Lattice Boltzmann methods as tools in Earth System Science

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Introduction

Performance increase of supercomputers [Dongarra, 2014] affords Earth System Models (ESMs) to expand the range of included processes (e.g. increase in spatial resolution [Spall, 2010] or incorporation of additional physical and geochemical processes [Stepanek and Lohmann, 2012]).
Here, we present the lattice Boltzmann method (LBM), as a novel modeling approach for some of the new processes included in ESMs. During the last two decades, LBM has been developed and successfully applied to many engineering fluid flow problems [Guo and Shu, 2013].

LBM :: Core Ideas

- relatively new class of numerical methods, inspired by kinetic theory $\rightsquigarrow$ simple algorithms:
  1. often explicit formulation
  2. easy to parallelize
  3. convenient handling of complex geometries
- historically related to Lattice Gas Cellular Automata (LGCA), but evolved separately, overcoming some limitations of LGCAs
- bottom-up approach to numerical modelling:
  1. formulate simple, discrete mesoscopic model. . .
  2. . . . such that the desired macroscopic equations are recovered

LBM :: Basic Algorithm

- discretize physical space ($\rightsquigarrow$ the “lattice”/”mesh”) and time
- discretize velocity space $\rightsquigarrow$ $\forall$ node of the lattice, we associate a finite set of probability distribution functions (PDFs)
- PDFs evolve according to simple rules: local collision (e.g. relaxation towards local Maxwell distribution), followed by spatial streaming

$$\underbrace{f_a(\vec{x}+\vec{e}_a\delta_t, t+\delta_t) = f_a(\vec{x}, t)}_{\text{Streaming}} - \underbrace{\frac{[f_a(\vec{x}, t) - f_a^{eq}(\vec{x}, t)]}{\tau}}_{\text{Collision}}, \qquad (1)$$

where $a \in [0, \beta - 1]$ is an index spanning the (discretized) momentum space and τ is a relaxation parameter (related to simulated viscosity)

- equilibrium PDFs based on local Maxwell-Boltzmann distribution

$$f_a^{eq}(\vec{x}) = w_a \rho(\vec{x}) \left[1 + 3\frac{\vec{e}_a \cdot \vec{u}}{c^2} + \frac{9}{2}\frac{(\vec{e}_a \cdot \vec{u})^2}{c^4} - \frac{3}{2}\frac{\vec{u}^2}{c^2}\right], \qquad (2)$$

where the weights w_a are lattice-dependent, and ρ, $\vec{u}$ are first moments of discrete PDFs

- multi-scale analysis shows $O(\delta_x^2, \delta_t^2)$-accurate recovery of Navier-Stokes equations

Sample discretizations of velocity-space

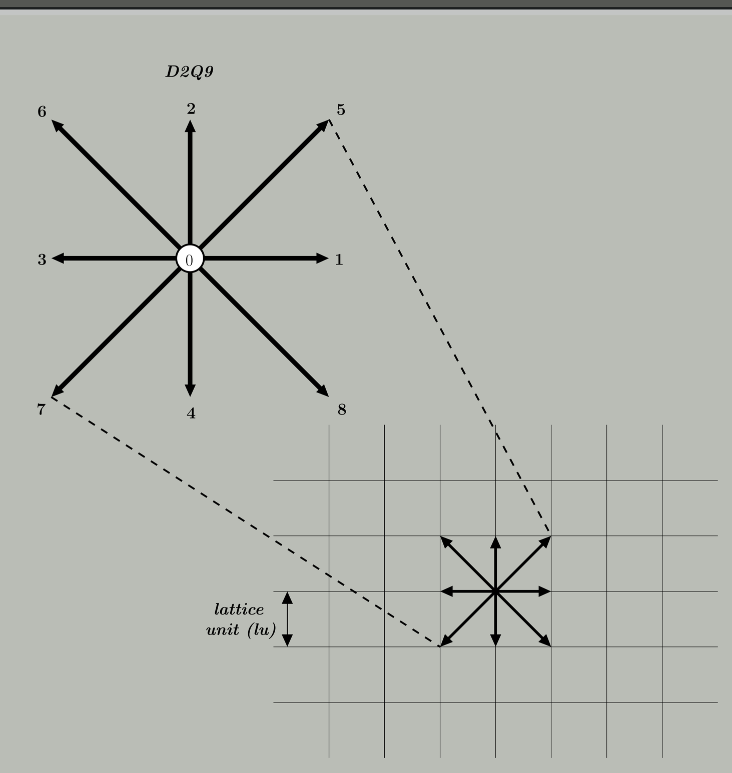

Figure : Illustration of space- and velocity-space-discretization for a **2D** lattice.

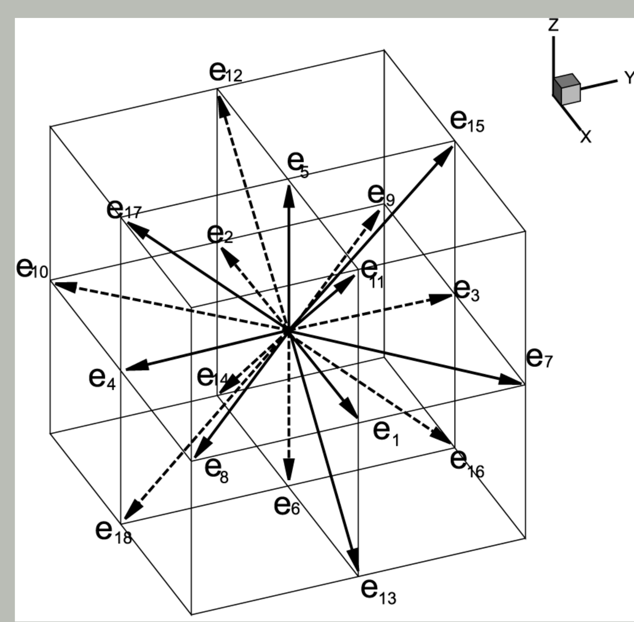

Figure : Illustration of velocity-space-discretization for a **3D** lattice.

