for this function:



#### 4.6.3 Variable Documentation

```
4.6.3.1 d_mask fp_t d_mask[5 * 5] [extern]
```

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

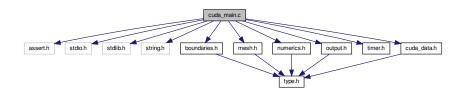
Definition at line 26 of file cuda\_discretization.cu.

## 4.7 cuda main.c File Reference

CUDA implementation of semi-infinite diffusion equation.

```
#include <assert.h>
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include "boundaries.h"
#include "mesh.h"
#include "numerics.h"
#include "output.h"
#include "timer.h"
#include "cuda_data.h"
```

Include dependency graph for cuda main.c:



## **Functions**

• int main (int argc, char \*argv[])

Run simulation using input parameters specified on the command line.

# 4.7.1 Detailed Description

CUDA implementation of semi-infinite diffusion equation.

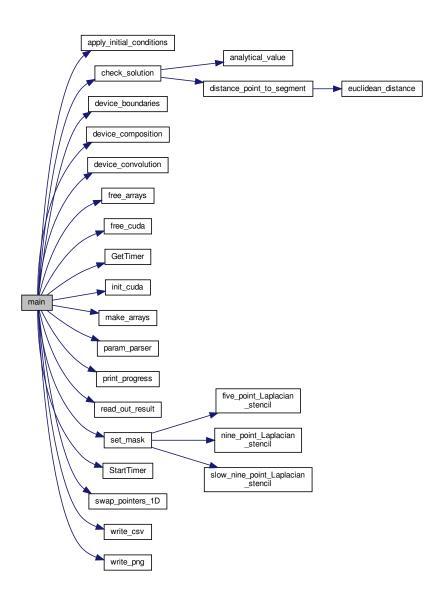
#### 4.7.2 Function Documentation

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

Run simulation using input parameters specified on the command line.

Definition at line 30 of file cuda\_main.c.

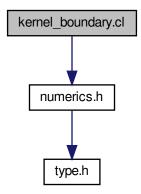
Here is the call graph for this function:



# 4.8 kernel\_boundary.cl File Reference

#include "numerics.h"

Include dependency graph for kernel\_boundary.cl:



#### **Functions**

• \_\_kernel void boundary\_kernel (\_\_global fp\_t \*d\_conc, const int nx, const int ny, const int nm)

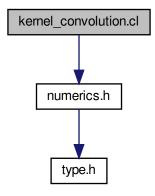
## 4.8.1 Function Documentation

Definition at line 24 of file kernel\_boundary.cl.

# 4.9 kernel\_convolution.cl File Reference

```
#include "numerics.h"
```

Include dependency graph for kernel\_convolution.cl:



#### **Functions**

```
    __kernel void convolution_kernel (__global fp_t *d_conc_old, __global fp_t *d_conc_lap, __constant fp_t *d_mask, __local fp_t *d_conc_tile, const int nx, const int ny, const int nm)
    __kernel void convolution_kernel (__global fp_t *d_conc_old, __global fp_t *d_conc_lap, __constant fp_t *d_mask, __local fp_t *d_conc_tile, const int nx, const int ny, const int nm)
```

#### 4.9.1 Function Documentation

Enable double-precision floats.

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.

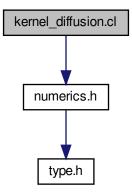
Note:

- The source matrix (d\_conc\_old) and destination matrix (d\_conc\_lap) must be identical in size
- · One OpenCL worker operates on one array index: there is no nested loop over matrix elements
- The halo (nm/2 perimeter cells) in d\_conc\_lap are unallocated garbage
- The same cells in *d\_conc\_old* are boundary values, and contribute to the convolution
- d\_conc\_tile is the shared tile of input data, accessible by all threads in this block
- The \_\_local specifier allocates the small d\_conc\_tile array in cache
- The \_\_constant specifier allocates the small d\_mask array in cache

Definition at line 37 of file kernel\_convolution.cl.

# 4.10 kernel\_diffusion.cl File Reference

#include "numerics.h"
Include dependency graph for kernel diffusion.cl:



#### **Functions**

\_\_kernel void diffusion\_kernel (\_\_global fp\_t \*d\_conc\_old, \_\_global fp\_t \*d\_conc\_new, \_\_global fp\_t \*d\_conc←
 \_lap, const int nx, const int ny, const int nm, const fp\_t D, const fp\_t dt)
 Enable double-precision floats.

#### 4.10.1 Function Documentation

# 4.10.1.1 diffusion\_kernel() \_\_kernel void diffusion\_kernel ( \_\_global fp\_t \* d\_conc\_old, \_\_global fp\_t \* d\_conc\_new, \_\_global fp\_t \* d\_conc\_lap, const int nx, const int ny, const int nm, const fp\_t D,

Enable double-precision floats.

Diffusion equation kernel for execution on the GPU

const fp\_t dt )

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

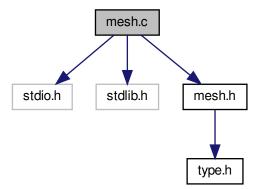
Definition at line 23 of file kernel\_diffusion.cl.

# 4.11 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, const int nx, const int ny, const 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 2D arrays.
```

void swap\_pointers\_1D (fp\_t \*\*conc\_old, fp\_t \*\*conc\_new)
 Swap pointers to data underlying 1D arrays.

## 4.11.1 Detailed Description

Implemenatation of mesh handling functions for diffusion benchmarks.

#### 4.11.2 Function Documentation

Free dynamically allocated memory.

Definition at line 44 of file mesh.c.

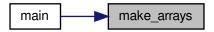


Allocate 2D arrays to store scalar composition values.

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 15 of file mesh.c.

Here is the caller graph for this function:



Swap pointers to 2D arrays.

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

Definition at line 59 of file mesh.c.



Swap pointers to data underlying 1D arrays.

Rather than copy data from  $fp_t* conc\_old[0]$  into  $fp_t* conc\_new[0]$ , an expensive operation, simply trade the top-most pointers. New becomes old, old becomes new, with no data lost and in almost no time.

Definition at line 68 of file mesh.c.

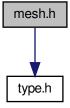
Here is the caller graph for this function:



# 4.12 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, const int nx, const int ny, const 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 2D arrays.
```

void swap\_pointers\_1D (fp\_t \*\*conc\_old, fp\_t \*\*conc\_new)
 Swap pointers to data underlying 1D arrays.

#### 4.12.1 Detailed Description

Declaration of mesh function prototypes for diffusion benchmarks.

#### 4.12.2 Function Documentation

Free dynamically allocated memory.

Definition at line 44 of file mesh.c.

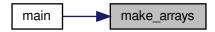


Allocate 2D arrays to store scalar composition values.

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 15 of file mesh.c.

Here is the caller graph for this function:



Swap pointers to 2D arrays.

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

Definition at line 59 of file mesh.c.



Swap pointers to data underlying 1D arrays.

Rather than copy data from  $fp_t* conc\_old[0]$  into  $fp_t* conc\_new[0]$ , an expensive operation, simply trade the top-most pointers. New becomes old, old becomes new, with no data lost and in almost no time.

Definition at line 68 of file mesh.c.

Here is the caller graph for this function:

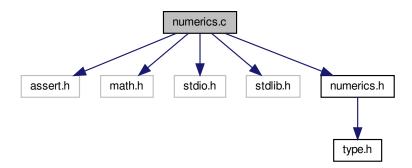


## 4.13 numerics.c File Reference

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**

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

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

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

Write 5-point Laplacian stencil into convolution mask.

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

Write 9-point Laplacian stencil into convolution mask.

