

Documentation

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1 How to run the program

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. Go to the `scenarios` folder and open the `project.dat` file 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 xlength^3 .
- **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 **rhoRef** of that component and the other to 0.0 in this cell, thus creating a random distribution of the 2 components.

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

- **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.
- **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 $\langle iProc*jProc*kProc \rangle$ 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.