Lattice Boltzmann Method for fluid flows

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**INNOCOLD project**

www.innocold.org

Using LBM method

1 PhD project: Simulation of the dispersion of leaked methane clouds over 1 sq. km

2 PhD projects: Modeling and Simulation of the source term and phase transition from liquid to gas
INNOCOLD project: Objective

Subject 3: Numerical Simulation of methane gas dispersion in atmosphere using Lattice Boltzmann Method, at LNG terminal in Dunkerque

- Risk assessment at Dunkerque site by providing LFL maps
- Reduce the investment cost of installing LNG industry
- Flexible numerical tool, suitable also for other installations and danger studies
Presentation outline

- INNOCOLD project
- Lattice Boltzmann Method (LBM)
  - Stream-collision algorithm
  - Finite Volume LBM (FVLBM) algorithm
- Comparison of LBM algorithms
  - Comparative study of the accuracy of different LBM algorithms
  - Validation of FVLBM: 3D Rayleigh-Benard Convection
- Perspectives
why LBM?

- Could be easily extended to multi-component, multi-phase flows
- Easy implementation for complex geometry: widely used in automobile industry eg. POWERFLOW
- Avoids solving heavy Poisson equation. Pressure and stress tensors are available locally
- Easy parallelization

Although, it has its own limitations

- Lower order of accuracy (2nd order in time and space)
- Limited to weakly compressible
- Based on equi-spaced cartesian grid
LBM

- Developed from the Lattice Gas Cellular Automaton
- LBM equation with BGK model – single relaxation time approximation

\[ \frac{\partial f_\alpha}{\partial t} + c_\alpha \cdot \nabla f_\alpha = \frac{1}{\tau} (f_\alpha^{eq} - f_\alpha) + F_\alpha \quad \text{where, } \alpha = 0, \ldots, N_{pop} \]

\[ \rho = \sum \alpha f_\alpha \quad \rho u = \sum \alpha c_\alpha f_\alpha \]

**Velocity Discretization**

- Fig: D2Q9 lattice arrangement
- Fig: D3Q19 lattice arrangement

**Space and time Discretization**

- Stream-collision algorithm
- Finite Volume approach
Stream-Collision algorithm

➢ Applying method of characteristics to LBM-PDE along the lines $x(t) = x(0) + c_\alpha t$

ODE :-->

\[
\frac{d}{dt} f_\alpha = \frac{1}{\tau} (f_{\alpha eq} - f_\alpha) + F_\alpha
\]

➢ Redefining the distribution functions for the lattice populations by,

\[
\tilde{f}_\alpha = f_\alpha - \frac{\Delta t}{2\tilde{\tau}} (f_{\alpha eq} - f_\alpha + \tau F_\alpha)
\]

\[
\tilde{f}_\alpha(x + c_\alpha \Delta t, t + \Delta t) = \tilde{f}_\alpha(x, t) + \frac{\Delta t}{\tilde{\tau}} (\tilde{f}_{\alpha eq}(x, t) - \tilde{f}_\alpha(x, t)) + \Delta t \left(1 - \frac{\Delta t}{2\tilde{\tau}}\right) F_\alpha
\]

where, $\tilde{\tau} = \tau + \Delta t/2 \quad \tilde{\tau} > \Delta t/2$

\[
\rho = \sum_\alpha \tilde{f}_\alpha
\]

\[
\rho u = \sum_\alpha c_\alpha (\tilde{f}_\alpha + \frac{\Delta t}{2} F_\alpha)
\]

\[
\nu = (\tilde{\tau} - \Delta t/2)c_s^2
\]
FVLBM algorithm

➢ Target: Applicable to stretched 3D cartesian grids

Fig: Grid Refinement (ParaView)
FVLBM algorithm (cell-centered)

- Integrating LBE over a volume $V$ (with surface $S$)

\[
\int_V \frac{\partial f_\alpha}{\partial t} \, dV + \int_S \mathbf{c}_\alpha \cdot \mathbf{n} \ f_\alpha \, dS = \int_V \frac{1}{\tau} (f_{\alpha}^{eq} - f_\alpha) \, dV + \int_V F_\alpha \, dV
\]

\[
\frac{\partial f_\alpha}{\partial t} + \frac{S_j}{V} \mathbf{c}_\alpha \cdot \mathbf{n}_j \ [f_\alpha]_j = \frac{1}{\tau} (f_{\alpha}^{eq} - f_\alpha) + F_\alpha
\]

Representation of 2-D structured FV grid

Fig: Schematic of the FV discretization with cell-centered lattice (2-D case)
FVLBM algorithm

Time discretization:

Applying explicit Euler scheme,
\[ \frac{\partial f_\alpha}{\partial t} = \frac{(f_\alpha^{(t+\Delta t)} - f_\alpha^{(t)})}{\Delta t} \]

\[ f_\alpha^{(t+\Delta t)} = f_\alpha^{(t)} - \Delta t \frac{S_j}{V} c_\alpha \cdot n_j \left[ f_\alpha^{(t)} \right]_j + \frac{\Delta t}{\tau} (f_\alpha^{eq(t)} - f_\alpha^{(t)}) + \Delta t F_\alpha \]

Space discretization:
At-least quadratic interpolation scheme required. QUICK scheme is chosen.

