User Guide - LBM with Multiphase

Daniel Lehmberg, Tord Kriznik Srensen, Vishal Sontakke

Open a terminal at the source folder and type in make to build the project with assertion checks enabled (recommended). These checks are done for negative distribution values. Alternatively one can also use make speed to build the project without assertion checks (not recommended if randomly chosen values for the parameter G are chosen).

Once the project is built, the scenario file needs to be set up. Open the project.dat file inside the scenarios folder with any text editor. This file already consists default values of the input parameters to the code. Following is a description of all the parameters:

- xlength: This is the size of the cubic domain. Each cell in the domain is a cube of length 1 and thus the parameter xlength gives the number of cells in each direction. The total number of cells would thus be xlength³.
- rhoRef0, rhoRef1: The reference density for the component(s).
- rhoFluct: When initializing a single component its density is initialized with a random perturbation of size rhoFluct around rhoRef.
- numComp: The number of components can be specified with this parameter. Currently initialization for numComp = 1 and 2 is supported¹. In case of a single component we have a density initialization with random perturbations. In case of 2 components, the initialization is based on randomly selecting a cell and putting density of one component to rhoRefof that component and the other to 0.0 in this cell, thus creating a random distribution of the 2 components.
- tau0, tau1: Based on the number of components one can provide a value for the relaxation time for the component(s). The components are numbered starting with a zero index and thus component 1 has relaxation time tau0 and component 2 has relaxation time tau1.
- m0,m1: This is the molecular mass of the component(s).
- G00, G01, G10, G11: This is the interaction matrix giving the value for the Green's function based on nearest neighbor interaction. The value of Gij gives the strength of the interacting potential between components i+1 and j+1 since the components are numbered with index 0.

¹Note: Multicomponent simulation is not fully supported without code adaptations

• psi0, psi1: This takes in integer values and uses the equation corresponding to that integer as the effective number density for that component as given below:

- 0:
$$\psi(x) = 1 - \exp(x)$$

- 1: $\psi(x) = x$

- timesteps: This gives the number of time steps the simulation should run for.
- timestepsPerPlotting: This gives the number of time steps after which an output file must be written for visualization.
- timestepDouble: Double the timestep between plot after each timestep where a plot happened if this does not equal 0.
- timestepMax: This gives the maximum number of timesteps between plots.
- iProc, jProc, kProc: These parameters specify the number of sub-domains in each direction for parallel computation. In the x direction the domain will be divided into iProc sub-domains, in the y direction jProc sub-domains, and in the z direction kProc sub-domains. Thus we have iProc*jProc*kProc number of processes, each working on a cuboid.

Once the parameters are set up, one can open the terminal in the source folder and type in

mpirun -np <iProc*jProc*kProc> ./lbsim scenarios/project.dat

where <iProc*jProc*kProc> is the product of the number of sub-domains in each direction, which equals the total number of processes that are to be used by MPI.

If the program runs successfully, one can use Paraview to visualize the result. In Paraview, the files with the extension *.pvts should be opened to view the entire domain at once. It is recommended to use the CelldataToPointdata filter to view a more smoother interpolated result.