continuumColony

15.3

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Here are the data structures with brief descriptions:

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Data Structure Documentation

2.1 blockDims Struct Reference

struct of block dimensions for CUDA kernels

Public Member Functions

- void makeBlockDims (int xl, int yl, int zl)
  make up struct of block dimentions for cuda kernels

Data Fields

- dim3 **defaultNumBlocks**
- dim3 **fbaNumBlocks**
- dim3 **diffNumBlocks**
- dim3 **syncTCLwithCLNumBlocks**
- dim3 **chemReactNumBlocks**
- dim3 **expandCellsNumBlocks**
- int **BCblocksWall**
- int **BCblocksFloor**

2.1.1 Detailed Description

struct of block dimensions for CUDA kernels

2.1.2 Member Function Documentation

2.1.2.1 void blockDims::makeBlockDims (int *xl*, int *yl*, int *zl*) [inline]

make up struct of block dimentions for cuda kernels

Parameters

xl	lattice length in x dimensions
yl	lattice length in y dimensions
zl	lattice length in z dimensions

Returns

Void

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

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2.2 cellLattice Struct Reference

Cell lattice struct. This contains a lattice of the local volume fraction of a single cell type, as well as the FBA table the cell uses.

Public Member Functions

- void readArbitraryVolumeFractionFilename (float *volumeFraction, string arbitraryVolumeFractionFilename, int ly, int lz)

  Initialize the starting geometry of a cell type using the an arbitrary volume fraction file.
- void buildCellLattice (fbaModel f, int x, int y, int z, float lambda, int start, string arbitraryVolumeFractionFilename, int startX, int startY, int startNumber, int agarHeight, float cellV)

  Build a cell lattice struct.

Data Fields

- float * **volumeFraction**
- float * **cVolumeFraction**
- float * **tempVolumeFraction**
- float * **cTempVolumeFraction**
- float * **fbaOuts** [11]
- float * **cFbaOuts** [11]
- fbaModel **fba**
- int **starterFlag**

2.2.1 Detailed Description

Cell lattice struct. This contains a lattice of the local volume fraction of a single cell type, as well as the FBA table the cell uses.

2.2.2 Member Function Documentation

2.2.2.1 void cellLattice::buildCellLattice (fbaModel *f,* int *x,* int *y,* int *z,* float *lambda,* int *start,* string *arbitraryVolumeFractionFilename,* int *startX,* int *startY,* int *startNumber,* int *agarHeight,* float *cellV*) [inline]

Build a cell lattice struct.

Parameters

f	An FBA table struct
x	Length of the lattice in the X-direction
y	Length of the lattice in the Y-direction
z	Length of the lattice in the Z-direction
lambda	Lattice Spacing (in meters)
start	Flag (0 or 1) indicating if this cell type is present at the start of a simulation
arbitrary-Volume-Fraction-Filename	Name of the arbitrary volume fraction file (can be ” if none)
startX	Starting X location (in units of the lattice spacing) for the cell (if start = 1 and arbitraryVolumeFractionFilename = ”)
startY	Starting Y location (in units of the lattice spacing) for the cell (if start = 1 and arbitraryVolumeFractionFilename = ”)
startNumber	Number of cells initially in the simulation (if start = 1 and arbitrary-VolumeFractionFilename = ”)
agarHeight	Height of the agar (in units of the lattice spacing)
cellV	Average cell volume

Returns

Void

2.2.2.2 void cellLattice::readArbitraryVolumeFractionFilename (float * *volumeFraction,* string *arbitraryVolumeFractionFilename,* int *ly,* int *lz*) [inline]

Initialize the starting geometry of a cell type using the an arbitrary volume fraction file.

Parameters

volume-Fraction	Pointer to a cell’s volume fraction lattice
arbitrary-Volume-Fraction-Filename	Name of the arbitrary volume fraction file
ly	Length of the lattice in the Y-direction
lz	Length of the lattice in the Z-direction

Returns

Void

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2.3 cellLattices Struct Reference

Cell lattices struct. This is a container struct for all the cell lattice structs in the simulation. It also stores to total volume fraction lattice.

Public Member Functions

- void buildCellLattices (float mvf, int x, int y, int z, float l, float t, int ah, float cellV, float cellM)

  Build the cellLattices struct.
- void **add** (cellLattice cL)

Data Fields

- int ∗ **typeFlags**
- int ∗ **cTypeFlags**
- float ∗ **totalVolumeFraction**
- float ∗ **cTotalVolumeFraction**
- int **numberCells**
- cellLattice **lattices** [10]
- float **maxVolFraction**
- float **conversionFactorConcPerSecondToMmolPerGDwtPerHr**
- int **xl**
- int **yl**
- int **zl**
- float **lambda**
- float **fbaTau**
- int **agarHeight**
- int **N**
- int **isRelaxed**

2.3.1 Detailed Description

Cell lattices struct. This is a container struct for all the cell lattice structs in the simulation. It also stores to total volume fraction lattice.

