Program description

MPI-style parallelized MATLAB programs for simulating Shan and Chen multicomponent multiphase lattice Boltzmann method [1].

Specifically, these programs simulate two-component two-phase fluid flows in 2D through empty domain or a domain with solid objects in it's interior. The programs can optionally run multiscale modeling procedure described in [2]. Details on the method, parallelization, multiscale modeling approach, and programs performance can be found in [3]. Short description of usage and programs can be found in programs themselves.

Programs were originally run on 12 Intel Xeon X5690 3.47 GHz processors on a desktop computer or 12 Intel Xeon CPU E5-2670 2.60GHz processors on a HPC cluster node. Developed parallel programs on 12 processors were at least 7.6 times faster than when run on a single processor yielding efficiency of 63%. Future developement may include transfering these programs into C or C++ with MPI.

Programs included here follow the simulation algorithm developed in [3]:

1. `bubble_ini_dev.m`
   Program for development of a bubble or droplet surrounded by continuous fluid in a shorter domain; used in all the later programs

2. `bubble_in_a_cage.m`
   Program for development of fluid flow field around the bubble/droplet trapped in a cage made of solid nodes. Domain should be the final architecture to be used in the next program.

3. `no_cage.m`
   Final step - simulation of bubble/droplet flow through i) array of solid features - pillars or posts ii) empty domain or iii) empty domain with multiscale modeling; Includes two options for treating architectural defects through fluid-solid interactions.

Besides functions for LBM computation, this set includes a program `staggered_geom.m` for creating a domain with circular, staggered pillars used in above programs when modeling domain with solid features. The geometry is introduced in a form that resembles macro substitution, which is not the best design choice and will be changed in the future versions of the program.

Directory `EMPTY` contains files as applied for modeling of an empty domain with multiscale modeling.

References

[1] Xiaowen Shan and Hudong Chen. Lattice boltzmann model for simulating flows with multiple phases and components. *Physical Review E*, 47(3):1815, 1993.

[2] Agnieszka Truszkowska, P Alex Greaney, and Goran Jovanovic. Multiscale lattice boltzmann modeling of two-phase flow and retention times in micro-patterned fluidic devices. *Computers & Chemical Engineering*, 95:249–259, 2016.

[3] Agnieszka Truszkowska. *Multiscale modeling of two-phase flows in microarchitectures with microfeatures.* PhD thesis, 2014.