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 $\texttt{xlength}^3$.

- `numComp`: The number of components can be specified with this parameter. Currently initialization for `numComp` $= 1$ and 2 is supported. In case of a single component we have a density initialization with 1% random perturbation. In case of 2 components, the initialization is based on randomly selecting a cell and putting density of one component to `1.0` 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`.

- `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.

- `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 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.