Parallel Molecular Dynamics with a Time-Reversible Nose-Hoover Thermostat on CPUs and GPUs

1.0

Generated by Doxygen 1.8.2

Sat Jan 4 2014 19:08:05

Contents

Chapter 1

CBEMDGPU

CBE MD on GPUs

by Nathan A. Mahynski, George A. Khoury, and Carmeline J. Dsilva

See main.cpp to set parameters which are documented by example in this file.

To compile the CPU version, type $ make MD

To compile the GPU version, type $ make -f Makefile_cuda

To compile tests, etc., type $ make ${var} where var is the suffix desired (see Makefile for details)

Chapter 2

Hierarchical Index

2.1 Class Hierarchy

This inheritance list is sorted roughly, but not completely, alphabetically:

Chapter 3

Class Index

3.1 Class List

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

Chapter 4

Class Documentation

4.1 atom Struct Reference

Structure of an atom.

```
#include <dataTypes.h>
```

Public Attributes

- float3 pos

  Position.
- float3 vel

  Velocity.
- float3 acc

  Acceleration.

4.1.1 Detailed Description

Structure of an atom.

Definition at line 28 of file dataTypes.h.

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

- /Users/nathanmahynski/Desktop/CBEMDGPU/dataTypes.h

4.2 cellList_cpu Class Reference

```
#include <cellList.h>
```

Public Member Functions

- cellList_cpu (const float3 &box, const float rc, const float rs)
- void checkUpdate (const systemDefinition &sys)

  Check if the neighbor list requires updating.
- int cell (const float3 &pos)

  Calculate the cell in which a given coordinate is located.
- int head (const int cell) const

Return the first atom (aka 'head') of each cell.

- int list (const int index) const

  Iterates through a linked list of particles, returns the index of the next atom in line.
- std::vector< int > neighbors (const int cellID) const

  Returns the indices of a cell's neighboring cells.

Public Attributes

- int3 nCells

  Number of cells in each direction.

4.2.1 Detailed Description

Cell Lists

Date

11/19/13

Maintains a linked list to track cells on the CPU

Definition at line 38 of file cellList.h.

4.2.2 Constructor & Destructor Documentation

4.2.2.1 cellList_cpu::cellList_cpu (const float3 & *box*, const float *rc*, const float *rs*)

Cell Lists

Date

11/19/13

Initialize a cell list on the CPUs.

Parameters

in	*box*	Box size
in	*rc*	Cutoff radius
in	*rs*	Skin Radius

Definition at line 154 of file cellList.cpp.

References nCells.

```
                                                                            {
    if (rc < 0.0) {
        throw customException("Cutoff radius must be > 0");
        return;
    }
    rc_ = rc;
    if (rs < 0.0) {
        throw customException("Skin radius must be > 0");
        return;
    }
    rs_ = rs;

    box_ = box;

    start_ = 1;
    lcell_.x = 1.01*(rc+rs);
    nCells.x = (int) floor (box.x/lcell_.x);
    lcell_.x = (box.x/nCells.x);

    lcell_.y = 1.01*(rc+rs);
    nCells.y = (int) floor (box.y/lcell_.y);
    lcell_.y = (box.y/nCells.y);

    lcell_.z = 1.01*(rc+rs);
    nCells.z = (int) floor (box.z/lcell_.z);
    lcell_.z = (box.z/nCells.z);

    if (lcell_.x <= (rc+rs) || lcell_.y <= (rc+rs) || lcell_.z < (rc+rs)) {
        throw customException("Cell width must exceed sum of
       cutoff and skin radius");
        return;
    }

    if (lcell_.x < 1) {
        throw customException ("Box dimension x too small
       relative to skin and cutoff radius to use cell lists");
        return;
    }
    if (lcell_.y < 1) {
        throw customException ("Box dimension y too small
       relative to skin and cutoff radius to use cell lists");
        return;
    }
    if (lcell_.z < 1) {
        throw customException ("Box dimension z too small
       relative to skin and cutoff radius to use cell lists");
        return;
    }

    if (nCells.x < 3 || nCells.y < 3 || nCells.z < 3) {
        throw customException("Must be able to have at least 3
       cells in each direction, change box size, skin, or cutoff radius");
        return;
    }

    try {
        head_.resize(nCells.x*nCells.y*nCells.z, -1);
    } catch (std::exception &e) {
        std::cerr << e.what() << std::endl;
        throw customException ("Unable to initialize head for
       cell list");
        return;
    }
    // build neighbors for each cell
    neighbor_.resize(nCells.x*nCells.y*nCells.z);
    for (unsigned int cellID = 0; cellID < nCells.x*nCells.y*nCells
      .z; ++cellID) {
        const int zref = floor(cellID/(nCells.x*nCells.y));
        const int yref = floor((cellID - zref*(nCells.x*nCells.y))/
      nCells.y);
        const int xref = floor(cellID - zref*(nCells.x*nCells.y) -
      yref*nCells.x);
        for (int dx = -1; dx <= 1; ++dx) {
            int xcell = xref + dx;
            if (xcell >= nCells.x) xcell = 0;
            if (xcell < 0) xcell = nCells.x-1;
            for (int dy = -1; dy <= 1; ++dy) {
                int ycell = yref + dy;
                if (ycell >= nCells.y) ycell = 0;
                if (ycell < 0) ycell = nCells.y-1;
                for (int dz = -1; dz <= 1; ++dz) {
                    int zcell = zref + dz;
                    if (zcell >= nCells.z) zcell = 0;
                    if (zcell < 0) zcell = nCells.z-1;
                    const int cellID2 = xcell + ycell*nCells.x + zcell*(
      nCells.x*nCells.y);
                    neighbor_[cellID].push_back(cellID2);
                }
            }
        }
    }
    for (unsigned int cellID = 0; cellID < nCells.x*nCells.y*nCells
      .z; ++cellID) {
    if (neighbor_[cellID].size() != 27) {
            throw customException ("Cell list initial build
       failed to find 27 neighbors (including self)");
            return;
        }
    }
}
```

4.2.3 Member Function Documentation

4.2.3.1 int cellList_cpu::cell (const float3 & *pos*)

Calculate the cell in which a given coordinate is located.

Calculates the cell (linear index of it) a position belongs to in a periodic box. The position does not need to be "inside" the box, boundary conditions are applied.

Parameters

in	*pos*	Position of atom

Returns

cell

Definition at line 250 of file cellList.cpp.

References nCells.

Referenced by checkUpdate(), and head().

```
                                        {
    float3 inBox = pbc(pos, box_);
    const int x = (int) floor(inBox.x/lcell_.x);
    const int y = (int) floor(inBox.y/lcell_.y);
    const int z = (int) floor(inBox.z/lcell_.z);
    return x + y*nCells.x + z*nCells.x*nCells.y;
}
```

4.2.3.2 void cellList_cpu::checkUpdate (const systemDefinition & *sys*)

Check if the neighbor list requires updating.

Checks to see if the cell list needs to be updated and if so, rebuilds Uses linked list, so algorithm in O(N)

Parameters

in	*sys*	System definition

Definition at line 264 of file cellList.cpp.

References systemDefinition::atoms, systemDefinition::box(), cell(), and systemDefinition::numAtoms().

Referenced by integrator::calcForce().

```
                                                          {
    int build = 0;
    if (start_) {
    const int natoms = sys.numAtoms();
    try {
            list_.resize(natoms, -1);
        } catch (std::exception& e) {
            std::cerr << e.what() << std::endl;
            throw customException ("Unable to initialize list
       for cell list");
            return;
        }
        try {
            posAtLastBuild_.resize(natoms);
        } catch (std::exception& e) {
            std::cerr << e.what() << std::endl;
            throw customException ("Unable to initialize
       position list for cell list");
            return;
        }
        start_ = 0;
        build = 1;
    } else {
        // check max displacements
        float drMax1_ = 0.0;
        float drMax2_ = 0.0;
        float3 dummy;
            for (unsigned int i = 0; i < sys.numAtoms(); ++i) {
                const float dr2 = pbcDist2 (sys.atoms[i].pos,
      posAtLastBuild_[i], dummy, sys.box());
                if (dr2 > drMax1_*drMax1_) {
                    drMax2_ = drMax1_;
                    drMax1_ = sqrt(dr2);
                } else if (dr2 > drMax2_*drMax2_) {
                    drMax2_ = sqrt(dr2);
                }
            }
        if (drMax1_+drMax2_ > rs_) {
            build = 1;
        } else {
            build = 0;
        }
    }

    if (build) {
        if (sys.numAtoms() != list_.size()) {
            throw customException ("Number of atoms in
     simulation has changed");
            return;
        }
        for (unsigned int i = 0; i < head_.size(); ++i) {
            head_[i] = -1;
        }
        for (unsigned int i = 0; i < sys.numAtoms(); ++i) {
            const int icell = cell(sys.atoms[i].pos);
            list_[i] = head_[icell];
            head_[icell] = i;
            posAtLastBuild_[i] = sys.atoms[i].pos;
        }
    }

    return;
}
```

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

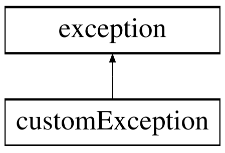
- /Users/nathanmahynski/Desktop/CBEMDGPU/cellList.h
- /Users/nathanmahynski/Desktop/CBEMDGPU/cellList.cpp

4.3 customException Class Reference

Error reporting.

`#include <common.h>`

Inheritance diagram for customException:



Public Member Functions

- const char ∗ what () const throw ()

  Return a message pertaining to what went wrong.
- customException (std::string m="custom exception occurred")

  Instantiate the object with a user specified message.

4.3.1 Detailed Description

Error reporting.

Common values, structures, etc.

Date

11/17/13

Definition at line 13 of file common.h.

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

- /Users/nathanmahynski/Desktop/CBEMDGPU/common.h

4.4 float3 Struct Reference

3 floating point numbers, same as defined for GPUs

```
#include <dataTypes.h>
```

Public Attributes

- float **x**
- float **y**
- float **z**

4.4.1 Detailed Description

3 floating point numbers, same as defined for GPUs

Requisite 'optimal' data types.

Date

11/21/13

Definition at line 15 of file dataTypes.h.

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

- /Users/nathanmahynski/Desktop/CBEMDGPU/dataTypes.h

4.5 int3 Struct Reference

3 integers, same as defined for GPUs

```
#include <dataTypes.h>
```

Public Attributes

- int **x**
- int **y**
- int **z**

4.5.1 Detailed Description

3 integers, same as defined for GPUs

Definition at line 21 of file dataTypes.h.

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

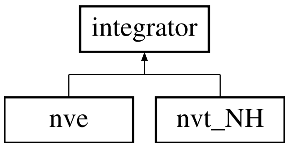
- /Users/nathanmahynski/Desktop/CBEMDGPU/dataTypes.h

4.6 integrator Class Reference

Base class for integrators such as NVT (Nose-Hoover) or NVE ensembles.

```
#include <integrator.h>
```

Inheritance diagram for integrator:



Public Member Functions

- void setTimestep (const float dt)

  Set the integrator timestep.
- void calcForce (systemDefinition &sys)

  Calculate the forces on each atom.
- virtual void step (systemDefinition &sys)=0

  Move the system forward a step in time.

Protected Attributes

- cellList_cpu cl_

  Cell or neighbor list.
- std::vector< float3 > lastAccelerations_

  Acceleration of particles on previous timestep (useful for NVE integrator)
- float dt_

  Timestep size.
- int start_

  Flag for whether this object has been initialized or not.

4.6.1 Detailed Description

Base class for integrators such as NVT (Nose-Hoover) or NVE ensembles.

Integrator

Date

11/17/13

Definition at line 14 of file integrator.h.

4.6.2 Member Function Documentation

4.6.2.1 void integrator::calcForce (**systemDefinition & *sys***)

Calculate the forces on each atom.

Integration

Date

11/19/13

Calculate the pairwise forces in a system. This also calculates the potential energy of a system. The kinetic energy is calculated during the verlet integration.

Parameters

in,out	*sys*	System definition

Definition at line 22 of file integrator.cpp.

References systemDefinition::atoms, systemDefinition::box(), cellList_cpu::checkUpdate(), cl_, cellList_cpu::head(), cellList_cpu::list(), systemDefinition::mass(), cellList_cpu::nCells, cellList_cpu::neighbors(), systemDefinition::numAtoms(), systemDefinition::potential, systemDefinition::potentialArgs(), systemDefinition::rcut(), and systemDefinition::setPotE().

Referenced by nve::step(), and nvt_NH::step().

```
                                                    {
// For cache coeherency allocate new space for calculations
float3 empty;
empty.x = 0; empty.y = 0; empty.z = 0;
std::vector <float3> acc (sys.numAtoms(), empty);
const float rc = sys.rcut();

// every time, check if the cell list needs to be updated first
cl_.checkUpdate(sys);

float Up = 0.0;
const float3 box = sys.box();
const float invMass = 1.0/sys.mass();

// traverse cell list and calculate total system potential energy
std::vector <float> args = sys.potentialArgs();
#pragma omp parallel for reduction(+:Up) schedule(dynamic, 1)
for (unsigned int cellID = 0; cellID < cl_.nCells.x*cl_.nCells
  .y*cl_.nCells.z; ++cellID) {
    int atom1 = cl_.head(cellID);
    while (atom1 >= 0) {
        std::vector < int > neighbors = cl_.neighbors(cellID);
        for (int index = 0; index < neighbors.size(); ++index) {
            const int cellID2 = neighbors[index];
            int atom2 = cl_.head(cellID2);
            while (atom2 >= 0) {
                if (atom1 > atom2) {
                    float3 pf;
                    Up += sys.potential (&sys.atoms[atom1].
  pos, &sys.atoms[atom2].pos, &pf, &box, &args[0], &rc);
                    acc[atom1].x -= pf.x*invMass;
                    acc[atom1].y -= pf.y*invMass;
                    acc[atom1].z -= pf.z*invMass;
                    acc[atom2].x += pf.x*invMass;
                    acc[atom2].y += pf.y*invMass;
                    acc[atom2].z += pf.z*invMass;
                }
                atom2 = cl_.list(atom2);
            }
        }
        atom1 = cl_.list(atom1);
    }
}

// save acceleration in array of atoms in system
#pragma omp parallel for
for (int i = 0; i < sys.numAtoms(); ++i) {
    sys.atoms[i].acc.x = -acc[i].x;
```

```
        sys.atoms[i].acc.y = -acc[i].y;
        sys.atoms[i].acc.z = -acc[i].z;
    }

    // set Up
    sys.setPotE(Up);
}
```

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

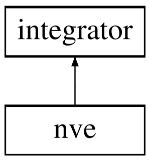
- /Users/nathanmahynski/Desktop/CBEMDGPU/integrator.h
- /Users/nathanmahynski/Desktop/CBEMDGPU/integrator.cpp

4.7 nve Class Reference

Integration scheme that preserves total energy of the system.

`#include <nve.h>`

Inheritance diagram for nve:



Public Member Functions

- void step (systemDefinition &sys)
- void setTimestep (const float dt)

    Set the integrator timestep.
- void calcForce (systemDefinition &sys)

    Calculate the forces on each atom.

Protected Attributes

- cellList_cpu cl_

    Cell or neighbor list.
- std::vector< float3 > lastAccelerations_

    Acceleration of particles on previous timestep (useful for NVE integrator)
- float dt_

    Timestep size.
- int start_

    Flag for whether this object has been initialized or not.

4.7.1 Detailed Description

Integration scheme that preserves total energy of the system.

NVE integration.

Date

11/18/13

Definition at line 13 of file nve.h.

4.7.2 Member Function Documentation

4.7.2.1 void integrator::calcForce (systemDefinition & *sys*) [inherited]

Calculate the forces on each atom.

Integration

Date

11/19/13

Calculate the pairwise forces in a system. This also calculates the potential energy of a system. The kinetic energy is calculated during the verlet integration.

Parameters

in,out	*sys*	System definition

Definition at line 22 of file integrator.cpp.

References systemDefinition::atoms, systemDefinition::box(), cellList_cpu::checkUpdate(), integrator::cl_, cellList-_cpu::head(), cellList_cpu::list(), systemDefinition::mass(), cellList_cpu::nCells, cellList_cpu::neighbors(), system-Definition::numAtoms(), systemDefinition::potential, systemDefinition::potentialArgs(), systemDefinition::rcut(), and systemDefinition::setPotE().

Referenced by step(), and nvt_NH::step().

```
                                                {
    // For cache coeherency allocate new space for calculations
    float3 empty;
    empty.x = 0; empty.y = 0; empty.z = 0;
    std::vector <float3> acc (sys.numAtoms(), empty);
    const float rc = sys.rcut();

    // every time, check if the cell list needs to be updated first
    cl_.checkUpdate(sys);

    float Up = 0.0;
    const float3 box = sys.box();
    const float invMass = 1.0/sys.mass();

    // traverse cell list and calculate total system potential energy
    std::vector <float> args = sys.potentialArgs();
    #pragma omp parallel for reduction(+:Up) schedule(dynamic, 1)
    for (unsigned int cellID = 0; cellID < cl_.nCells.x*cl_.nCells
      .y*cl_.nCells.z; ++cellID) {
        int atom1 = cl_.head(cellID);
        while (atom1 >= 0) {
            std::vector < int > neighbors = cl_.neighbors(cellID);
            for (int index = 0; index < neighbors.size(); ++index) {
                const int cellID2 = neighbors[index];
                int atom2 = cl_.head(cellID2);
                while (atom2 >= 0) {
                    if (atom1 > atom2) {
                        float3 pf;
                        Up += sys.potential (&sys.atoms[atom1].
      pos, &sys.atoms[atom2].pos, &pf, &box, &args[0], &rc);
                        acc[atom1].x -= pf.x*invMass;
                        acc[atom1].y -= pf.y*invMass;
                        acc[atom1].z -= pf.z*invMass;
                        acc[atom2].x += pf.x*invMass;
                        acc[atom2].y += pf.y*invMass;
                        acc[atom2].z += pf.z*invMass;
                    }
                    atom2 = cl_.list(atom2);
                }
            }
            atom1 = cl_.list(atom1);
        }
    }

    // save acceleration in array of atoms in system
    #pragma omp parallel for
    for (int i = 0; i < sys.numAtoms(); ++i) {
        sys.atoms[i].acc.x = -acc[i].x;
        sys.atoms[i].acc.y = -acc[i].y;
        sys.atoms[i].acc.z = -acc[i].z;
    }

    // set Up
    sys.setPotE(Up);
}
```

4.7.2.2 void nve::step (systemDefinition & *sys*) [virtual]

Do NVE integration

Date

11/18/13

Integrate a single timestep forward using Velocity-Verlet integration scheme. Update the positions and velocities using velocity verlet integration. This uses the accelerations stored on each atom. Creates a cell list the first time it is called.

Parameters

in,out	*sys*	System definition

Implements integrator.

Definition at line 22 of file nve.cpp.

References systemDefinition::atoms, integrator::calcForce(), integrator::dt_, integrator::lastAccelerations_, systemDefinition::mass(), systemDefinition::numAtoms(), systemDefinition::setKinE(), integrator::start_, and systemDefinition::updateInstantTemp().

```
                                     {
    if (start_) {
        try {
            lastAccelerations_.resize(sys.numAtoms())
  ;
        } catch (std::exception &e) {
            std::cerr << e.what() << std::endl;
            throw customException("Failed to initialize
   integrator due to memory constraints");
            return;
        }
        // calculate the forces initially (sets Up)
        calcForce (sys);

        // also get initial T
        #pragma omp parallel
        {
            #pragma omp for shared(sys.atoms) schedule(dynamic, OMP_CHUNK)
            for (unsigned int i = 0; i < sys.numAtoms(); ++i) {
                sys.atoms[i].vel.x += dt_*0.5*(lastAccelerations_
  [i].x+sys.atoms[i].acc.x);
                sys.atoms[i].vel.y += dt_*0.5*(lastAccelerations_
  [i].y+sys.atoms[i].acc.y);
                sys.atoms[i].vel.z += dt_*0.5*(lastAccelerations_
  [i].z+sys.atoms[i].acc.z);
            }
        }

        float tmp = 0.0, Uk = 0.0;
        #pragma omp parallel
        {
            #pragma omp reduction(+:Uk) schedule(dynamic, OMP_CHUNK)
            for (unsigned int i = 0; i < sys.numAtoms(); ++i) {
                Uk += (sys.atoms[i].vel.x*sys.atoms[i].vel.x)+(sys.
  atoms[i].vel.y*sys.atoms[i].vel.y)+(sys.atoms[i].vel.z*sys.atoms
  [i].vel.z);
            }
        }
        Uk *= sys.mass();
        tmp = Uk;
        Uk *= 0.5;
        tmp /= (3.0*(sys.numAtoms()-1.0));
        sys.updateInstantTemp(tmp);
        sys.setKinE(Uk);
        start_ = 0;
    }

    // update positions based on current positions
    #pragma omp parallel
    {
        #pragma omp for shared(sys.atoms) schedule(dynamic, OMP_CHUNK)
        for (unsigned int i = 0; i < sys.numAtoms(); ++i) {
            sys.atoms[i].pos.x += dt_*(sys.atoms[i].vel.x+0.5*dt_
  *sys.atoms[i].acc.x);
            sys.atoms[i].pos.y += dt_*(sys.atoms[i].vel.y+0.5*dt_
  *sys.atoms[i].acc.y);
            sys.atoms[i].pos.z += dt_*(sys.atoms[i].vel.z+0.5*dt_
  *sys.atoms[i].acc.z);
            lastAccelerations_[i] = sys.atoms[i].acc;
        }
    }

    // calculate new forces at new positions
    calcForce (sys);

    // update velocities and get Uk and kinetic temperature
    #pragma omp parallel
    {
        #pragma omp for shared(sys.atoms) schedule(dynamic, OMP_CHUNK)
        for (unsigned int i = 0; i < sys.numAtoms(); ++i) {
            sys.atoms[i].vel.x += dt_*0.5*(lastAccelerations_
  [i].x+sys.atoms[i].acc.x);
            sys.atoms[i].vel.y += dt_*0.5*(lastAccelerations_
  [i].y+sys.atoms[i].acc.y);
            sys.atoms[i].vel.z += dt_*0.5*(lastAccelerations_
  [i].z+sys.atoms[i].acc.z);
        }
    }

    // get temperature and kinetic energy
    float tmp = 0.0, Uk = 0.0;
    #pragma omp parallel
    {
        #pragma omp reduction(+:Uk) schedule(dynamic, OMP_CHUNK)
        for (unsigned int i = 0; i < sys.numAtoms(); ++i) {
            Uk += (sys.atoms[i].vel.x*sys.atoms[i].vel.x)+(sys.atoms
  [i].vel.y*sys.atoms[i].vel.y)+(sys.atoms[i].vel.z*sys.atoms[i].
  vel.z);
        }
    }
    Uk *= sys.mass();
    tmp = Uk;
    Uk *= 0.5;
    tmp /= (3.0*(sys.numAtoms()-1.0));
    sys.updateInstantTemp(tmp);
    sys.setKinE(Uk);
}
```

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

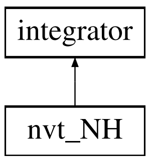
- /Users/nathanmahynski/Desktop/CBEMDGPU/nve.h
- /Users/nathanmahynski/Desktop/CBEMDGPU/nve.cpp

4.8 nvt_NH Class Reference

Uses Nose-Hover integration method to thermostat a system (constant T rather than E)

```
#include <nvt.h>
```

Inheritance diagram for nvt_NH:



Public Member Functions

- nvt_NH (const float Q)
- void step (systemDefinition &sys)
- void setTimestep (const float dt)

  Set the integrator timestep.
- void calcForce (systemDefinition &sys)

  Calculate the forces on each atom.

Protected Attributes

- cellList_cpu cl_

  Cell or neighbor list.
- std::vector< float3 > lastAccelerations_

  Acceleration of particles on previous timestep (useful for NVE integrator)
- float dt_

  Timestep size.
- int start_

  Flag for whether this object has been initialized or not.

4.8.1 Detailed Description

Uses Nose-Hover integration method to thermostat a system (constant T rather than E)

NVT integration with Nose-Hoover thermostat.

Date

11/18/13

Definition at line 13 of file nvt.h.

4.8.2 Constructor & Destructor Documentation

4.8.2.1 nvt_NH::nvt_NH (const float *Q*)

Do NVT integration with Nose-Hoover thermostat.

Date

11/18/13

Initialize integrator

Parameters

in	*Q*	Thermal mass for thermostat

Definition at line 20 of file nvt.cpp.

References integrator::start_.

```
                                        {
    Q_ = Q;
    gamma_ = 0.0;
    start_ = 1;
}
```

4.8.3 Member Function Documentation

4.8.3.1 void integrator::calcForce (**systemDefinition & *sys*)** [inherited]

Calculate the forces on each atom.

Integration

Date

11/19/13

Calculate the pairwise forces in a system. This also calculates the potential energy of a system. The kinetic energy is calculated during the verlet integration.

Parameters

in,out	*sys*	System definition

Definition at line 22 of file integrator.cpp.

References systemDefinition::atoms, systemDefinition::box(), cellList_cpu::checkUpdate(), integrator::cl_, cellList-_cpu::head(), cellList_cpu::list(), systemDefinition::mass(), cellList_cpu::nCells, cellList_cpu::neighbors(), system-Definition::numAtoms(), systemDefinition::potential, systemDefinition::potentialArgs(), systemDefinition::rcut(), and systemDefinition::setPotE().

Referenced by nve::step(), and step().

```
                                                    {
    // For cache coeherency allocate new space for calculations
    float3 empty;
    empty.x = 0; empty.y = 0; empty.z = 0;
    std::vector <float3> acc (sys.numAtoms(), empty);
    const float rc = sys.rcut();

    // every time, check if the cell list needs to be updated first
    cl_.checkUpdate(sys);

    float Up = 0.0;
    const float3 box = sys.box();
    const float invMass = 1.0/sys.mass();

    // traverse cell list and calculate total system potential energy
    std::vector <float> args = sys.potentialArgs();
    #pragma omp parallel for reduction(+:Up) schedule(dynamic, 1)
    for (unsigned int cellID = 0; cellID < cl_.nCells.x*cl_.nCells
      .y*cl_.nCells.z; ++cellID) {
        int atom1 = cl_.head(cellID);
        while (atom1 >= 0) {
            std::vector < int > neighbors = cl_.neighbors(cellID);
            for (int index = 0; index < neighbors.size(); ++index) {
                const int cellID2 = neighbors[index];
                int atom2 = cl_.head(cellID2);
                while (atom2 >= 0) {
                    if (atom1 > atom2) {
                        float3 pf;
                        Up += sys.potential (&sys.atoms[atom1].
      pos, &sys.atoms[atom2].pos, &pf, &box, &args[0], &rc);
                        acc[atom1].x -= pf.x*invMass;
                        acc[atom1].y -= pf.y*invMass;
                        acc[atom1].z -= pf.z*invMass;
                        acc[atom2].x += pf.x*invMass;
                        acc[atom2].y += pf.y*invMass;
                        acc[atom2].z += pf.z*invMass;
                    }
                    atom2 = cl_.list(atom2);
                }
            }
            atom1 = cl_.list(atom1);
        }
    }

    // save acceleration in array of atoms in system
    #pragma omp parallel for
    for (int i = 0; i < sys.numAtoms(); ++i) {
        sys.atoms[i].acc.x = -acc[i].x;
        sys.atoms[i].acc.y = -acc[i].y;
        sys.atoms[i].acc.z = -acc[i].z;
    }

    // set Up
    sys.setPotE(Up);
}
```

4.8.3.2 void nvt_NH::step (systemDefinition & *sys*) [virtual]

Integrate a single timestep forward using Velocity-Verlet integration scheme. This is NOT identical since some intermediate bookkeeping needs to be handled for thermostat. Creates a cell list the first time it is called.

Parameters

in,out	*sys*	System definition

Implements integrator.

Definition at line 32 of file nvt.cpp.

References systemDefinition::atoms, systemDefinition::box(), integrator::calcForce(), integrator::cl_, integrator::dt-_, systemDefinition::instantT(), systemDefinition::mass(), systemDefinition::numAtoms(), systemDefinition::rcut(), systemDefinition::rskin(), systemDefinition::setKinE(), integrator::start_, systemDefinition::targetT(), and system-Definition::updateInstantTemp().

```
                                    {
    int chunk = OMP_CHUNK;
    if (start_) {
        try {
            cellList_cpu tmpCL (sys.box(), sys.rcut(), sys.
  rskin());
            cl_ = tmpCL;
        } catch (std::exception &e) {
            std::cerr << e.what() << std:: endl;
            throw customException("Failed to integrate on first
   step");
        }

        gamma_ = 0.0;
        for (unsigned int i = 0; i < sys.numAtoms(); ++i)  {
            gamma_ += (sys.atoms[i].vel.x*sys.atoms[i].vel.x)+(sys.
  atoms[i].vel.y*sys.atoms[i].vel.y)+(sys.atoms[i].vel.z*sys.atoms
  [i].vel.z);
        }
        gamma_ -= (3.0*(sys.numAtoms()-1.0))*sys.instantT();
        gamma_ /= Q_;

        // get initial temperature
        calcForce(sys);
        float tmp=0.0, Uk = 0.0;
        #pragma omp parallel for reduction(+:Uk)
        for (unsigned int i = 0; i < sys.numAtoms(); ++i) {
            Uk += (sys.atoms[i].vel.x*sys.atoms[i].vel.x)+(sys.atoms
  [i].vel.y*sys.atoms[i].vel.y)+(sys.atoms[i].vel.z*sys.atoms[i].
  vel.z);
        }
        Uk *= sys.mass();
        tmp = Uk;
        Uk *= 0.5;
        tmp /= (3.0*(sys.numAtoms()-1.0));
        sys.updateInstantTemp(tmp);
        sys.setKinE(Uk);
        start_ = 0;
        gammadot_ = 0.0;
        gammadd_ = 0.0;
    }

    tau2_ = Q_/ ((3.0*(sys.numAtoms()-1.0))*sys.targetT());
    gammadd_ = 1/tau2_*(sys.instantT()/sys.targetT()-1);

    // (1) update thermostat velocity and thermostat position
    // velocity half-step
    gammadot_ += dt_*0.5*gammadd_;

    // position step
    gamma_ += gammadot_*dt_;
    // (2) evolve particle velocities
    #pragma omp parallel shared(sys)
    {
        #pragma omp for schedule(dynamic,OMP_CHUNK)
        for (unsigned int i = 0; i < sys.numAtoms(); ++i) {
            sys.atoms[i].vel.x = sys.atoms[i].vel.x*exp(-gammadot_*
      dt_*0.5) + 0.5*dt_*(sys.atoms[i].acc.x);
            sys.atoms[i].vel.y = sys.atoms[i].vel.y*exp(-gammadot_*
      dt_*0.5) + 0.5*dt_*(sys.atoms[i].acc.y);
            sys.atoms[i].vel.z = sys.atoms[i].vel.z*exp(-gammadot_*
      dt_*0.5) + 0.5*dt_*(sys.atoms[i].acc.z);
        }

        // (3) evolve particle positions
        #pragma omp for schedule(dynamic,OMP_CHUNK)
        for (unsigned int i = 0; i < sys.numAtoms(); ++i) {
            sys.atoms[i].pos.x += sys.atoms[i].vel.x*dt_;
            sys.atoms[i].pos.y += sys.atoms[i].vel.y*dt_;
            sys.atoms[i].pos.z += sys.atoms[i].vel.z*dt_;
        }
    }

    // (4) calc force
    calcForce(sys);

    // (5) evolve particle velocities
    #pragma omp parallel shared(sys)
    {
    #pragma omp for schedule(dynamic,OMP_CHUNK)
    for (unsigned int i = 0; i < sys.numAtoms(); ++i) {
        sys.atoms[i].vel.x = (sys.atoms[i].vel.x+sys.atoms[i].
      acc.x*dt_*0.5)*exp(-gammadot_*dt_*0.5);
        sys.atoms[i].vel.y = (sys.atoms[i].vel.y+sys.atoms[i].
      acc.y*dt_*0.5)*exp(-gammadot_*dt_*0.5);
        sys.atoms[i].vel.z = (sys.atoms[i].vel.z+sys.atoms[i].
      acc.z*dt_*0.5)*exp(-gammadot_*dt_*0.5);
        }
    }
    float Uk = 0.0;
    float tmp = 0.0;

    #pragma omp parallel for reduction(+:Uk)
    // get temperature and kinetic energy
    for (unsigned int i = 0; i < sys.numAtoms(); ++i) {
        Uk += (sys.atoms[i].vel.x*sys.atoms[i].vel.x)+(sys.atoms
      [i].vel.y*sys.atoms[i].vel.y)+(sys.atoms[i].vel.z*sys.atoms[i].
      vel.z);
    }

    Uk *= sys.mass();
    tmp = Uk;
    Uk *= 0.5;
    tmp /= (3.0*(sys.numAtoms()-1.0));
    sys.updateInstantTemp(tmp);
    sys.setKinE(Uk);

    // (6) update thermostat velocity
    gammadd_ = 1/tau2_*(sys.instantT()/sys.targetT()-1);
    gammadot_ += dt_*0.5*gammadd_;
}
```

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

- /Users/nathanmahynski/Desktop/CBEMDGPU/nvt.h
- /Users/nathanmahynski/Desktop/CBEMDGPU/nvt.cpp

4.9 systemDefinition Class Reference

Contains all information pertaining to a system being simulated.

`#include <system.h>`

Public Member Functions

- void initRandom (const int N, const int rngSeed)

- void initThermal (const int N, const float Tset, const int rngSeed, const float dx)
- void updateInstantTemp (const float T)

  Manually set the instantaneous temperature.
- void setTemp (const float T)

  Assign the target temperature for NVT simulations.
- void setMass (const float m)

  Assign the mass of each particle.
- void setRcut (const float rc)

  Assign the cutoff radius of the pair potential.
- void setRskin (const float rs)

  Assign the skin radius as a buffer for the neighbor/cell lists.
- void setBox (const float x, const float y, const float z)

  Assign the simulation box size.
- void printBox ()

  Print the box dimesions to stdout.
- float3 box () const

  Report the box dimensions.
- float instantT () const

  Report the instantaneous temperature.
- float targetT () const

  Report the target temperature for NVT simulations.
- float mass () const

  Report the particle's mass.
- float PotE () const

  Report the instantaneous potential energy of the system.
- void setPotE (const float Up)

  Assign the potential energy.
- void setKinE (const float Uk)

  Assign the kinetic energy.
- float KinE () const

  Report the instantaneous kinetic energy of the system.
- float rskin () const

  Report the skin radius for the neighbor/cell lists.
- float rcut () const

  Report the pair potential function cutoff radius.
- void writeSnapshot ()

  Print a snapshot of the system.
- int numAtoms () const

  Report the pair potential function cutoff radius.
- void setPotentialArgs (const std::vector$<$ float $>$ args)

  Assign additional arguments to the pair potential function.
- std::vector$<$ float $>$ potentialArgs ()

  Report additional arguments to the pair potential function.
- void setPotential (pointFunction_t pp)

  Assign pair potential function.

Public Attributes

- pointFunction_t potential

  Pointer to pair potential function.
- std::vector$<$ atom $>$ atoms

  Vector of atoms in the system.

4.9.1 Detailed Description

Contains all information pertaining to a system being simulated.

System definition

Date

11/17/13

Definition at line 16 of file system.h.

4.9.2 Member Function Documentation

4.9.2.1 void systemDefinition::initRandom (const int *N*, const int *rngSeed*)

Initialize a system of N atoms with random velocities and positions on a lattice. Net momeentum is automatically initialized to zero.

Parameters

in	*N*	Number of atoms to create
in	*rngSeed*	Random number generator seed

Definition at line 31 of file system.cpp.

References atoms.

```
                                                                            {
    float3 totMomentum;
    totMomentum.x = 0; totMomentum.y = 0; totMomentum.z = 0;

    if (N < 1) {
        throw customException ("N must be > 0");
        return;
    }

    srand(rngSeed);
    int chunk = OMP_CHUNK;
    unsigned int i;
    atoms.resize(N);
    #pragma omp parallel private(i)
    {
    #pragma omp for schedule(dynamic, chunk)
    for (i = 0; i < N; ++i) {
        if (i < N-1) {
            atoms[i].vel.x = (RNG-0.5);
            atoms[i].vel.y = (RNG-0.5);
            atoms[i].vel.z = (RNG-0.5);
            totMomentum.x += atoms[i].vel.x;
            totMomentum.y += atoms[i].vel.y;
            totMomentum.z += atoms[i].vel.z;
        } else {
            atoms[i].vel.x = -totMomentum.x;
            atoms[i].vel.y = -totMomentum.y;
            atoms[i].vel.z = -totMomentum.z;
        }
        atoms[i].pos.x = (RNG)*box_.x;
        atoms[i].pos.y = (RNG)*box_.y;
        atoms[i].pos.z = (RNG)*box_.z;
        atoms[i].acc.x = 0;
        atoms[i].acc.y = 0;
        atoms[i].acc.z = 0;
    }
    }
}
```

4.9.2.2 void systemDefinition::initThermal (const int *N*, const float *Tset*, const int *rngSeed*, const float *dx*)

Initialize a system of N atoms with random velocities to meet a desired temperature and positions on a lattice. Net momentum is automatically initialized to zero.

Parameters

in	*N*	Number of atoms to create
in	*rngSeed*	Random number generator seed

Definition at line 77 of file system.cpp.

References atoms.

```
                              {
    float3 totMomentum;
    totMomentum.x = 0; totMomentum.y = 0; totMomentum.z = 0;

    if (N < 1) {
        throw customException ("N must be > 0");
        return;
    }

    srand(rngSeed);
    atoms.resize(N);

    // maxwell boltzmann distribution has mean 0 stdev kT/m in each dimension
    typedef std::tr1::linear_congruential<int, 16807, 0, (int)((1U << 31) -1 )
      > Myceng;
    Myceng eng;
    float sig = sqrt(Tset/mass_);
    std::tr1::normal_distribution<float> distribution(0.0,sig);
    float rannum = 0.0;
    float tmpT = 0.0;
    int index = 0;
    const int xs = floor(box_.x/dx);
    const int ys = floor(box_.y/dx);
    const int zs = floor(box_.z/dx);

    // initialize particle positions on a simple cubic lattice
    for (unsigned int x = 0; x < xs; ++x) {
        for (unsigned int y = 0; y < ys; ++y) {
            for (unsigned int z = 0; z < zs; ++z) {
                if (index < N) {
                    atoms[index].pos.x = x*dx;
                    atoms[index].pos.y = y*dx;
                    atoms[index].pos.z = z*dx;
                } else {
                    x = xs;
                    y = ys;
                    z = zs;
                    break;
                }
                index++;
            }
        }
    }

    for (unsigned int i = 0; i < N; ++i) {
        atoms[i].acc.x = 0;
        atoms[i].acc.y = 0;
        atoms[i].acc.z = 0;
        if (i < N-1) {
            atoms[i].vel.x = distribution(eng);
            atoms[i].vel.y = distribution(eng);
            atoms[i].vel.z = distribution(eng);
            totMomentum.x += atoms[i].vel.x;
            totMomentum.y += atoms[i].vel.y;
            totMomentum.z += atoms[i].vel.z;
        } else {
            atoms[i].vel.x = -totMomentum.x;
            atoms[i].vel.y = -totMomentum.y;
            atoms[i].vel.z = -totMomentum.z;
        }
        tmpT += (atoms[i].vel.x*atoms[i].vel.x + atoms[i].vel.y*
      atoms[i].vel.y + atoms[i].vel.z*atoms[i].vel.z);
    }

    // do velocity rescaling to get exactly the right T
    tmpT *= mass_/(3.0*(N-1));
    tmpT /= Tset;
    tmpT = 1.0/tmpT;
    for (unsigned int i = 0; i < N; i ++ ) {
        atoms[i].vel.x = atoms[i].vel.x*sqrt(tmpT);
        atoms[i].vel.y = atoms[i].vel.y*sqrt(tmpT);
        atoms[i].vel.z = atoms[i].vel.z*sqrt(tmpT);
    }
}
```

4.9.2.3 void systemDefinition::setPotential (pointFunction_t *pp*)

Assign pair potential function.

Sets the "host" pair potential function which also sets the GPU equivalent in integrator.cu if using CUDA.

Parameters

in	*pp*	Pointer to pair potential function

Definition at line 20 of file system.cpp.

References potential.

```
                                                           {
    potential = pp;
}
```

4.9.2.4 void systemDefinition::writeSnapshot ( )

Print a snapshot of the system.

Write instantaneous snapshot of the system to a file called "trajectory.xyz" This file is appended not overwritten consecutively.

Definition at line 154 of file system.cpp.

References atoms.

```
                                         {
    static int snapNum = 0;
    if (snapFile_ == NULL) {
        snapFile_ = fopen("trajectory.xyz", "w");
    }

    fprintf(snapFile_, "%d\nSnapshot #%d\n", atoms.size(), snapNum);

    for (unsigned int i = 0; i < atoms.size(); ++i) {
        fprintf(snapFile_, "%s\t%g\t%g\t%g\n", "A", atoms[i].pos.x, atoms
      [i].pos.y, atoms[i].pos.z);
    }

    snapNum++;
}
```

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

- /Users/nathanmahynski/Desktop/CBEMDGPU/system.h
- /Users/nathanmahynski/Desktop/CBEMDGPU/system.cpp

4.10 systemProps Class Reference

Holds all information about the CPU and GPU the simulation is being performed on.

`#include <cudaHelper.h>`

Public Member Functions

- **systemProps** (std::string fname)
- void displayAllProps ()

  Display cpu host and device (if using GPUs) properties.
- __host__ void displayCudaProps ()

Display the properties of the GPU being used.
- void displayHost ()

  Display host name and other properties.
- int maxThreadsPerBlock (const int devID)

  Returns the maximum number of threads per block on the GPU.
- int maxGridDimX (const int devID)

  Returns the maximum number of blocks per grid on the GPU.
- int numDevices () const

  Returns the number of GPUs found attached to the CPU.

4.10.1 Detailed Description

Holds all information about the CPU and GPU the simulation is being performed on.

Functions to assist in using CUDA and/or GPUs

Date

11/21/13

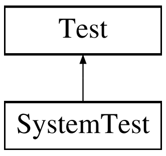
Definition at line 25 of file cudaHelper.h.

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

- /Users/nathanmahynski/Desktop/CBEMDGPU/cudaHelper.h

4.11 SystemTest Class Reference

Inheritance diagram for SystemTest:



Protected Member Functions

- virtual void **SetUp** ()

Protected Attributes

- systemDefinition **a**
- int **natoms**
- float **mass**
- float **L**
- float **eps**
- float **sigma**
- nvt_NH **integrate**

4.11.1 Detailed Description

Definition at line 11 of file unittests.cpp.

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

- /Users/nathanmahynski/Desktop/CBEMDGPU/unittests.cpp