

## The coarse-grained time stepper for a lattice Boltzmann model

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In some applications, one wants to study the macroscopic behavior of a system, but only microscopic or mesoscopic evolution laws are available. Kevrekidis *et al.* developed a coarse-grained time stepper [1] which evolves the macroscopic variables for such a system over a certain time interval using only these microscopic or mesoscopic evolution laws. For this procedure, it is assumed that a closed macroscopic description exists conceptually such that the macroscopic behavior can be described by a few macroscopic variables. A coarse-grained time step consists of three substeps. First, the microscopic variables are initialized from the given macroscopic state in the *lifting* or *reconstruction* step. These microscopic variables are then evolved over the desired time interval using the microscopic simulator. Finally, the macroscopic variables are computed from the final microscopic values. The procedure relies on a separation of time scales between the macroscopic variables and the other variables that are only relevant at the microscopic scales. As an example, we will use a lattice Boltzmann model (LBM) for the one-dimensional FitzHugh-Nagumo reaction-diffusion system. For this system, a macroscopic (PDE) description in terms of the density, i.e., the lowest-order moment of the LBM distributions, does exist.

The initialization of the microscopic model in the reconstruction step is crucial. Since the microscopic simulator needs more information than provided by the initial macroscopic variables, this missing information has to be filled in. Due to the time scale separation, the higher-order moments of the state become slaved to, i.e., become functionals of, the lowest-order moments (the macroscopic variables) very quickly, irrespective of the quality of the initialization. However, when the reconstruction is not optimal, the macroscopic time trajectory can differ significantly from the intended one, i.e., the trajectory for the full LBM, even after slaving has been obtained. We will show that it is important to reconstruct the missing initial higher-order moments as close as possible to their correctly slaved values (slaved with respect to the initial macroscopic variables). In this way the reconstruction-induced errors will be small and the trajectory for the coarse-grained time stepper will approximate the desired one well. Consequently, good macroscopic information along the trajectory can already be obtained after a very short time interval. This can be an important benefit for numerical techniques build on top of the coarse-grained time stepper, like time stepper based numerical bifurcation analysis [2] and acceleration techniques for time integration, e.g., *projective integration* [1].

### References

- [1] I. G. Kevrekidis, C. W. Gear, J. M. Hyman, P. G. Kevrekidis, O. Runborg and C. Theodoropoulos. Equation-free, coarse-grained multiscale computation: Enabling microscopic simulators to perform system-level analysis. *Comm. Math. Sci.*, 1(4):715–762, 2003.
- [2] P. Van Leemput, K. Lust and I. G. Kevrekidis. Coarse-grained numerical bifurcation analysis of lattice Boltzmann models. *in preparation*.