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

Write 9-point Laplacian stencil into convolution mask.

• fp\_t euclidean\_distance (const fp\_t ax, const fp\_t ay, const fp\_t bx, const fp\_t by)

Compute Euclidean distance between two points, a and b.

• fp\_t manhattan\_distance (const fp\_t ax, const fp\_t ay, const fp\_t bx, const fp\_t by)

Compute Manhattan distance between two points, a and b.

fp\_t distance\_point\_to\_segment (const fp\_t ax, const fp\_t ay, const fp\_t bx, const fp\_t by, const fp\_t px, const fp\_t px, const fp\_t px

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

void analytical\_value (const fp\_t x, const fp\_t t, const fp\_t D, fp\_t \*c)

Analytical solution of the diffusion equation for a carburizing process.

void check\_solution (fp\_t \*\*conc\_new, fp\_t \*\*conc\_lap, const int nx, const int ny, const fp\_t dx, const fp\_t dx,

Compare numerical and analytical solutions of the diffusion equation.

#### 4.13.1 Detailed Description

Implementation of Laplacian operator and analytical solution functions.

#### 4.13.2 Function Documentation

# 

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  $c_{\infty}$  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 109 of file numerics.c.

Here is the caller graph for this function:



## 4.13.2.2 check\_solution() void check\_solution (

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

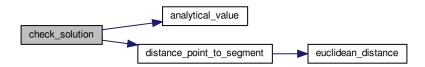
Compare numerical and analytical solutions of the diffusion equation.

#### 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 114 of file numerics.c.



Here is the caller graph for this function:



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 96 of file numerics.c.

Here is the call graph for this function:





Compute Euclidean distance between two points, a and b.

Definition at line 84 of file numerics.c.

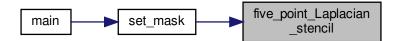
Here is the caller graph for this function:



Write 5-point Laplacian stencil into convolution mask.

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

Definition at line 37 of file numerics.c.



Compute Manhattan distance between two points, a and b.

Definition at line 90 of file numerics.c.

Write 9-point Laplacian stencil into convolution mask.

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

Definition at line 48 of file numerics.c.

Here is the caller graph for this function:



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

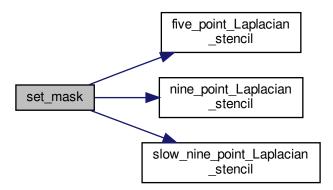
The mask corresponding to the numerical code will be applied. The suggested encoding is mask width as the ones digit and value count as the tens digit, *e.g.* 53 specifies five\_point\_Laplacian\_stencil(), while 93 specifies nine\_point\_Laplacian\_stencil().

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 17 of file numerics.c.

Here is the call graph for this function:



Here is the caller graph for this function:



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\_Laplacian\_stencil().

Definition at line 65 of file numerics.c.

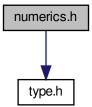
Here is the caller graph for this function:



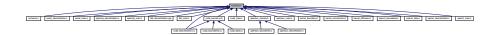
#### 4.14 numerics.h File Reference

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 (const fp\_t dx, const fp\_t dy, const int code, fp\_t \*\*mask\_lap, const int nm)

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

void five point Laplacian stencil (const fp t dx, const fp t dy, fp t \*\*mask lap, const int nm)

Write 5-point Laplacian stencil into convolution mask.

void nine point Laplacian stencil (const fp t dx, const fp t dy, fp t \*\*mask lap, const int nm)

Write 9-point Laplacian stencil into convolution mask.

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

Write 9-point Laplacian stencil into convolution mask.

void compute\_convolution (fp\_t \*\*const conc\_old, fp\_t \*\*conc\_lap, fp\_t \*\*const mask\_lap, const int nx, const int ny, const int nm)

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

void update\_composition (fp\_t \*\*conc\_old, fp\_t \*\*conc\_lap, fp\_t \*\*conc\_new, const int nx, const int nx, const int nm, const fp\_t D, const fp\_t dt)

Update composition field using explicit Euler discretization (forward-time centered space)

fp\_t euclidean\_distance (const fp\_t ax, const fp\_t ay, const fp\_t bx, const fp\_t by)

Compute Euclidean distance between two points, a and b.

fp\_t manhattan\_distance (const fp\_t ax, const fp\_t ay, const fp\_t bx, const fp\_t by)

Compute Manhattan distance between two points, a and b.

fp\_t distance\_point\_to\_segment (const fp\_t ax, const fp\_t ay, const fp\_t bx, const fp\_t bx, const fp\_t px, const fp\_t px, const fp\_t px

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

void analytical\_value (const fp\_t x, const fp\_t t, const fp\_t D, fp\_t \*c)

Analytical solution of the diffusion equation for a carburizing process.

void check\_solution (fp\_t \*\*conc\_new, fp\_t \*\*conc\_lap, const int nx, const int ny, const fp\_t dx, const fp\_t dx, const fp\_t dx, const fp\_t elapsed, const fp\_t D, fp\_t \*rss)

Compare numerical and analytical solutions of the diffusion equation.

#### 4.14.1 Detailed Description

Declaration of Laplacian operator and analytical solution functions.

## 4.14.2 Macro Definition Documentation

## 4.14.2.1 MAX\_MASK\_H #define MAX\_MASK\_H 5

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

Definition at line 26 of file numerics.h.

## 4.14.2.2 MAX\_MASK\_W #define MAX\_MASK\_W 5

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

Definition at line 21 of file numerics.h.

#### 4.14.3 Function Documentation

## 4.14.3.1 analytical\_value() void analytical\_value (

```
const fp_t x,
const fp_t t,
const fp_t D,
fp_t * c )
```

Analytical solution of the diffusion equation for a carburizing process.

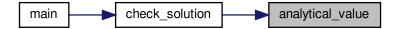
For 1D diffusion through a semi-infinite domain with initial and far-field composition  $c_{\infty}$  and boundary value  $c(x=0,t)=c_0$  with constant diffusivity D, the solution to Fick's second law is

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

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 109 of file numerics.c.



## 4.14.3.2 check\_solution() void check\_solution (

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

Compare numerical and analytical solutions of the diffusion equation.

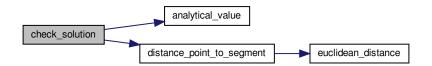
#### Returns

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 114 of file numerics.c.

Here is the call graph for this function:





# 4.14.3.3 compute\_convolution() void compute\_convolution (

```
fp_t **const conc_old,
fp_t ** conc_lap,
fp_t **const mask_lap,
const int nx,
const int ny,
const 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 17 of file serial\_discretization.c.

Here is the caller graph for this function:



#### 4.14.3.4 distance\_point\_to\_segment() fp\_t distance\_point\_to\_segment (

```
const fp_t ax,
const fp_t ay,
const fp_t bx,
const fp_t by,
const fp_t px,
const 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 96 of file numerics.c.



Here is the caller graph for this function:



Compute Euclidean distance between two points, a and b.

Definition at line 84 of file numerics.c.

Here is the caller graph for this function:

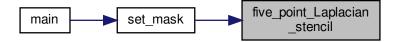


Write 5-point Laplacian stencil into convolution mask.

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

Definition at line 37 of file numerics.c.

Here is the caller graph for this function:



Compute Manhattan distance between two points, a and b.

Definition at line 90 of file numerics.c.

Write 9-point Laplacian stencil into convolution mask.

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

Definition at line 48 of file numerics.c.



