Toward High Performance Computing of Compressible Flows using Lattice Boltzmann Method

Gabriel Nastac
Robert Tramel
Kord Technologies, Inc.

Advanced Modeling & Simulation Seminar Series
NASA Ames Research Center
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Kord Technologies, Inc.

- Founded in 2008 in Huntsville, AL
- Employs over 250 personnel throughout the US
- Kord supports efforts by:
  - US Army
  - US Navy
  - US Airforce
  - MDA
  - DHS
  - NASA
  - SMDC
- Kord also supports Boeing on SLS in thermal analysis, stress analysis, fracture modeling, design engineering, and CFD.
Kord CFD

- High Speed Aerodynamics
- High Speed Aerothermodynamics
  - Conjugate Heat Transfer
  - Tightly Coupled Fluid-Structure Interactions
- Cryogenic Propellant Systems
  - Ascent Venting (AV) Models
- Shock Capturing Schemes (HLLE++)
  - NASA OVERFLOW
  - DoD Kestrel/Helios
- Rotorcraft Turbulence
  - Consistent LES
  - Low-Artificial Dissipation Algorithms
- Volcanic Ash Deposition in GT Engines
- Solvers:
  - In-House Unstructured and Structured Compressible NS
  - Government (DoD, NASA)
  - Commercial (ANSYS Fluent)
- Hardware:
  - In-house cluster
  - Government HPC resources

Map of volcanic ash cloud from the eruption of Eyjafjallajökull (red dot) in April 2010 [Met Office, 2017].

Helicopter Landing in Ship Airwake

Turbulence / Shock Waves / Acoustics
Overview

• Motivation
• Boltzmann Equation
• Low-Mach Lattice Boltzmann Method (LBM)
• Existing Low-Mach LBM Results
• LBM extensions to transonic and supersonic flows
• Upcoming Work and Preliminary 2D Results
• Future Work
Motivation (1/3)
Solve Our Problems

Flows we are interested in
Flows where we think LBM can be utilized today

LBM Benefits
- Excellent Advection
- Low Numerical Dissipation
- Local Operations

Rotorcraft Aerodynamics
- Top: Helicopter Landing in Ship Airwake
- Bottom: Vortex Preserving and Consistent LES Algorithms

High Speed Aerodynamics
- Monolithic CHT and TC FSI

1 Coupled Flight Simulator and CFD Calculations of Ship Airwake using HPCMP CREATE™-AV Kestrel. Forsythe, et al. 2015
Effectively utilize current and future parallel architecture

**Motivation (2/3)**

- 40 years of microprocessor data normalized to average processing power in 1980 [NVIDIA, 2018].

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**NVIDIA**

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V = 0.44 m x 0.48 m x 0.83 m
Motivation (3/3)

NASA LAVA Team Results

• Recent results by NASA LAVA show promise in the method for aerospace engineering analysis

• Massively parallel 3D Cartesian AMR Simulations

• Shown to dramatically reduce computational costs due to run-time and mesh generation

• Low numerical dissipation which paves way to higher fidelity LES

• Existing implementation is Low-Mach LBM

• Literature currently exists on extension of LBM to compressible flows - what is the efficiency of the method for compressible flows compared to existing solutions?

Vorticity colored by Mach number.
[Barad, Kocheemoolayil, Stich, Kiris, 2018].

Low-Mach LBM of Landing Gear
[Barad, Kocheemoolayil, Kiris, 2018].
Boltzmann Equation

• Density Distribution Function:
  \[ f(x, \xi, t) \]

• Macroscopic variables are moments of the distribution function, e.g.:
  \[
  \rho(x, t) = \int f(x, \xi, t) d^3\xi \\
  \rho(x, t)u(x, t) = \int \xi f(x, \xi, t) d^3\xi \\
  \rho(x, t)E(x, t) = \frac{1}{2} \int |\xi|^2 f(x, \xi, t) d^3\xi
  \]