2.3.2 Member Function Documentation

2.3.2.1 void cellLattices::buildCellLattices (float *mvf*, int *x*, int *y*, int *z*, float *l*, float *t*, int *ah*, float *cellV*, float *cellM*) [inline]

Build the cellLattices struct.

Parameters

mvf	Maximum volume fraction parameter
x	Length of the lattice in the X-direction
y	Length of the lattice in the Y-direction
z	Length of the lattice in the Z-direction
l	Lattice Spacing (in meters)
t	FBA timestep
ah	Agar height in units of the lattice spacing
cellV	Average cell volume
cellM	Average cell mass

Returns

Void

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

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2.4 chemCognate Struct Reference

Chem cognate struct.

Data Fields

- int **reactChemIdx**
- int **prodChemIdx**

2.4.1 Detailed Description

Chem cognate struct.

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

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2.5 chemLattice Struct Reference

Cell lattice struct. This contains a lattice of chem concentrations, a lattice of diffusion rates, and info about time steps, boundary conditions, and other such things.

Public Member Functions

- void buildChemLattice (float dw, float da, float l, float t, int x, int y, int z, int agar, float initAg, float initAir, int isInt, int cicli, int isHin, float cellVol, int wallBcFlag, int floorBcFlag)

  Build a chem lattice struct.

Data Fields

- float * **lattice**
- float * **tempLattice**
- float * **cLattice**
- float * **cTempLattice**
- float * **Dlattice**
- float * **cDlattice**
- float **Dwater**
- float **Dagar**
- float **initialAgar**
- float **initialAir**
- float **tau**
- int **isIntracellular**
- int **cellIdxChemLivesIn**
- int **isHindered**
- int **refWallBcFlag**
- int **refFloorBcFlag**

2.5.1 Detailed Description

Cell lattice struct. This contains a lattice of chem concentrations, a lattice of diffusion rates, and info about time steps, boundary conditions, and other such things.

2.5.2 Member Function Documentation

2.5.2.1 void chemLattice::buildChemLattice (float *dw,* float *da,* float *l,* float *t,* int *x,* int *y,* int *z,* int *agar,* float *initAg,* float *initAir,* int *isInt,* int *cicli,* int *isHin,* float *cellVol,* int *wallBcFlag,* int *floorBcFlag*) [inline]

Build a chem lattice struct.

Parameters

dw	The diffusion rate in water
da	The diffusion rate in agar
l	The lattice spacing
t	The timestep
x	Number of lattice sites in the x direction
y	Number of lattice sites in the y direction
z	Number of lattice sites in the z direction
agar	The height (in lattice sites) of the agar
initAg	The initial concentration of the chemical in the agar
initAir	The initial concentration of the chemical in the air
isInt	Flag determining if the chemical species is intracellular (1) or extracellular (0)
cicli	Cell index the chemical lives is--if a chemical species is intracellular, this int denotes the index of the cell type where the chemical resides
isHin	Flag determining if a chemical experiences hindered diffusion around cells (1) of does not experience hindered diffusion (0)
cellVol	Volume of the cell (in meters^3)
wallBcFlag	Flag determining if a chemical will experience reflective boundary conditions at the 4 walls of the simulation box (1) or will experience fixed-concentration boundary conditions (0)
floorBcFlag	Flag determining if a chemical will experience reflective boundary conditions at the floor of the simulation box (1) or will experience fixed-concentration boundary conditions (0)

Returns

Void

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

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2.6 chemLattices Struct Reference

Chem lattices struct. This is a container struct for all the chem lattice structs in the simulation.

Public Member Functions

- void buildChemLattices (int x, int y, int z, float l, float t, int ah)

  Build the chem lattices struct.
- void add (chemLattice cl)

  Add a chem lattice to this container struct of chem lattices.

Data Fields

- int **xl**
- int **yl**
- int **zl**
- float **lambda**
- float **fbaTau**
- int **agarHeight**
- int **N**
- int **numberChems**
- chemLattice **lattices** [10]

2.6.1 Detailed Description

Chem lattices struct. This is a container struct for all the chem lattice structs in the simulation.

2.6.2 Member Function Documentation

2.6.2.1 void chemLattices::add (chemLattice *cl*) [inline]

Add a chem lattice to this container struct of chem lattices.

Parameters

cl	chem lattice

Returns

Void

2.6.2.2 void chemLattices::buildChemLattices (int *x*, int *y*, int *z*, float *l*, float *t*, int *ah*) [inline]

Build the chem lattices struct.