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

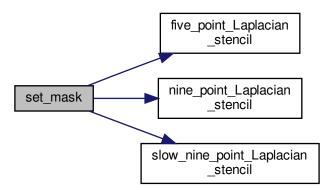
The mask corresponding to the numerical code will be applied. The suggested encoding is mask width as the ones digit and value count as the tens digit, *e.g.* 53 specifies five\_point\_Laplacian\_stencil(), while 93 specifies nine\_point\_Laplacian\_stencil().

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 17 of file numerics.c.

Here is the call graph for this function:





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\_Laplacian\_stencil().

Definition at line 65 of file numerics.c.

Here is the caller graph for this function:



Update composition field using explicit Euler discretization (forward-time centered space)

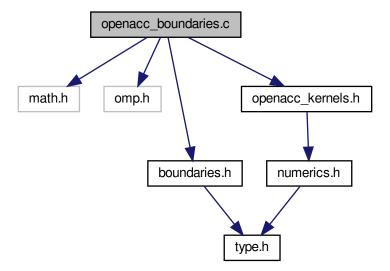
Definition at line 33 of file serial\_discretization.c.



# 4.15 openacc\_boundaries.c File Reference

Implementation of boundary condition functions with OpenMP threading.

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



## **Functions**

- void apply\_initial\_conditions (fp\_t \*\*conc, const int nx, const int ny, const int nm)

  Initialize flat composition field with fixed boundary conditions.
- void boundary\_kernel (fp\_t \*\*\_\_restrict\_\_ conc, const int nx, const int ny, const int nm)
- void apply\_boundary\_conditions (fp\_t \*\*conc, const int nx, const int ny, const int nm) Set fixed value  $(c_{hi})$  along left and bottom, zero-flux elsewhere.

## 4.15.1 Detailed Description

Implementation of boundary condition functions with OpenMP threading.

#### 4.15.2 Function Documentation

# $\textbf{4.15.2.1} \quad \textbf{apply\_boundary\_conditions()} \quad \texttt{void apply\_boundary\_conditions} \quad ($

```
fp_t ** conc,
const int nx,
const int ny,
const int nm )
```

Set fixed value  $\left(c_{hi}\right)$  along left and bottom, zero-flux elsewhere.

Definition at line 90 of file openacc\_boundaries.c.

Here is the call graph for this function:



Here is the caller graph for this function:

```
main apply_boundary_conditions
```

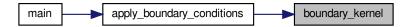
Initialize flat composition field with fixed boundary conditions.

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 16 of file openacc\_boundaries.c.

Definition at line 37 of file openacc boundaries.c.

Here is the caller graph for this function:

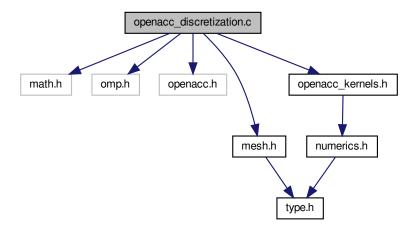


# 4.16 openacc\_discretization.c File Reference

Implementation of boundary condition functions with OpenACC threading.

```
#include <math.h>
#include <omp.h>
#include <openacc.h>
#include "mesh.h"
#include "openacc_kernels.h"
```

Include dependency graph for openacc\_discretization.c:



#### **Functions**

void convolution\_kernel (fp\_t \*\*conc\_old, fp\_t \*\*conc\_lap, fp\_t \*\*mask\_lap, const int nx, const int ny, const int nm)

Tiled convolution algorithm for execution on the GPU.

void diffusion\_kernel (fp\_t \*\*conc\_old, fp\_t \*\*conc\_new, fp\_t \*\*conc\_lap, const int nx, const int ny, const int nm, const fp\_t D, const fp\_t dt)

Vector addition algorithm for execution on the GPU.

#### 4.16.1 Detailed Description

Implementation of boundary condition functions with OpenACC threading.

#### 4.16.2 Function Documentation

Tiled convolution algorithm for execution on the GPU.

Definition at line 17 of file openacc discretization.c.

Vector addition algorithm for execution on the GPU.

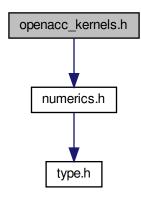
Definition at line 41 of file openacc\_discretization.c.

# 4.17 openacc\_kernels.h File Reference

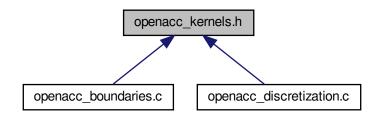
Declaration of functions to execute on the GPU (OpenACC kernels)

#include "numerics.h"

Include dependency graph for openacc\_kernels.h:



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



#### **Functions**

- void boundary\_kernel (fp\_t \*\*conc, const int nx, const int ny, const int nm)

  Boundary condition kernel for execution on the GPU.
- void convolution\_kernel (fp\_t \*\*conc\_old, fp\_t \*\*conc\_lap, fp\_t \*\*mask\_lap, const int nx, const int ny, const int nm)

Tiled convolution algorithm for execution on the GPU.

• void diffusion\_kernel (fp\_t \*\*conc\_old, fp\_t \*\*conc\_new, fp\_t \*\*conc\_lap, const int nx, const int ny, const int nm, const fp\_t D, const fp\_t dt)

Vector addition algorithm for execution on the GPU.

## 4.17.1 Detailed Description

Declaration of functions to execute on the GPU (OpenACC kernels)

## 4.17.2 Function Documentation

Boundary condition kernel for execution on the GPU.

```
4.17.2.2 convolution_kernel() void convolution_kernel (
    fp_t ** conc_old,
    fp_t ** conc_lap,
    fp_t ** mask_lap,
    const int nx,
    const int ny,
    const int nm )
```

Tiled convolution algorithm for execution on the GPU.

Definition at line 17 of file openacc\_discretization.c.

Vector addition algorithm for execution on the GPU.

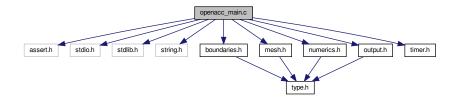
Definition at line 41 of file openacc\_discretization.c.

# 4.18 openacc\_main.c File Reference

OpenACC implementation of semi-infinite diffusion equation.

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

Include dependency graph for openacc\_main.c:



## **Functions**

• int main (int argc, char \*argv[])

Run simulation using input parameters specified on the command line.

## 4.18.1 Detailed Description

OpenACC implementation of semi-infinite diffusion equation.

#### 4.18.2 Function Documentation

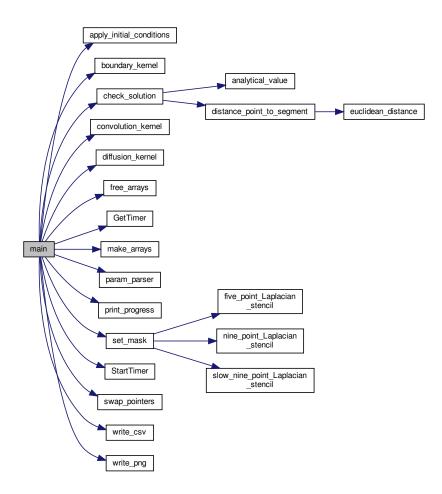
```
4.18.2.1 main() int main ( int argc, char * argv[])
```

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 33 of file openacc\_main.c.

Here is the call graph for this function:

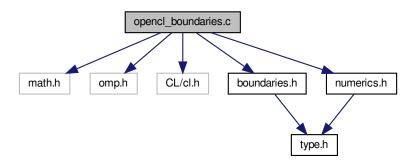


# 4.19 opencl boundaries.c File Reference

Implementation of boundary condition functions with OpenCL acceleration.

```
#include <math.h>
#include <omp.h>
#include <CL/cl.h>
#include "boundaries.h"
#include "numerics.h"
```

Include dependency graph for opencl\_boundaries.c:



#### **Functions**

void apply\_initial\_conditions (fp\_t \*\*conc, const int nx, const int ny, const int nm)
 Initialize flat composition field with fixed boundary conditions.