• Evolution of \( f \) in time given by Boltzmann Equation:
  \[
  \frac{df(x, \xi, t)}{dt} = \frac{\partial f}{\partial t} + \xi_j \frac{\partial f}{\partial x_j} + \frac{F_j}{\rho} \frac{\partial f}{\partial \xi_j} = \Omega(f(x, \xi, t))
  \]

ℋ-Theorem

- ℋ-Theorem originally introduced by Boltzmann in 1872:

\[ ℋ(f) = \int f \ln f \, d^3\xi \]

- The ℋ-Theorem is directly related to entropy density:

\[ \rho_s = -Rℋ \]

- Boltzmann showed that the quantity ℋ can only decrease and reaches a minima at equilibrium (in other words, equilibrium occurs at maximum entropy).

- Collisions drive the density distribution function towards equilibrium.
Collision Operator

• The collision operator represents the non-linear local redistribution of $f$ due to collisions.

• The operator conserves mass, momentum, and energy (elastic):

$$\int \Omega(f) d^3 \xi = 0$$
$$\int \xi \Omega(f) d^3 \xi = 0$$
$$\int |\xi|^2 \Omega(f) d^3 \xi = 0$$

• The Bhatnagar-Gross-Krook (BGK) operator [Bhatnagar, 1954] is given as a relaxation towards equilibrium (Maxwell-Boltzmann Distribution):

$$\Omega(f) = -\frac{1}{\tau} (f - f^{eq})$$
Lattice Boltzmann Method

• We first develop a velocity distribution lattice:
  \[
  \frac{\partial f}{\partial t} + \xi_j \frac{\partial f}{\partial x_j} = \Omega(f) \rightarrow \frac{\partial f_i}{\partial t} + \xi_{ij} \frac{\partial f_i}{\partial x_j} = \Omega_i(f)
  \]

• At each point, we now have a lattice of dimension $D_dQ_n$, where $d$ is the dimension and $n$ is the number of lattice velocities

• We have a hyperbolic ODE which we can simplify using MOC:
  \[
  f_i(x + \xi_i, t + 1) - f_i(x, t) = \Omega_i(f_i(x, t))
  \]

\[
\begin{align*}
\xi_4 &= (-1,1) & f_4 \\
\xi_3 &= (0,1) & f_3 \\
\xi_2 &= (1,1) & f_2 \\
\xi_5 &= (-1,0) & f_5 \\
\xi_1 &= (1,0) & f_1 \\
\xi_6 &= (-1,-1) & f_6 \\
\xi_7 &= (0,-1) & f_7 \\
\xi_8 &= (1,-1) & f_8
\end{align*}
\]

D2Q9 lattice with outer distribution values and lattice velocities.
Lattice Boltzmann Method (cont.)

\[ f_i(x + \xi_i, t + 1) - f_i(x, t) = \Omega_i(f_i(x, t)) \]

- The above equation is two main steps: collision and streaming
- Collision:
  \[ f'_i(x, t) = f_i(x, t) + \Omega_i(f_i(x, t)) \]
- Streaming:
  \[ f_i(x + \xi_i, t + 1) = f'_i(x, t) \]

Streaming step of Lattice Boltzmann for D2Q9 Lattice. The inner four cells are consistently colored to visualize the propagation.
LBM Collision Operator

\[ \Omega(f) = -\frac{1}{\tau}(f - f^{eq}) \rightarrow \Omega_i(f_i) = -\frac{1}{\tau}(f_i - f_i^{eq}) \]

- What is the equilibrium distribution, \( f_i^{eq} \)? The continuous equilibrium distribution is the Maxwell-Boltzmann distribution. The discrete form is developed by discretizing the continuous velocity space. The moments of interest must be conserved\(^1\).

\[ f^{eq}(\rho, u, \xi) = \frac{\rho}{(2\pi)^{\frac{3}{2}}} \exp\left[-\frac{(\xi - u)^2}{2}\right] \]

- Low-Mach Equilibrium distribution (\( c_s \) is particle speed, \( W_i \) are lattice weights):

\[ f_i^{eq} = W_i\rho \left(1 + \frac{\xi_i \cdot u}{c_s^2} + \frac{(\xi_i \cdot u)^2}{2c_s^4} - \frac{|u|^2}{2c_s^2}\right) \]

- Macroscopic variables can be computed based on existing distribution values:

\[ \rho = \sum_{i=1}^{n} f_i = \sum_{i=1}^{n} f_i^{eq} \]

\[ \rho u = \sum_{i=1}^{n} \xi_i f_i = \sum_{i=1}^{n} \xi_i f_i^{eq} \]

- The relaxation time is a function of the viscosity.

\(^1\)The LBM: Principles and Practice. Krüger, et. al.
Recovering Navier-Stokes

- Multiple methods in literature can be used to determine macroscopic governing equations.
- Chapman-Enskog expansion (1910~1920) is a popular approach and commonly used.
- Essentially a linearization of Boltzmann distribution based on the Knudsen number:
  \[ Kn = \frac{\lambda}{L} \sim \epsilon \]
  \[ f_i = f_i^{eq} + \epsilon f_i^{(1)} + \epsilon^2 f_i^{(2)} + \cdots \]
- It can be shown that the method described thus far recovers the unsteady isothermal weakly compressible (essentially incompressible) Navier-Stokes equations with \( O(Ma^2) \) error:
  \[ \partial_t (\rho) + \partial_j (\rho u_j) = 0 \]
  \[ \partial_t (\rho u_i) + \partial_j (\rho u_i u_j + \delta_{ij} p - 2\mu S_{ij}) = 0 \]
Benefits and Downsides

**Benefits**

- No Poisson equation – a bottleneck in typical incompressible NS solvers
- Simple explicit algorithm
- Collisions are entirely local
- Essentially perfect advection by construction
- Low-Numerical Dissipation

**Downsides**

- The error terms are of $O(Ma^2)$ → extensions must be done to simulate compressible flow ($Ma \geq 0.3$)
- Prandtl number, $Pr = 1$
- Method is based on translational energy modes (monatomic gases) and consequently the specific heat ratio is fixed ($\gamma = 5/3$ for 3D)
- Unsteady by construction
- Resolving wall is prohibitive with Cartesian AMR → Wall Models or Dual-Mesh
Low Mach LBM in NASA LAVA

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<th>Method</th>
<th>CPU Cores (type)</th>
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<th>Core Days to 0.19 seconds</th>
<th>Relative SBU Expense</th>
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GCM: Ghost Cell Method  
IIM: Immersed Interface Method

![Near Field PSD](image)

[Barad, Kocheemoolayil, Kiris, 2018]

Unoptimized LBM with 1.6 billion cells 2~ faster than NS with 300 million cells
LBM for Compressible Flow

- There are numerous research groups around the world working on compressible flow extensions to LBM
- The method which we think has the most promise currently is the Entropic Compressible LBM by N. Frapolli, S. S. Chikatamarla, and I. V. Karlin of ETH Zurich (2016)
- Key components of the method:
  - Unconditionally stable (enables high Re simulations)
  - Increases Mach number limit by an order of magnitude (up to 3.0)
  - Variable Prandtl number and Specific Heat Ratio (e.g. Pr = 0.71, γ = 1.4 for standard air)
  - Entropic component adds artificial dissipation for shock capturing without sensors
- Method was tested and validated on 2D and 3D geometry using AMR:
  - 2D Inviscid/Viscous Transonic & Supersonic NACA0012
  - 3D Inviscid Onera M6 Wing
  - 3D Compressible Homogeneous Isotropic Turbulence
- Potential issues of the method:
  - Computational Efficiency. How does the method compare to existing methods?
  - Entropic methods in general (including low-Mach) add artificial viscosity in under-resolved areas similar to sub-grid scale (SGS) LES models – not really an issue.

Objectives and Upcoming Work

• Implement compressible LBM\textsuperscript{1}

• