SPH-DEM Documentation

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1 Introduction

SPH-DEM is primarily an implementation of the SPH method, described in more detail in the following papers [1, 4, 2]. It has the following main features

- Written in C++
- Modular structure separates the parallel data structure from the SPH/DEM equation. Uses C++ templates to efficiently apply arbitrary functions on particles and their neighbours
- Fully parallel implementation using MPI
- Output files use VTK format
- SPH Functionality
 - Weakly compressible formulation, as described in [4]
 - Lenard-Jones type boundary particles, periodic boundaries and ghost boundaries
 - Variety of different viscosity terms and kernel options
 - First order corrected kernel derivatives
- DEM Functionality
 - Linear Spring Dashpot and Lubrication contact models
 - SPH boundary particles can be used for walls
- SPH-DEM coupling based on Locally Averaged Navier-Stokes Eqns.
 Drag terms: De Felice, Ergun and Stokes. Details of this implementation can be found in [3]

2 Basic Usage

Each project/simulation has its own directory under the root source directory for SPH-DEM. For example, to create a new project called *testProject*:

```
1 cd $SPH-DEM_SOURCE_DIR
2 mkdir testProject
3 cd test Project
```

It is helpful to simply copy the contents of an older project in order to initialise the new project. For example, using the taylor green vortex test case taylorGreen:

```
1 cp taylorGreen/* testProject/
```

Then navigate to the new project, edit the configuration files (not shown, see Section 3 for details), and then compile the project

```
cd testProject
...edit configuration files...
make
```

You can setup the initial state of the project using the setup executable, and then run the simulation using run.

```
1 ./setup INITDATA_NAME
2 ./run INITDATA_NAME START_TIMESTEP OUTPUTDATA_NAME
```

Here INITDATA_NAME is the name given to the initial data files, START_TIMESTEP is the timestep to start the simulation (normally 0 if you are not restarting a simulation) and OUTPUTDATA_NAME is the name given to the output data files. See Section 5 for more details of the input/output data formats.

3 Project Description

This sections describes the per-project configuration and setup. The main configuration options can be set in customConstants.h and setup.cpp. The header file customConstants.h contains a list of c++ constants and #defines that can customise each simulation. The source file setup.cpp is compiled to an executable that constructs and writes out the initial data for the simulation.

Each project also has two classes *customSim* and *customOutput* that allow the user to customise the simulation.

3.1 Custom Constants

Different options in SPH-DEM are controlled by #define statements and constants defined in the *customConstants.h* file in each project subdirectory. For example, here is a listing for the included *taylorGreen* project.

```
#ifndef CUSTOMCONSTANTS_H
  #define CUSTOMCONSTANTS.H
3
4
  #include <cmath>
5
6 #define _2D_
  #define NDIM 2
  #define INCOMPRESS
10
  const double PI = 3.14159265;
12 const double RMIN[NDIM] = \{0,0\};
  const double RMAX[NDIM] = \{1.0, 1.0\};
13
15 #define TIME_OVERIDE 0
16 #define START_TIME 0
17 #define NSTEP_OVERIDE 0
18 #define START_NSTEP 0
  const double GAMMA = 1.4;
  const double HFAC = 1.5;
22
23
  const int PERIODIC[NDIM] = \{1,1\};
24
25
  const double DENS = 1000.0;
26 const double REFD = 1000.0;
  const int GHOST[2*NDIM] = \{0,0,0,0,0\};
28
  const double DENS_DROP[NDIM] = \{0,0\};
29
30 #define WENDLAND
31 #define VISC_MONAGHAN
32 #define VORTLEASTSQUARES
```

```
33
34 #define NO_ANTICLUMPING
35 #define CONST_H
36
  const double MAXTIME = 6;
37
  const double DAMPTIME = 0;
  const int OUTSTEP = 100;
40 const int RESTART_EVERY_N_STEPS = 100;
41 const int REINIT_DENS_EVERY_N_STEPS = 2000000;
  const int REINIT_DENS_AT_N_STEPS = 2000000;
  const int DAMP_STEPS = 0;
45 const double NVORT = 2;
46 const double REYNOLDS.NUMBER = 100;
  const double VREF = 1.0;
  const double VMAX = VREF;
  const double VISCOSITY = VREF*(RMAX[0]-RMIN[0]) /REYNOLDS_NUMBER;
49
  const double CSFAC = 10.0;
  const double SPSOUND = CSFAC*VMAX;
  const double PRB = pow(REFD/DENS,6)*pow(SPSOUND,2)*REFD/7.0;
53
54
55
  const int NX = 20;
56 const int NY = 20;
57
  const double PSEP = (RMAX[0] - RMIN[0]) / NX;
  const double H = HFAC*(RMAX[0] - RMIN[0]) / NX;
59
  const double BFAC = 1.0;
  const int MAX_NUM_PARTICLES_PER_CPU = NX*NY+1;
61
  const double GRIDSEP = PSEP;
```

This file is a mix of define statements and constants that are used for the main SPH-DEM program, and others (e.g. NVORT, REYNOLDS_NUMBER) that are only used within the *taylorGreen* project directory.

The rest of the section is devoted to listing all the available defines and constants used by the SPH-DEM program. The comments describe each option and the code gives an example of use.

3.1.1 Simulation Geometry

```
number of spatial dimensions. Can be 1, 2 or 3.
3
   * /
4 #define NDIM 2
5
   * RMIN and RMAX are arrays containing the minimum and maximum
6
7
   * of the simulation
8
   */
9
  const double RMIN[NDIM] = \{0,0\};
10 const double RMAX[NDIM] = \{1.0, 1.0\};
11
12
   * The intial (and average) particle spacing between sph
13
        particles
14
   */
15
  const double PSEP = (RMAX[0] - RMIN[0]) / NX;
16
17
   * spacing between boundary particles
18
```

```
20 const double BFAC = 1.0;

21 /*

22 /*

23 * The spacing of the regular grid (if used)

24 */

25 const double GRIDSEP = PSEP;
```

3.1.2 Boundary Conditions

```
1
   * Each entry in PERIODIC (0 or 1) tells the program if the
2
        simulation
   * domain is periodic in that spatial dimension
3
4
   */
  \mathbf{const} int PERIODIC[NDIM] = {1,1};
5
6
7
   * Each entry in GHOST (0 or 1) tells the program if that
8
        boundary \ is \ a \ ghost \ or
   st mirror boundary. Entries 0 and 1 refer to the lower and upper
9
         boundaries
10
    st in the x direction, 2 and 3 refer to the lower and upper
        boundaries in the y
11
   * direction, and so on.
12
13
14 const int GHOST[2*NDIM] = {0,0,0,0};
15
16
   * Each entry in DENS_DROP gives the relative density drop
17
        experianced by the
18
    * SPH particles as they cross the periodic boundary in that
        spatial dimension
19
   const double DENS_DROP[NDIM] = \{10,0\};
20
```

3.1.3 Timing

```
1
3
   * Time at which simulation ends
  const double MAXTIME = 6;
5
6
7
   * Time at which damping ends (0 for no damping)
8
9
  10
11
12
13
   * Number of output timesteps (time between output timesteps is
        therefore
   * constant during the simulation
14
15
16 | \mathbf{const} | \mathbf{int} | \mathbf{OUTSTEP} = 100;
17
18
19
   * After RESTART_EVERY_N_STEPS timesteps, a restart file is
       written out
20
   st so that the simulation can be restarted at this point
21
22 const int RESTART_EVERY_N_STEPS = 100;
```

```
23
24
   * TIME_OVERIDE (0 or 1) tells the program to override the
        starting time read in
26
   * from the datafiles
27
   * START_TIME is the time used if TIME_OVERRIDE = 1
28
29
30 #define TIME_OVERIDE 0
31 #define START_TIME 0
32
33
   * NSTEP_OVERIDE (0 or 1) tells the program to override the
34
        starting\ timestep
35
   * number read in from the datafiles
36
   * START\_NSTEP is the timestep number used if NSTEP\_OVERRIDE = 1
37
38
   */
39 #define NSTEP_OVERIDE 0
40 #define START_NSTEP 0
```

3.1.4 SPH options

```
* GAMMA is the exponent used in the SPH pressure equation of
3
   * /
4
  const double GAMMA = 1.4;
5
6
   st REFD is the reference density used in the pressure equation
        of state
8
   \textbf{const double} \ \text{REFD} = \ 1000.0; 
g
10
11
   * The speed of sound. This is artificialy set for
12
        incompressible \ simulation
13
   * to 10 times the maximum velocity.
14
15 const double SPSOUND = CSFAC*VMAX;
16
17
   * PRB is the multiplicative constant in the pressure equation
18
        of state.
19
   */
20
  const double PRB = pow(REFD/DENS, 6) *pow(SPSOUND, 2) *REFD / 7.0;
21
22
23
   * Each SPH smoothing length is HFAC times the average particle
        spacing\ PSEP
24
   */
25
  const double HFAC = 1.5;
26
27
28
   st Options to re-initialise the sph particle density ever n
        steps or once
29
   st at step n. If REINIT_DENS_MLS is set use a Moving Least
        Squares kernel
30
   * to reinit the density. Otherwise use a normal sph density sum
31
   */
  const int REINIT_DENS_EVERY_N_STEPS = 2000000;
33 const int REINIT_DENS_AT_N_STEPS = 2000000;
34 #define RINIT_DENS_MLS
```

```
35
36
     Different sph kernels. If none are chosen the standard cubic
37
        spline is used
38
39 #define WENDLAND
40 #define QUINTIC
41 #define HANN
42
43
44
   * Different viscosity terms. At least one must be chosen. The
       ARTIFICIAL
45
     viscosity can be added to any of the others.
46
47 #define VISC_MONAGHAN
48 #define VISC_MORRIS
49 #define VISC_CLEARY
50 #define VISC_ARTIFICIAL
  const double ALPHA_ARTIFICIAL = 0.1;
52
53
   *\ kinematic\ vicosity\ of\ the\ fluid
54
55
  const double VISCOSITY = VREF*(RMAX[0] - RMIN[0]) / REYNOLDS_NUMBER;
56
57
58
59
   * Do not use the monaghan anti-clumping term (this is used by
        default)
60
61 #define NO_ANTICLUMPING
62
63
   * Do not vary the particle smoothing length h with density
64
65
66 #define CONST_H
67
68
69
   * Use the variable h correction terms proposed in
70
   * Price, D., 2012. Smoothed particle hydrodynamics and
        magnetohydrody-
   * namics. Journal of Computational Physics 231, 759 794.
71
72
73 #define VAR_H_CORRECTION
74
75
   * Use the corrected kernel gradient terms proposed in
76
   * J. Bonet, T.-S.L. Lok, Variational and momentum preservation
77
        aspects of
   * Smooth Particle Hydrodynamic formulations, Computer Methods
78
        in Applied
   * Mechanics and Engineering, Volume 180, Issues 1 2, 15
79
        November 1999, Pages
   * 97-115
80
81
82 #define CORRECTED_GRADIENT
```

3.2 Setup

Below is shown an example of the code neccessary to write out initialisation data for SPH-DEM. Note that this is not a neccessary step to running a simulation. If the initialisation data can be obtained in another fashion, or from a restart file from a previously run simulation, then this can be used to start another SPH-DEM simulation.

```
1 int main(int argc, char *argv[]) {
      if (argc != 2) {
 2
         cout << "Usage: setup outfilename" << endl;
3
4
         return(-1);
 5
6
      string filename = argv[1];
 7
 8
      vector < C particle > ps;
9
      Cparticle p;
10
      for (int i=0; i \le NX; i++) {
11
         for (int j=0; j< NY; j++) {
12
13
             p.tag = ps.size()+1;
             p.r = (i+0.5)*PSEP+RMIN[0], (j+0.5)*PSEP+RMIN[1];
14
15
             p.dens = DENS;
            p.mass = PSEP*PSEP*DENS;
16
17
             p.h = H;
             p.v = -VREF*cos(2.0*PI*p.r[0])*sin(2.0*PI*p.r[1]), VREF*
18
                 \sin (2.0*PI*p.r[0])*\cos (2.0*PI*p.r[1]);
19
             p.vhat = p.v;
20
             p.iam = sph;
21
             ps.push_back(p);
22
23
      }
24
25
      vector < vector < double > > vprocDomain;
26
      vector<Array<int ,NDIM> > vprocNeighbrs;
27
      vector<particleContainer > vps;
28
      vectInt split;
29
      split = 1,1;
      Nmisc::splitDomain(ps, split, vps, vprocDomain, vprocNeighbrs);
30
31
32
      CglobalVars globals;
33
      Cio_data_vtk ioFile(filename.c_str(),&globals);
34
35
      int nProc = product(split);
36
      for (int i=0; i< nProc; i++) {
37
         globals.mpiRank = i;
38
         for (int j=0; j<NDIM*2; j++)
39
             globals.procDomain [\ j\ ] \ = \ vprocDomain [\ i\ ] [\ j\ ];
40
          globals.procNeighbrs = vprocNeighbrs[i];
         ioFile.setFilename(filename.c_str(),&globals);
41
42
         ioFile.writeGlobals(0,&globals);
43
         ioFile.writeRestart(0, vps[i],&globals);
44
         ioFile.writeDomain(0,\&globals);
45
46
```

The above code example can be split into three sections. In the first the sph particles are created and added to the vector of particles. In the second the particles and domain are spit evenly among the number of CPUs chosen by the user. In the third the result is written to the data files

3.2.1 Creating new SPH particles

```
vector < C particle > ps;
Cparticle p;

for (int i = 0; i < NX; i++) {
    for (int j = 0; j < NY; j++) {
        p.tag = ps.size()+1;
        p.r = (i+0.5)*PSEP+RMIN[0],(j+0.5)*PSEP+RMIN[1];</pre>
```

```
8
                    p.dens = DENS;
 9
                    p.mass = PSEP*PSEP*DENS;
10
                    p.h = H;
                    {\rm p.v} \, = \, - \text{VREF*} \cos \left( \, 2.0 \, * \, \text{PI*p.r} \, [\, 0 \, ] \, \right) \, * \sin \left( \, 2.0 \, * \, \text{PI*p.r} \, [\, 1 \, ] \, \right) \, , \\ \text{VREF*}
11
                           \sin(2.0*PI*p.r[0])*\cos(2.0*PI*p.r[1]);
12
                    p.vhat = p.v;
13
                    p.iam = sph;
14
                    ps.push_back(p);
15
16
```

The class *Cparticle* contains all the data for a single sph particle. Here we are creating a 2D regular grid of particles that completly fill the simulation domain. So we loop through the number of particles chosen (using NX and NY) and create the particles. We are simulating a taylor green vortex, so the initial velocity of the particles is set using the analytical expression for the vortex velocity field.

Each particle has a volume equal to a square of side PSEP, which along with the density DENS gives the particle mass. The smoothing length is given by H (which in turn is given by HFAC*PSEP) and the particle type is set to "sph". The two velocities, v and vhat, are set equal. The former is the "true" velocity field (used to calculate viscosity) while the latter is an (optionally) smoothed velocity which is used to update the particle positions (and also used to calculate the change in density with time).

3.2.2 Split data among CPUs

```
vector < double > vprocDomain;
vector < Array < int ,NDIM> > vprocNeighbrs;
vector < particleContainer > vps;
vectInt split;
split = 1,1;
particleContainer ps;
Nmisc:: splitDomain(ps, split, vps, vprocDomain, vprocNeighbrs);
```

The *splitDomain* procedure splits the particles among equal sized subdomains according to the *split* vector given by the user. This example only uses one CPU. If two CPUs were required, then this could be modified to

```
1 split = 2,1;
```

The vectors *vprocDomain* and *vprocNeighbrs* contain the side min/max point information of the domains and neighbourhood information (i.e. which domains are next to each other). The resultant vector of vector of particles is given in *vps*.

3.2.3 Write Data

```
CglobalVars globals;
Cio_data_vtk ioFile(filename.c_str(),&globals);

int nProc = product(split);
for (int i=0;i<nProc;i++) {
    globals.mpiRank = i;
    for (int j=0;j<\nDIM*2;j++)
        globals.procDomain[j] = vprocDomain[i][j];
```

```
globals.procNeighbrs = vprocNeighbrs[i];

ioFile.setFilename(filename.c_str(),&globals);

ioFile.writeGlobals(0,&globals);

ioFile.writeRestart(0,vps[i],&globals);

ioFile.writeDomain(0,&globals);

}
```

This code segment writes out the particles, domain information and global variables to restart files, which can then be used to initialise the simulation. Note that this is the same procedure used when writing periodic restart information while the simulation is running, so the initialisation and restart procedure for SPH-DEM are identical.

3.3 Custom Simulation and Outputs

Within each project directory are defined two classes, *customSim* and *customOutput*. These allow the user to add arbitrary code into the simulation to, for example, move boundary particles, insert/remove particles or apply a custom postprocessing algorithm. They are both derived from base classes which do nothing, so if no modification to the base simulation is neccessary the user only has to leave the classes empty.

The base class for *customSim* is as follows:

```
class CcustomSimBase {
      public:
2
3
         CcustomSimBase(CdataLL *_data, double _time): data(_data),
             time(_time) {}
         double getTime() { return time; }
4
5
         virtual void beforeStart(double newTime) { time = newTime;
6
         virtual void beforeMiddle(double newTime) { time = newTime
         virtual void beforeEnd(double newTime) { time = newTime; }
7
 8
         virtual void afterEnd(double newTime) { time = newTime; }
9
         virtual vect vFilter(const vect vin, const vect rin) {
             return vin; }
10
         virtual vect rFilter(const vect rin) { return rin; }
11
12
      protected:
13
         double time:
         CdataLL *data;
14
15
  };
```

This class defines a number of virtual functions, beforeStart, beforeMiddle etc. which are called either before or after the start, middle or end of each timestep. Users can reimplement these functions in the customSim class to insert code at these points. In addition, the vFilter and rFilter functions can be used to filter the position and velocity of each particles respectively before they are writen to output files.

The protected variable data is a pointer to the main particle data structure, and the description for its use can be seen in Section 4.

The listing for the base class for *customOutput* is given below.

```
class CcustomOutputBase {
   public:
        CcustomOutputBase(CdataLL *_data): data(_data) {}
```

This contains one function, *calcOutput* which is called just before the files are written every output timestep. Users can therefore apply any custom post-processing here.

4 Writing New Functions

In order to add custom simulation and/or post-processing code to the simulation the user will need to use the included particle data structure CdataLL, described in dataLL.h, dataLL.cpp and dataLL.impl.h in the main source code directory. This class holds the particle data and handles the domain geometry, parallel processing and the application of custom operations to the particle data. It is the latter functionality we will use in this section.

Two of *CdataLL*'s methods are:

The first applies the function The funct to all the particles in the simulation that satisfy the function If funct. The second applies the function The funct to all the particles (that satisfy If funct and their neighbouring particles in the simulation. The template class T and the corresponding input variable are optional and are used to pass data to the functions.

In order to use the first method, *traverse*, we first need to define an inline function to apply to the particles.

```
inline void addGravity(Cparticle &p,CglobalVars &g) {
   p. ff [2] -= 9.81;
   p. f [2] -= 9.81;
}
```

This is a simple function that adds gravity to a single particle. Too apply this function to all the particles in the simulation we use data, which is a pointer to the main CdataLL datastructure, to call the traverse method. We also use the ifSph function to only apply addGravity to the sph particles in the simulation.

```
1 data->traverse<addGravity, Nsph::ifSph>();
```

Looking at the *customSim* and *customOutput*, you can see that the *data* pointer is a member variable in each class. As described previously, this points to the main particle data structure of the simulation.

To use the *neighboursGroup* method, we once again define an inline function to apply to the particles. But this time the definition of the function is slightly different.

```
1 inline void calcDensity (Cparticle &p, vector < Cparticle *> &
         neighbrs, CglobalVars &g) {
        p.dens = p.mass*W(0,p.h);
        for (int i=0;i<neighbrs.size();i++) {
3
 4
             Cparticle *pn = neighbrs[i];
            \label{eq:continue} \textbf{if} \ ((\,\texttt{pn->} \texttt{iam} \ != \ \texttt{sph}\,) \&\&(\texttt{pn->} \texttt{iam} \ != \ \texttt{sph}\, \texttt{Boundary}\,)\,) \ \ \textbf{continue}\,;
 5
 6
            vect dr = p.r-pn->r;
 7
            double r = len(dr);
 8
            p.dens += pn->mass*W(r/p.h,p.h);
 9
10
```

This function loops over all the neighbouring particles and calculates a standard sph density interpolation.

To use this function, we simple call the *neighboursGroup* method from the main particle datastructure. We will also use the *ifSphOrSphBoundary* function to only apply *calcDensity* to the sph or boundary sph particles.

```
data->neighboursGroup<calcDensity,ifSphOrSphBoundary>();
```

5 IO Format

The datafiles written by SPH-DEM are organised around a base filename, given by the user. As an example for the rest of this section, we will use *results* as a base filename. Using this, the list of datafiles are

resultsDDDDD_NN.vtu: These

These are the particle properties (position, velocity, density etc) written in the VTK file format. DDDDD is the timestep number and NN is the CPU number. Each CPU writes its own particles to a separate file

resultsDDDDD.pvtu:

These are small files that just point to each $resultsDDDDD_NN.vtu$ file for timestep DDDDD

resultsGlobalsNN.dat:

These are csv text files, using spaces for separators instead of a comma, that contain the global variables for each timestep. Things like total kinetic energy, momentum, time, CPU time, timestep etc. Each CPU writes out a different globals datafile, but the results Globals 0.dat file is the file that is of main interest, since all the "total" variables are summed across the CPUs in this file. See the first line in the file to see the list of global variables written.

resultsDomainNN.dat:

This is a text file containing the domain extents for each CPU. This is primarily for internal use by SPH-DEM.

resultsRestartDDDDD_NN.vtu:

These are sim-ilar to resultsDDDDD_NN.vtu, but are used to restart the program. They therefore use better accuracy (doubles instead of floats) and contain more particle properties that the normal output datafiles.

6 SPH DEM Functionality

This section describes the DEM functionality added to SPH-DEM and the new user options for both DEM and the coupling between the sph and dem particles.

6.1 Dem Particle

A new particle type *dem* has been added. When creating this new particle, create a new particle as per the sph particle, but with the following changes:

```
1 ...
p.dens = DEM_DENS;
p.h = DEM_SEARCH_RADIUS;
p.mass = DEM_VOL*DEM_DENS;
p.iam = dem;
...
```

To help with the initialisation of dem projects, a few helper functions are included in misc.h. These are:

```
1
 2
     Add regular grid of dem particles within the rectangular
         block defined by
     the points minRange and maxRange. The grid spacing is
 3
        calculated using the
   * desired porosity
 4
5
   */
   \mathbf{void} \ \ \mathbf{addGridDEMparticles} \ (\ \mathbf{vector} < \mathbf{Cparticle} > \ \& \mathbf{ps} \ , \mathbf{const} \ \ \mathbf{double}
6
       minRange [NDIM], const double maxRange [NDIM], const double
       porosity);
7
 8
9
    * Add dem particles randomly within the rectangle defined by
        the points
     minRange and maxRange. The number of particles inserted is
10
        calculated
11
   * using the desired porosity
12
   void addRandomDEMparticles (CdataLL *data, const double minRange [
13
       NDIM], const double maxRange[NDIM], const double porosity);
14
15
   st Add dem particles randomly within a vertical cylinder. The
16
        origin point,
    * radius and height define the cylinder dimensions. The number
17
        of particles
18
      inserted is calculated using the desired porosity
19
20
   void addRandomDEMparticlesCyl(CdataLL *data, const vect origin,
       const double radius, const double height, int n);
```

6.2 New Custom Constants

Some new constants and options are included to handle the new dem and sph-dem functionality. These are described below.

6.2.1 DEM

```
/*
* Radius of dem particles. Used in dem-dem contact calculation
and

* dem-sph drag caculation

*/
const double DEM_RADIUS = 0.0005;

/*
* Volume of dem particles.
```

```
10 const double DEM_VOL = (4.0/3.0)*PI*pow(DEM_RADIUS,3);
11
12
13
  * Density of dem particles
14
15 const double DEM_DENS = DENS*1.5;
16
17
18
   * reduced mass of dem particles. since all dem particles
19
   * have equal mass this will be equal to 0.5*dem_mass
201
  const double DEM_MIN_REDUCED_MASS = 0.5*DEM_MASS;
22
23
24
   * spring and damping constants for linear spring dash-pot
   * Also used for lubrication contact force if particles are
25
   * in direct contact
27
28 const double DEM_K = 1.0e01;
29
  const double DEMGAMMA = 0.0004;
30
  * max number of dem particles. Used to allocate memory
32
33
34 const int MAX_NUM_DEM_PARTICLES = 1.0*NDEM;
35
36
37
   * all dem particles are fixed in space
38
39 #define FIXED_DEM
40
41
   * no dem-dem contacts
42
43
44 #define NO_DEM_CONTACTS
45
46
47
   * All dem particles translate as a solid block
   * Use to simulate a porous block
49
50 #define DEM_BLOCK
51
52
53
   * Two different contact models implemented. LINEAR is a
  *\ linear\ spring-dashpot\ model\ and\ LUBRICATION\ models
54
  * lubrication force between particles immersed in water.
  st ROUGHNESS_EPSILON is the separation distance, scaled
57
   * by particle radius, at which the lubrication force swaps
58
   * to a spring-dashpot model.
59
   */
60 #define LINEAR
61 #define LUBRICATION
62 const double ROUGHNESS_EPSILON = 0.01;
```

6.2.2 SPH-DEM Coupling

```
1 /*
2 * Necessary to switch on sph-dem coupling and
3 * any dem functionality
4 */
5 #define LIQ.DEM
6 /*
```

```
* defines the coupling radius used for sph-dem coupling.
9
   * This is used when calculating porosity and interpolating
10
   * particle drag from dem to sph phases.
11
12 const double LIQ_DEM_COUPLING_RADIUS = 8*DEM_RADIUS;
13
14
   * Normally the dem particles collide with any boundary
15
16
   * particle boundaries. This turns this off so that the user
17
   st can define their own custom dem boundaries (in customSim)
18
19 #define LIQ_DEM_CUSTOM_WALL_CONTACTS
20
21
22
   * Normally the drag calculated on the dem particles is
        transferred
23
   * to the sph particles via a kernel interpolation. This turns
24
   st off and calculates the drag separatly on the sph particles
25
  #define LIQ_DEM_SEPARATE_DRAGS
26
27
28
29
   * Turns off the drag on the sph particles
30
31 #define LIQ_DEM_ONE_WAY_COUPLE
32
33
34
   st Uses a variable timestep condition for the liq-dem coupling
35
  #define LIQ_DEM_VARIABLE_TIMESTEP
```

References

- [1] R. A. Gingold and J. J. Monaghan. Smoothed particle hydrodynamic: theory and application to non-spherical stars. *Monthly Notices of the Royal Astronomical Society*, 181:375–389, 1977.
- [2] J. J. Monaghan. Smoothed particle hydrodynamics. Reports of Progress in Physics, 68:1703–1759, August 2005.
- [3] M. Robinson, S. Luding, and M. Ramaioli. Fluid-particle flow modelling and validation using two-way-coupled mesoscale SPH-DEM. *submitted to Int. Journal of Multiphase Flow*, 2012.
- [4] M. Robinson and J.J. Monaghan. Direct numerical simulation of decaying two-dimensional turbulence in a no-slip square box using smoothed particle hydrodynamics. *International Journal for Numerical Methods in Fluids*, 2011.