## 4.19.1 Detailed Description

Implementation of boundary condition functions with OpenCL acceleration.

## 4.19.2 Function Documentation

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 17 of file opencl\_boundaries.c.

Here is the caller graph for this function:

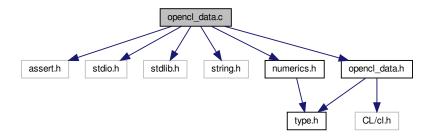


## 4.20 opencl\_data.c File Reference

Implementation of functions to create and destroy OpenCLData struct.

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

Include dependency graph for opencl\_data.c:



## **Functions**

- void report\_error (cl\_int status, const char \*message)
  - Report error code when status is not CL\_SUCCESS.
- void init\_opencl (fp\_t \*\*conc\_old, fp\_t \*\*mask\_lap, const int nx, const int ny, const int nm, struct OpenCLData \*dev)

Initialize OpenCL device memory before marching.

void build\_program (const char \*filename, cl\_context \*context, cl\_device\_id \*gpu, cl\_program \*program, cl\_int \*status)

Build kernel program from text input.

void free\_opencl (struct OpenCLData \*dev)

Free OpenCL device memory after marching.

### 4.20.1 Detailed Description

Implementation of functions to create and destroy OpenCLData struct.

#### 4.20.2 Function Documentation

Build kernel program from text input.

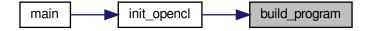
Source follows the OpenCL Programming Book, https://www.fixstars.com/en/opencl/book/Open←CLProgrammingBook/calling-the-kernel/

Definition at line 137 of file opencl\_data.c.

Here is the call graph for this function:



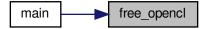
Here is the caller graph for this function:



Free OpenCL device memory after marching.

Definition at line 211 of file opencl\_data.c.

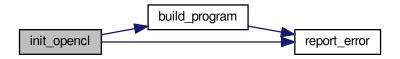
Here is the caller graph for this function:



Initialize OpenCL device memory before marching.

Definition at line 37 of file opencl\_data.c.

Here is the call graph for this function:



Here is the caller graph for this function:

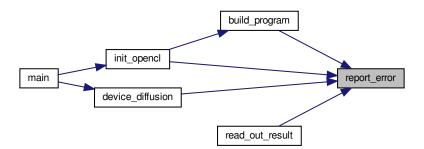


Report error code when status is not CL\_SUCCESS.

Refer to https://streamhpc.com/blog/2013-04-28/opencl-error-codes/ for help interpreting error codes.

Definition at line 18 of file opencl\_data.c.

Here is the caller graph for this function:

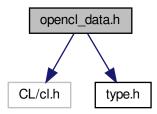


### 4.21 opencl\_data.h File Reference

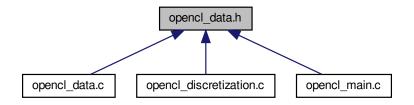
Declaration of OpenCL data container.

```
#include <CL/cl.h>
#include "type.h"
```

Include dependency graph for opencl\_data.h:



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



#### **Classes**

struct OpenCLData

Container for GPU array pointers and parameters.

#### **Functions**

• void report\_error (cl\_int error, const char \*message)

Report error code when status is not CL\_SUCCESS.

• void build\_program (const char \*filename, cl\_context \*context, cl\_device\_id \*gpu, cl\_program \*program, cl\_int \*status)

Build kernel program from text input.

void init\_opencl (fp\_t \*\*conc\_old, fp\_t \*\*mask\_lap, const int nx, const int ny, const int nm, struct OpenCLData \*dev)

Initialize OpenCL device memory before marching.

• void device\_boundaries (struct OpenCLData \*dev, const int flip, const int nx, const int ny, const int nm, const int bx, const int by)

Apply boundary conditions on OpenCL device.

void device\_convolution (struct OpenCLData \*dev, const int flip, const int nx, const int ny, const int nm, const int bx, const int by)

Compute convolution on OpenCL device.

• void device\_diffusion (struct OpenCLData \*dev, const int flip, const int nx, const int ny, const int nm, const int bx, const int by, const fp\_t D, const fp\_t dt)

Solve diffusion equation on OpenCL device.

- void read\_out\_result (struct OpenCLData \*dev, const int flip, fp\_t \*\*conc\_new, const int nx, const int ny)
   Copy data out of OpenCL device.
- void free\_opencl (struct OpenCLData \*dev)

Free OpenCL device memory after marching.

#### 4.21.1 Detailed Description

Declaration of OpenCL data container.

#### 4.21.2 Function Documentation

Build kernel program from text input.

Source follows the OpenCL Programming Book, https://www.fixstars.com/en/opencl/book/Open←CLProgrammingBook/calling-the-kernel/

Definition at line 137 of file opencl\_data.c.

Here is the call graph for this function:



Here is the caller graph for this function:



Apply boundary conditions on OpenCL device.

Definition at line 27 of file opencl\_discretization.c.

Compute convolution on OpenCL device.

Definition at line 54 of file opencl\_discretization.c.

### 

Solve diffusion equation on OpenCL device.

const int by,
const fp\_t D,
const fp\_t dt )

Definition at line 83 of file opencl\_discretization.c.

Here is the call graph for this function:



Here is the caller graph for this function:



Free OpenCL device memory after marching.

Definition at line 211 of file opencl\_data.c.

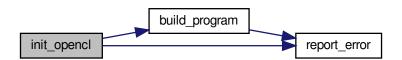
Here is the caller graph for this function:



Initialize OpenCL device memory before marching.

Definition at line 37 of file opencl\_data.c.

Here is the call graph for this function:



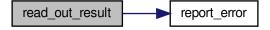
Here is the caller graph for this function:



Copy data out of OpenCL device.

Definition at line 114 of file opencl\_discretization.c.

Here is the call graph for this function:

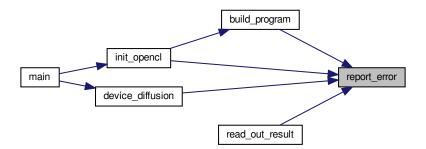


Report error code when status is not CL\_SUCCESS.

Refer to https://streamhpc.com/blog/2013-04-28/opencl-error-codes/ for help interpreting error codes.

Definition at line 18 of file opencl\_data.c.

Here is the caller graph for this function:

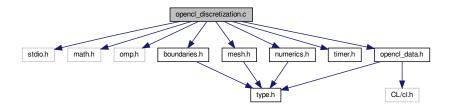


### 4.22 opencl\_discretization.c File Reference

Implementation of boundary condition functions with OpenCL acceleration.

```
#include <stdio.h>
#include <math.h>
#include <omp.h>
#include "boundaries.h"
#include "mesh.h"
#include "numerics.h"
#include "timer.h"
#include "opencl_data.h"
```

Include dependency graph for opencl\_discretization.c:



#### **Functions**

• void device\_boundaries (struct OpenCLData \*dev, const int flip, const int nx, const int ny, const int nm, const int bx, const int by)

Apply boundary conditions on OpenCL device.

• void device\_convolution (struct OpenCLData \*dev, const int flip, const int nx, const int ny, const int nm, const int bx, const int by)

Compute convolution on OpenCL device.