LBM algorithms relevant to Earth System Science (ESS)

The method has been successful in modeling complex phenomena, e.g.:

- multi-phase and multi-component flows [Sankaranarayanan et al., 2003]
- melting processes [Huber et al., 2008]
- porous media [Ahrenholz et al., 2006]
- direct numerical simulation (DNS) of turbulence [Peng et al., 2010]

New modeling-framework (GeLB) :: Motivation

- a wide variety of LBM algorithms exist. . .
- . . . but, experimentation and inter-comparison is not trivial (changing core algorithm and, especially, boundary-conditions $\rightsquigarrow$ effectively rewrite of the software)
- technical side-issues (parallelization, efficient I/O, flexible geometry) increase the amount of work

GeLB :: Basic Architecture

Components of GeLB:

- *Core*-library (C++), which supports parallelization, efficient I/O, simulation-restart, etc.
- *source-to-source compiler*, which takes as input simulation-description files (readable for non-specialist) and produces a C++ program that uses the *GeLB-Core* library
- simulation-description is expressed using a small set of abstractions (*Initializer*, *Dynamics*, *Gauge*)

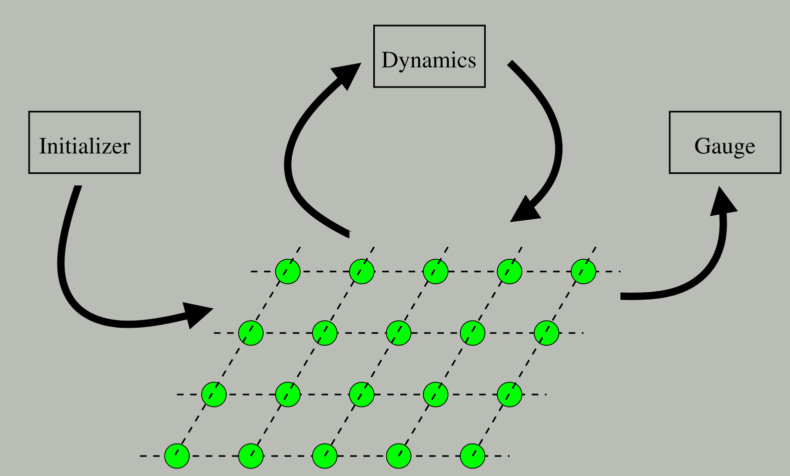

Figure : Roles of Initializer, Dynamics, and Gauge in GeLB

GeLB :: Sample results (preliminary)

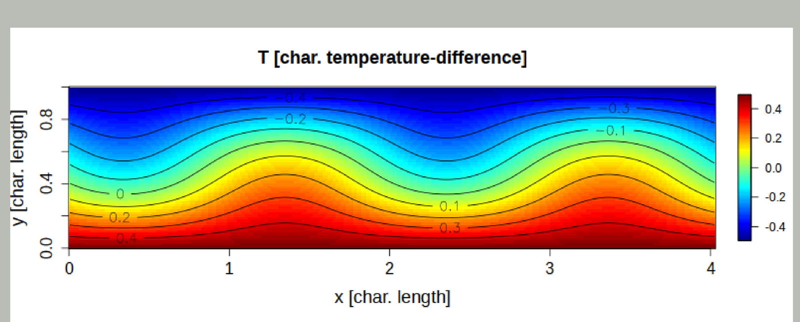

Figure : **2D** Rayleigh-Benard convection ($Ra = 1900$)

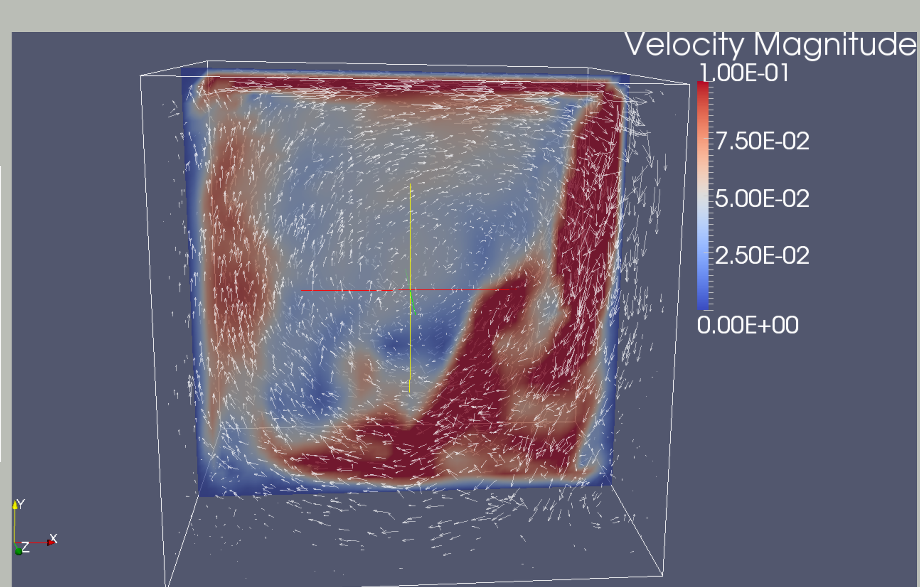

Figure : **3D** lid-driven cavity, $Re = 1.03E4$ (Smagorinsky LES)

Conclusions and Outlook

- extensive model-validation for benchmark-problems
- DNS simulations of double-diffusive instability
- addition of ***GPGPU*** parallel-execution backend

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