Parameters

x	Number of lattice sites in the x direction
y	Number of lattice sites in the y direction
z	Number of lattice sites in the z direction
l	The lattice spacing in meters
t	The simulation timestep
ah	The agar height in lattice sites

Returns

Void

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

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2.7 chemReaction Struct Reference

Chem uptake reaction struct.

Public Member Functions

- void buildChemReaction (float m, float cat, float e, int type, int react, int prod, float cellV)

  Build an uptake reaction struct.

Data Fields

- float **km**
- float **kcat**
- float **E**
- int **cellType**
- int **reactant**
- int **product**

2.7.1 Detailed Description

Chem uptake reaction struct.

2.7.2 Member Function Documentation

2.7.2.1 void chemReaction::buildChemReaction (float *m,* float *cat,* float *e,* int *type,* int *react,* int *prod,* float *cellV*) [inline]

Build an uptake reaction struct.

Parameters

m	Michaelis constant for a michaelis-menten uptake reaction
cat	Kcat for a michaelis-menten uptake reaction
e	Number of uptake enzymes on an average cell
type	The index of the cell type that does this uptake reaction
react	The index of the chem type that is uptaken
prod	The index of the chem type that is produced (intercellular)
cellV	The cell volume of the cell type

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2.8 chemReactions Struct Reference

container struct for all the uptake reaction structs

Public Member Functions

- void add (chemReaction cR)

  add an uptake reaction to the container struct

Data Fields

- int **numberReactions**
- chemReaction **reactions** [10]

2.8.1 Detailed Description

container struct for all the uptake reaction structs

2.8.2 Member Function Documentation

2.8.2.1 void chemReactions::add (chemReaction *cR*) [inline]

add an uptake reaction to the container struct

Parameters

cR	The uptake reaction struct to be added

Returns

Void

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

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2.9 fbaModel Struct Reference

fbaModel struct. This is a struct that contains an FBA table and the parameters needed to index into it.

Public Member Functions

- void buildFbaModel (string inputFilename)

  build the FBA table using an FBA table file.

Data Fields

- int **nInputs**
- int **nOutputs**
- int **inputIndexes** [10]
- int **outputIndexes** [11]
- int **numberOfTabledValues** [10]
- float **inputStride** [10]
- int **indexMultipliers** [10]
- float * **fbaTable**
- float * **cFbaTable**

2.9.1 Detailed Description

fbaModel struct. This is a struct that contains an FBA table and the parameters needed to index into it.

2.9.2 Member Function Documentation

2.9.2.1 void fbaModel::buildFbaModel (string *inputFilename*) [inline]

build the FBA table using an FBA table file.

Parameters

filename	The name of the FBA table file

Returns

Void

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

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2.10 regReaction Struct Reference

Regulation reaction struct.

Public Member Functions

- void buildRegReaction (int chem1, int chem2, int reactCell, int prodCell, string mults)

  Build a regulation reaction.
- void fillChemCognate (string cogs)

  Regulation reactions turn one cell type into another; the intracellular species within the reactant cell type also need to transform into the intracellular species of the product cell type.

Data Fields

- float **multipliers** [10]
- chemCognate **cognates** [10]
- int **numChemCognates**
- int **chemType1**
- int **chemType2**
- int **reactantCell**
- int **productCell**

2.10.1 Detailed Description

Regulation reaction struct.

2.10.2 Member Function Documentation

2.10.2.1 void regReaction::buildRegReaction (int *chem1,* int *chem2,* int *reactCell,* int *prodCell,* string *mults*) [inline]

Build a regulation reaction.

Parameters

chem1	Index of the first chemical species a cell is assumed to change regulatory state in response to
chem2	Index of the second chemical species a cell is assumed to change regulatory state in response to
reactCell	Index of the cell type transformed by this regulation reaction
prodCell	Index of the cell type produced by this regulation reaction
mults	Coefficients for the polynomial rate law that governs this reaction

Returns

Void

2.10.2.2 void regReaction::fillChemCognate (string *cogs*) [inline]

Regulation reactions turn one cell type into another; the intracellular species within the reactant cell type also need to transform into the intracellular species of the product cell type.

Parameters

cogs	Tab delimited set of indexes of the intracellular chem index in the reactant cell (first) and product cell (second)

Returns

Void

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2.11 regReactions Struct Reference

container struct for the regulation reactions

Public Member Functions

- void add (regReaction reg)

  add a regulation reaction to this container struct

Data Fields

- int **numberReactions**
- regReaction **reactions** [10]

2.11.1 Detailed Description

container struct for the regulation reactions

2.11.2 Member Function Documentation

2.11.2.1 void regReactions::add (regReaction *reg*) [inline]

add a regulation reaction to this container struct

Parameters

reg	The regulation reaction struct to be added

Returns

Void

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

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