• void device\_diffusion (struct OpenCLData \*dev, const int flip, const int nx, const int ny, const int nm, const int bx, const int by, const fp\_t D, const fp\_t dt)

Solve diffusion equation on OpenCL device.

void read\_out\_result (struct OpenCLData \*dev, const int flip, fp\_t \*\*conc, const int nx, const int ny)
 Copy data out of OpenCL device.

### 4.22.1 Detailed Description

Implementation of boundary condition functions with OpenCL acceleration.

### 4.22.2 Function Documentation

# **4.22.2.1 device\_boundaries()** void device\_boundaries ( struct OpenCLData \* dev,

```
const int flip,
const int nx,
const int ny,
const int nm,
const int bx,
const int by)
```

Apply boundary conditions on OpenCL device.

Definition at line 27 of file opencl\_discretization.c.

### 4.22.2.2 device\_convolution() void device\_convolution (

```
struct OpenCLData * dev,
const int flip,
const int nx,
const int ny,
const int nm,
const int bx,
const int by)
```

Compute convolution on OpenCL device.

Definition at line 54 of file opencl\_discretization.c.

#### 4.22.2.3 device\_diffusion() void device\_diffusion (

```
struct OpenCLData * dev,
const int flip,
const int nx,
const int ny,
const int nm,
const int bx,
const int by,
const fp_t D,
const fp_t dt )
```

Solve diffusion equation on OpenCL device.

Definition at line 83 of file opencl\_discretization.c.

Here is the call graph for this function:



Here is the caller graph for this function:



Copy data out of OpenCL device.

Definition at line 114 of file opencl\_discretization.c.

Here is the call graph for this function:

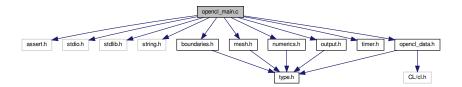


### 4.23 opencl\_main.c File Reference

OpenCL implementation of semi-infinite diffusion equation.

```
#include <assert.h>
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include "boundaries.h"
#include "mesh.h"
#include "numerics.h"
#include "output.h"
```

```
#include "timer.h"
#include "opencl_data.h"
Include dependency graph for opencl_main.c:
```



### **Functions**

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

Run simulation using input parameters specified on the command line.

### 4.23.1 Detailed Description

OpenCL implementation of semi-infinite diffusion equation.

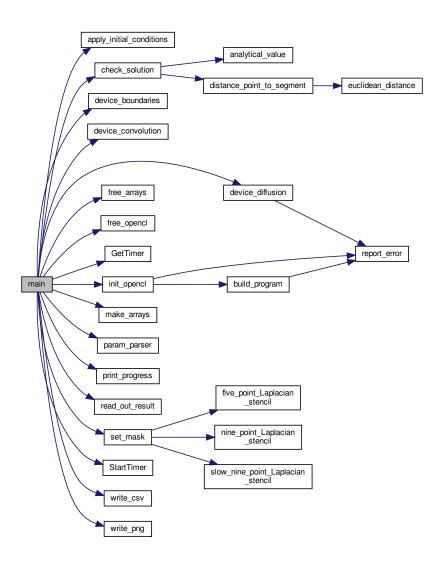
### 4.23.2 Function Documentation

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

Run simulation using input parameters specified on the command line.

Definition at line 30 of file opencl\_main.c.

Here is the call graph for this function:

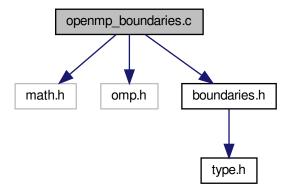


### 4.24 openmp\_boundaries.c File Reference

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 apply\_initial\_conditions (fp\_t \*\*conc, const int nx, const int ny, const int nm)

  Initialize flat composition field with fixed boundary conditions.
- void apply\_boundary\_conditions (fp\_t \*\*conc, const int nx, const int ny, const int nm) Set fixed value  $(c_{hi})$  along left and bottom, zero-flux elsewhere.

### 4.24.1 Detailed Description

Implementation of boundary condition functions with OpenMP threading.

### 4.24.2 Function Documentation

Set fixed value  $(c_{hi})$  along left and bottom, zero-flux elsewhere.

Definition at line 36 of file openmp boundaries.c.

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.

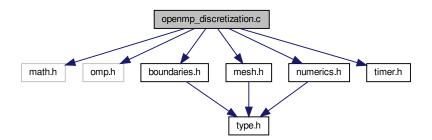
Definition at line 15 of file openmp\_boundaries.c.

### 4.25 openmp\_discretization.c File Reference

Implementation of boundary condition functions with OpenMP threading.

```
#include <math.h>
#include <omp.h>
#include "boundaries.h"
#include "mesh.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, const int nx, const int nx, const int nm, const int nm)

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

void update\_composition (fp\_t \*\*conc\_old, fp\_t \*\*conc\_lap, fp\_t \*\*conc\_new, const int nx, const int n

Update composition field using explicit Euler discretization (forward-time centered space)

### 4.25.1 Detailed Description

Implementation of boundary condition functions with OpenMP threading.

### 4.25.2 Function Documentation

### 

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 18 of file openmp discretization.c.

### 4.25.2.2 update\_composition() void update\_composition (

```
fp_t ** conc_old,
fp_t ** conc_lap,
fp_t ** conc_new,
const int nx,
const int ny,
const int nm,
const fp_t D,
const fp_t dt )
```

Update composition field using explicit Euler discretization (forward-time centered space)

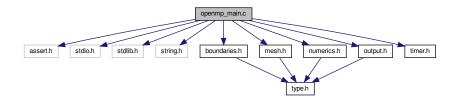
Definition at line 38 of file openmp discretization.c.

### 4.26 openmp\_main.c File Reference

OpenMP implementation of semi-infinite diffusion equation.

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

Include dependency graph for openmp\_main.c:



### **Functions**

• int main (int argc, char \*argv[])

Run simulation using input parameters specified on the command line.

### 4.26.1 Detailed Description

OpenMP implementation of semi-infinite diffusion equation.

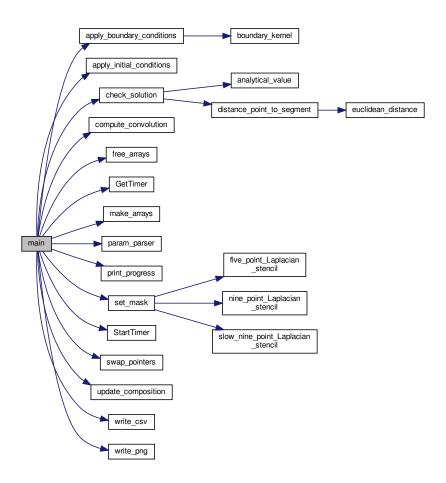
#### 4.26.2 Function Documentation

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

Run simulation using input parameters specified on the command line.

Definition at line 25 of file openmp\_main.c.

Here is the call graph for this function:

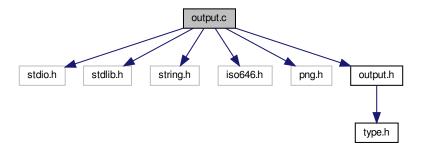


### 4.27 output.c File Reference

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 \*bx, int \*by, int \*checks, int \*code, fp\_t \*D, fp\_t \*dx, fp\_t \*dy, fp\_t \*linStab, int \*nm, int \*nx, int \*ny, int \*steps)

Read parameters from file specified on the command line.

- 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, const int nx, const int ny, const fp t dx, const fp t dy, const int step)

Writes scalar composition field to diffusion.??????csv.

• void write\_png (fp\_t \*\*conc, const int nx, const int ny, const int step)

Writes scalar composition field to diffusion. ???????.png.

### 4.27.1 Detailed Description

Implementation of file output functions for diffusion benchmarks.

### 4.27.2 Function Documentation

#### 4.27.2.1 param\_parser() void param\_parser (

```
int argc,
char * argv[],
int * bx,
int * by,
int * checks,
int * code,
fp_t * D,
```

```
fp_t * dx,
fp_t * dy,
fp_t * linStab,
int * nm,
int * nx,
int * ny,
int * steps )
```

Read parameters from file specified on the command line.

Definition at line 18 of file output.c.

Here is the caller graph for this function:



```
4.27.2.2 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++)  $\{$ 

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

Definition at line 124 of file output.c.

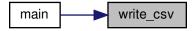
Here is the caller graph for this function:



Writes scalar composition field to diffusion.??????csv.

Definition at line 148 of file output.c.

Here is the caller graph for this function:



Writes scalar composition field to diffusion.??????ng.

Definition at line 181 of file output.c.

Here is the caller graph for this function:

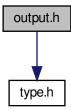


### 4.28 output.h File Reference

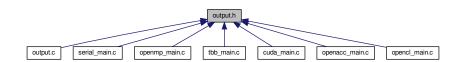
Declaration of output function prototypes for diffusion benchmarks.

#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 \*bx, int \*by, int \*checks, int \*code, fp\_t \*D, fp\_t \*dx, fp\_t \*dy, fp\_t \*linStab, int \*nm, int \*nx, int \*ny, int \*steps)

Read parameters from file specified on the command line.

void print\_progress (const int step, const int steps)

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

 $\bullet \ \ \text{void write\_csv} \ (\text{fp\_t} \ **conc, \ const \ int \ nx, \ const \ int \ ny, \ const \ fp\_t \ dx, \ const \ fp\_t \ dy, \ const \ int \ step)\\$ 

Writes scalar composition field to diffusion.??????csv.

• void write\_png (fp\_t \*\*conc, const int nx, const int ny, const int step)

Writes scalar composition field to diffusion.???????.png.

### 4.28.1 Detailed Description

Declaration of output function prototypes for diffusion benchmarks.

### 4.28.2 Function Documentation

Read parameters from file specified on the command line.

Definition at line 18 of file output.c.

Here is the caller graph for this function:



```
4.28.2.2 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;
}</pre>
```

Definition at line 124 of file output.c.

Here is the caller graph for this function:



Writes scalar composition field to diffusion.??????csv.

Definition at line 148 of file output.c.

Here is the caller graph for this function:



Writes scalar composition field to diffusion.??????ng.

Definition at line 181 of file output.c.

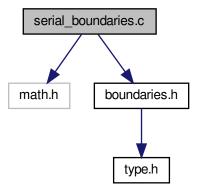
Here is the caller graph for this function:



### 4.29 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 apply\_initial\_conditions (fp\_t \*\*conc, const int nx, const int ny, const int nm)

  Initialize flat composition field with fixed boundary conditions.
- void apply\_boundary\_conditions (fp\_t \*\*conc, const int nx, const int ny, const int nm) Set fixed value  $(c_{hi})$  along left and bottom, zero-flux elsewhere.

### 4.29.1 Detailed Description

Implementation of boundary condition functions without threading.

#### 4.29.2 Function Documentation

Set fixed value  $(c_{hi})$  along left and bottom, zero-flux elsewhere.

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

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 14 of file serial boundaries.c.

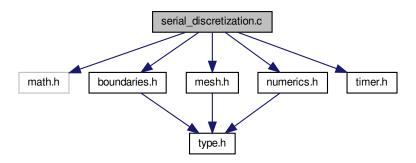
### 4.30 serial\_discretization.c File Reference

Implementation of boundary condition functions without threading.

```
#include <math.h>
#include "boundaries.h"
#include "mesh.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, const int nx, const int ny, const int nm)

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

void update\_composition (fp\_t \*\*conc\_old, fp\_t \*\*conc\_lap, fp\_t \*\*conc\_new, const int nx, const int n

Update composition field using explicit Euler discretization (forward-time centered space)

#### 4.30.1 Detailed Description

Implementation of boundary condition functions without threading.

### 4.30.2 Function Documentation

### 

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 17 of file serial discretization.c.

const int nm )

#### 4.30.2.2 update\_composition() void update\_composition (

```
fp_t ** conc_old,
fp_t ** conc_lap,
fp_t ** conc_new,
const int nx,
const int nm,
const int p,
const fp_t D,
const fp_t dt )
```

Update composition field using explicit Euler discretization (forward-time centered space)

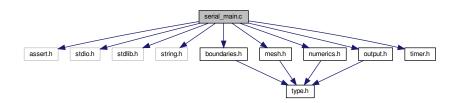
Definition at line 33 of file serial\_discretization.c.

### 4.31 serial main.c File Reference

Serial implementation of semi-infinite diffusion equation.

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

Include dependency graph for serial\_main.c:



#### **Functions**

• int main (int argc, char \*argv[])

Run simulation using input parameters specified on the command line.

### 4.31.1 Detailed Description

Serial implementation of semi-infinite diffusion equation.

#### 4.31.2 Function Documentation

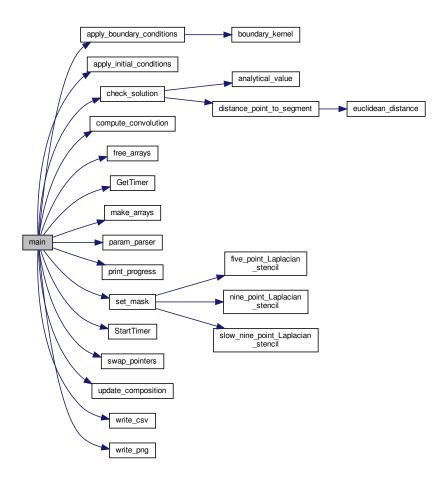
```
4.31.2.1 main() int main ( int argc, char * argv[])
```

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 33 of file serial\_main.c.

Here is the call graph for this function:

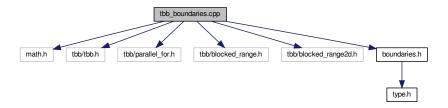


### 4.32 tbb\_boundaries.cpp File Reference

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 apply\_initial\_conditions (fp\_t \*\*conc, const int nx, const int ny, const int nm)

  Initialize flat composition field with fixed boundary conditions.
- void apply\_boundary\_conditions (fp\_t \*\*conc, const int nx, const int ny, const int nm) Set fixed value  $(c_{hi})$  along left and bottom, zero-flux elsewhere.

#### 4.32.1 Detailed Description

Implementation of boundary condition functions with TBB threading.

#### 4.32.2 Function Documentation

Set fixed value  $(c_{hi})$  along left and bottom, zero-flux elsewhere.

Definition at line 54 of file tbb boundaries.cpp.

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 18 of file tbb\_boundaries.cpp.

### 4.33 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 "mesh.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, const int nx, const int nx, const int nm)

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

void update\_composition (fp\_t \*\*conc\_old, fp\_t \*\*conc\_lap, fp\_t \*\*conc\_new, const int nx, const int nx, const int nm, const fp\_t D, const fp\_t dt)

Update composition field using explicit Euler discretization (forward-time centered space)

• void check\_solution\_lambda (fp\_t \*\*conc\_new, fp\_t \*\*conc\_lap, const int nx, const int ny, const fp\_t dx, const fp\_t dy, const int nm, const fp\_t elapsed, const fp\_t D, fp\_t \*rss)

### 4.33.1 Detailed Description

Implementation of boundary condition functions with TBB threading.

#### 4.33.2 Function Documentation

Definition at line 59 of file tbb\_discretization.cpp.

const fp\_t D,
fp\_t \* rss )

Here is the caller graph for this function:

```
main _____ check_solution_lambda
```

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 22 of file tbb\_discretization.cpp.

Here is the caller graph for this function:



### 4.33.2.3 update\_composition() void update\_composition (

```
fp_t ** conc_old,
fp_t ** conc_lap,
fp_t ** conc_new,
const int nx,
const int ny,
const int nm,
const fp_t D,
const fp_t dt )
```

Update composition field using explicit Euler discretization (forward-time centered space)

Definition at line 43 of file tbb\_discretization.cpp.

Here is the caller graph for this function:



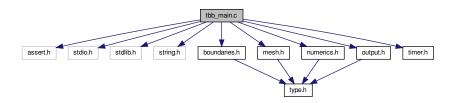
### 4.34 tbb\_main.c File Reference

Threading Building Blocks implementation of semi-infinite diffusion equation.

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

```
#include <string.h>
#include "boundaries.h"
#include "mesh.h"
#include "numerics.h"
#include "output.h"
#include "timer.h"
```

Include dependency graph for tbb\_main.c:



#### **Functions**

- void check\_solution\_lambda (fp\_t \*\*conc\_new, fp\_t \*\*conc\_lap, const int nx, const int nx, const int nx, const fp\_t dx, const fp\_t dy, const int nm, const fp\_t elapsed, const fp\_t D, fp\_t \*rss)
- int main (int argc, char \*argv[])

Run simulation using input parameters specified on the command line.

#### 4.34.1 Detailed Description

Threading Building Blocks implementation of semi-infinite diffusion equation.

#### 4.34.2 Function Documentation

#### 4.34.2.1 check\_solution\_lambda() void check\_solution\_lambda (

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

Definition at line 59 of file tbb\_discretization.cpp.

Here is the caller graph for this function:



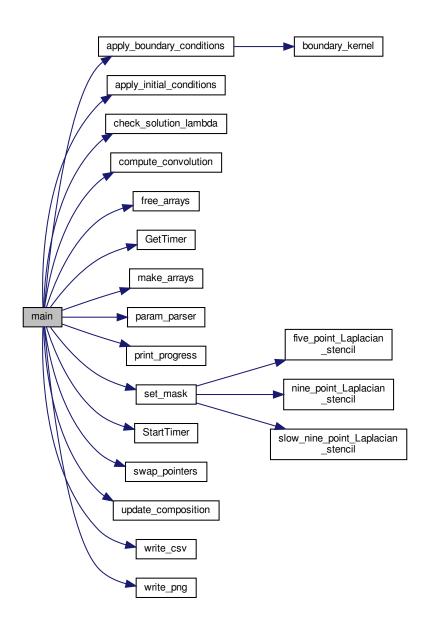
```
4.34.2.2 main() int main ( int argc, char * argv[] )
```

Run simulation using input parameters specified on the command line.

Definition at line 29 of file tbb\_main.c.

4.35 timer.c File Reference 105

Here is the call graph for this function:



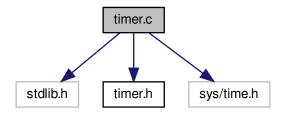
### 4.35 timer.c File Reference

High-resolution cross-platform machine time reader.

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

#include <sys/time.h>

Include dependency graph for timer.c:



### **Macros**

- #define \_\_USE\_BSD
- #define \_\_USE\_MISC

#### **Functions**

void StartTimer ()

Set CPU frequency and begin timing.

• double GetTimer ()

Return elapsed time in seconds.

### **Variables**

· struct timeval timerStart

### 4.35.1 Detailed Description

High-resolution cross-platform machine time reader.

Author

**NVIDIA** 

### 4.35.2 Macro Definition Documentation

4.35 timer.c File Reference 107

### 4.35.2.1 \_\_USE\_BSD #define \_\_USE\_BSD

Definition at line 37 of file timer.c.

### 4.35.2.2 \_\_USE\_MISC #define \_\_USE\_MISC

Definition at line 40 of file timer.c.

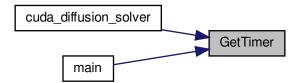
#### 4.35.3 Function Documentation

### 4.35.3.1 GetTimer() double GetTimer ( )

Return elapsed time in seconds.

Definition at line 71 of file timer.c.

Here is the caller graph for this function:



### 4.35.3.2 StartTimer() void StartTimer ( )

Set CPU frequency and begin timing.

Definition at line 55 of file timer.c.

Here is the caller graph for this function:



### 4.35.4 Variable Documentation

### 4.35.4.1 timerStart struct timeval timerStart

Platform-dependent data type of hardware time value

Definition at line 1 of file timer.c.

#### 4.36 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.

### 4.36.1 Detailed Description

Declaration of timer function prototypes for diffusion benchmarks.

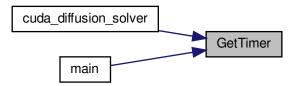
### 4.36.2 Function Documentation

### 4.36.2.1 GetTimer() double GetTimer ( )

Return elapsed time in seconds.

Definition at line 71 of file timer.c.

Here is the caller graph for this function:



### 4.36.2.2 StartTimer() void StartTimer ()

Set CPU frequency and begin timing.

Definition at line 55 of file timer.c.

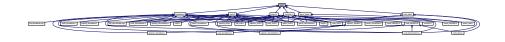
Here is the caller graph for this function:



### 4.37 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

### 4.37.1 Detailed Description

Definition of scalar data type and Doxygen diffusion group.

### 4.37.2 Typedef Documentation

### $\textbf{4.37.2.1} \quad \textbf{fp\_t} \quad \texttt{typedef double fp\_t}$

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 22 of file type.h.

## Index

USE_BSD	tbb_discretization.cpp, 101
timer.c, 106	conc_lap
USE_MISC	CudaData, 4
timer.c, 107	OpenCLData, 6
	conc_new
analytical_value	CudaData, 4
numerics.c, 44	OpenCLData, 6
numerics.h, 52	conc_old
apply_boundary_conditions	CudaData, 4
boundaries.h, 10	OpenCLData, 6
openacc_boundaries.c, 59	context
openmp_boundaries.c, 83	OpenCLData, 6
serial_boundaries.c, 95	conv
tbb_boundaries.cpp, 99	Stopwatch, 8
apply_initial_conditions	convolution kernel
boundaries.h, 10	cuda_discretization.cu, 23
cuda_boundaries.cu, 12	cuda_kernels.cuh, 29
openacc_boundaries.c, 60	kernel_convolution.cl, 35
opencl_boundaries.c, 67	openacc_discretization.c, 62
openmp_boundaries.c, 83	openacc_kernels.h, 64
serial boundaries.c, 95	OpenCLData, 6
tbb_boundaries.cpp, 99	convolution_program
_ ,,,	OpenCLData, 7
boundaries.h, 9	cuda_boundaries.cu, 11
apply_boundary_conditions, 10	apply_initial_conditions, 12
apply_initial_conditions, 10	boundary_kernel, 13
boundary_kernel	cuda_data.cu, 14
cuda_boundaries.cu, 13	free_cuda, 14
cuda_kernels.cuh, 29	init_cuda, 15
kernel_boundary.cl, 34	cuda_data.h, 16
openacc_boundaries.c, 60	cuda_diffusion_solver, 17
openacc_kernels.h, 64	device_boundaries, 18
OpenCLData, 5	device composition, 18
boundary_program	device_convolution, 19
OpenCLData, 5	free_cuda, 19
build_program	init cuda, 20
opencl_data.c, 69	read out result, 20
opencl_data.h, 73	cuda_diffusion_solver
	cuda_data.h, 17
check_solution	cuda discretization.cu, 23
numerics.c, 45	cuda_discretization.cu, 21
numerics.h, 52	compute convolution, 22
check_solution_lambda	convolution_kernel, 23
tbb_discretization.cpp, 101	cuda_diffusion_solver, 23
tbb_main.c, 103	d mask, 27
commandQueue	device boundaries, 24
OpenCLData, 6	device_composition, 25
compute_convolution	device_composition, 25 device_convolution, 25
cuda_discretization.cu, 22	device_convolution, 25 diffusion_kernel, 26
numerics.h, 53	
openmp_discretization.c, 85	read_out_result, 27
serial_discretization.c, 96	cuda_kernels.cuh, 27

112 INDEX

boundary_kernel, 29	mesh.c, 38
convolution_kernel, 29	mesh.h, 41
d_mask, 31	free_cuda
diffusion_kernel, 30	cuda_data.cu, 14
cuda_main.c, 31	cuda_data.h, 19
main, 32	free_opencl
CudaData, 3	opencl_data.c, 69
conc_lap, 4	opencl_data.h, 75
conc new, 4	. —
conc old, 4	GetTimer
	timer.c, 107
d_mask	timer.h, 108
cuda_discretization.cu, 27	
cuda_kernels.cuh, 31	init_cuda
device_boundaries	cuda_data.cu, 15
cuda_data.h, 18	cuda_data.h, 20
cuda_discretization.cu, 24	init_opencl
opencl_data.h, 74	opencl_data.c, 70
opencl_discretization.c, 78	opencl_data.h, 76
device_composition	
cuda_data.h, 18	kernel_boundary.cl, 33
cuda_discretization.cu, 25	boundary_kernel, 34
device convolution	kernel_convolution.cl, 34
cuda_data.h, 19	convolution_kernel, 35
cuda_discretization.cu, 25	kernel_diffusion.cl, 36
opencl_data.h, 74	diffusion_kernel, 36
opencl_discretization.c, 79	
device diffusion	main
opencl_data.h, 74	cuda_main.c, 32
opencl_discretization.c, 79	openacc_main.c, 65
diffusion kernel	opencl_main.c, 81
cuda discretization.cu, 26	openmp_main.c, 86
cuda_kernels.cuh, 30	serial_main.c, 98
kernel diffusion.cl, 36	tbb_main.c, 104
openacc_discretization.c, 62	make_arrays
openacc_kernels.h, 64	mesh.c, 38
OpenCLData, 7	mesh.h, 41
diffusion_program	manhattan_distance
OpenCLData, 7	numerics.c, 47
distance_point_to_segment	numerics.h, 56
numerics.c, 46	mask
numerics.h, 54	OpenCLData, 7
numeriositi, or	MAX_MASK_H
euclidean_distance	numerics.h, 51
numerics.c, 46	MAX_MASK_W
numerics.h, 55	numerics.h, 52
,	mesh.c, 37
file	free_arrays, 38
Stopwatch, 8	make_arrays, 38
five_point_Laplacian_stencil	swap_pointers, 39
numerics.c, 47	swap_pointers_1D, 39
numerics.h, 55	mesh.h, 40
fp_t	free_arrays, 41
type.h, 110	make_arrays, 41
free_arrays	swap_pointers, 42

INDEX 113

swap_pointers_1D, 42	free_opencl, 75 init_opencl, 76
nine_point_Laplacian_stencil	read_out_result, 76
numerics.c, 48	report_error, 77
numerics.h, 56	opencl_discretization.c, 78
numerics.c, 43	• —
analytical_value, 44	device_boundaries, 78
check_solution, 45	device_convolution, 79
distance point to segment, 46	device_diffusion, 79
euclidean_distance, 46	read_out_result, 80
five_point_Laplacian_stencil, 47	opencl_main.c, 80
manhattan_distance, 47	main, 81
	OpenCLData, 4
nine_point_Laplacian_stencil, 48	boundary_kernel, 5
set_mask, 48	boundary_program, 5
slow_nine_point_Laplacian_stencil, 49	commandQueue, 6
numerics.h, 50	conc_lap, 6
analytical_value, 52	conc_new, 6
check_solution, 52	conc_old, 6
compute_convolution, 53	context, 6
distance_point_to_segment, 54	convolution_kernel, 6
euclidean_distance, 55	convolution_program, 7
five_point_Laplacian_stencil, 55	diffusion kernel, 7
manhattan_distance, 56	diffusion program, 7
MAX_MASK_H, 51	mask, 7
MAX_MASK_W, 52	openmp_boundaries.c, 82
nine_point_Laplacian_stencil, 56	apply_boundary_conditions, 83
set_mask, 56	apply_initial_conditions, 83
slow_nine_point_Laplacian_stencil, 57	openmp_discretization.c, 84
update_composition, 58	compute_convolution, 85
. – ,	update_composition, 85
openacc_boundaries.c, 59	openmp_main.c, 86
apply_boundary_conditions, 59	main, 86
apply_initial_conditions, 60	output.c, 87
boundary_kernel, 60	•
openacc_discretization.c, 61	param_parser, 88 print_progress, 89
convolution_kernel, 62	
diffusion kernel, 62	write_csv, 89
openacc_kernels.h, 63	write_png, 90
boundary_kernel, 64	output.h, 91
convolution_kernel, 64	param_parser, 92
diffusion_kernel, 64	print_progress, 92
openacc_main.c, 65	write_csv, 93
main, 65	write_png, 93
opencl_boundaries.c, 66	
apply_initial_conditions, 67	param_parser
opencl data.c, 68	output.c, 88
build program, 69	output.h, 92
_, •	print_progress
free_opencl, 69	output.c, 89
init_opencl, 70	output.h, 92
report_error, 71	
opencl_data.h, 71	read_out_result
build_program, 73	cuda_data.h, 20
device_boundaries, 74	cuda_discretization.cu, 27
device_convolution, 74	opencl_data.h, 76
device diffusion, 74	opencl discretization.c, 80

114 INDEX

report_error	StartTimer, 109
opencl_data.c, 71	timerStart
opencl_data.h, 77	timer.c, 108
	type.h, 109
serial_boundaries.c, 94	fp_t, 110
apply_boundary_conditions, 95	
apply_initial_conditions, 95	update_composition
serial_discretization.c, 95	numerics.h, 58
compute_convolution, 96	openmp_discretization.c, 85
update_composition, 96	serial_discretization.c, 96
serial_main.c, 97	tbb_discretization.cpp, 102
main, 98	
set_mask	write_csv
numerics.c, 48	output.c, 89
numerics.h, 56	output.h, 93
slow_nine_point_Laplacian_stencil	write_png
numerics.c, 49	output.c, 90
numerics.h, 57	output.h, 93
soln	
Stopwatch, 8	
StartTimer	
timer.c, 107	
timer.h, 109	
Stepwatch 8	
Stopwatch, 8 Stopwatch, 7	
conv, 8	
file, 8	
soln, 8	
step, 8 swap_pointers	
mesh.c, 39	
mesh.h, 42	
swap_pointers_1D	
mesh.c, 39	
mesh.h, 42	
1110011.11, 42	
tbb_boundaries.cpp, 99	
apply_boundary_conditions, 99	
apply_initial_conditions, 99	
tbb_discretization.cpp, 100	
check_solution_lambda, 101	
compute_convolution, 101	
update_composition, 102	
tbb_main.c, 102	
check_solution_lambda, 103	
main, 104	
timer.c, 105	
USE_BSD, 106	
USE_MISC, 107	
GetTimer, 107	
StartTimer, 107	
timerStart, 108	
timer.h, 108	
GetTimer, 108	