Fig: Test of accuracy of different numerical methods for standard Poiseuille flow. Velocity profile comparison for mesh size 1X64.
FVLBM algorithm

Major drawback:

![Graph showing the relationship between $d_{\text{max}}/\tau$ and $\tau$ for different values of $\tau$ for FVLBM. The graph includes a line and data points, with the equation $2*\exp(-\tau)$ plotted as well.]

**Fig:** Decaying Kolmogorov flow: $(d_{\text{max}}/\tau$ vs $\tau$) measure of maximum threshold stable time step for different values of $\tau$ for FVLBM

$$2 > \frac{\Delta t}{\tau} > 0$$
FVLBM algorithm: Improvement

➢ Semi-implicit integration scheme

\[ f^{(t+\Delta t)}_\alpha = f_\alpha - \Delta t \frac{S_j}{V} c_\alpha \cdot n_j \left[ f_\alpha + \frac{\Delta t}{2\tilde{\tau}} (f^{eq}_\alpha - f_\alpha) \right]_j + \frac{\Delta t}{\tilde{\tau}} (f^{eq}_\alpha - f_\alpha) + \Delta t \ F_\alpha \]

where, \( \tilde{\tau} = \tau + \frac{\Delta t}{2} \), \( \tilde{\tau} > \frac{\Delta t}{2} \)

➢ Further improvement with Heun scheme for advection term

- Greater stability criteria
- Increased accuracy

\[ f^{(t+\Delta t)}_\alpha = f_\alpha - \Delta t \frac{S_j}{V} c_\alpha \cdot n_j \left( \frac{[f^{*}_\alpha + \frac{\Delta t}{2\tilde{\tau}} (f^{eq\ast}_\alpha - f^{*}_\alpha)]_j + [f_\alpha + \frac{\Delta t}{2\tilde{\tau}} (f^{eq}_\alpha - f_\alpha)]_j}{2} \right) + \frac{\Delta t}{\tilde{\tau}} (f^{eq}_\alpha - f_\alpha) + \Delta t \ F_\alpha \]

\[ \nu = \tau \ c_s^2 = \left( \tilde{\tau} - \frac{\Delta t}{2} \right) c_s^2 \]
stream-collision

- Well-known; highly tested
- Restricted to homogenous grid
- Streaming along characteristics performed at almost zero cost

FV-LBM algorithm

- Not well explored
- Allows non-homogenous grids
- Addition of a heavy advection term in the calculation

Comparison
efficiency, accuracy, performance, stability
Comparative study of the accuracy of FV-LBM and standard LBM algorithms

Viscosity evaluation

**Fig:** Decaying Kolmogorov flow: Relative error measurement. Finite Volume case: \( dt = 1 \) for \( \tau \geq 0.13 \) (marked with a vertical line) and \( dt = 0.1 \) for \( \tau < 0.13 \). Streaming case: \( dt = 1 \) always. **Inset:** the absolute value of the same error in log-log scale. FVLBM is less accurate but there is an optimal region of application (\( \tau = 0.5 \)).
Comparative study of the accuracy of FV-LBM and standard LBM algorithms

Accuracy of velocity (bounded flow)

**Fig:** *Poiseuille Flow:* Relative error on the Re = 10 velocity Poiseuille flow profile at changing the number of grid points (N) and keeping Δx = 1.

FV is same order in space as stream-collision (i.e. second order accurate) but less accurate of a factor 8 to 10.
Comparative study of the accuracy of FV-LBM and standard LBM algorithms

**Fig:** *Poiseuille flow*: Relative error measurement on the $Re = 10$ velocity Poiseuille flow profile. Here domain size and forcing is varied keeping $Re$ constant. Also grid points are kept constant. At average $dt$ of 10, the FV can be even 100 times more accurate than stream-collision.
FVLBM algorithm: 3D flows

- 3D Rayleigh-Benard System

- Ra=2.5\times10^6; Pr=1; Aspect ratio=2
- Grid : 128X128X64
- Hyperbolic sine grid refinement at the walls
- No-slip BC at walls
- Periodic BC in x,y directions
- Constant upper and lower wall temperatures to be -1 and 1 respectively
3D Validation: Rayleigh-Benard convection

**Fig:** Mean temperature profile $T_m$ - averaged over time and horizontal planes - as a function of the height $z$ in the cell. Profiles only the lower/upper 10% of the cell.
3D Validation: Rayleigh-Benard convection

**Fig:** Root-mean-square temperature profiles $T_{rms}$, averaged over time and horizontal planes, as a function of the cell height $z$. Profiles only the lower/upper 10% of the cell.
3D Validation: Rayleigh-Benard convection

**Fig:** Turbulent kinetic energy $k = 0.5* (u^2)$, averaged over time and horizontal planes, as a function of the cell height $z$. 
Perspectives

➢ Performance comparison

➢ Simulation of fully turbulent Channel flow by FVLBM

- $\text{Re}_{(\tau)} = 180$
- Grid 128 X 128 X 256
- No-slip BC at top and bottom walls
- Periodic BC in x-y directions
- Inlet initiated with parabolic velocity profile

**Fig:** Fully-developed turbulent channel flow simulation domain

➢ Further enhancing the stability of the method
Thank You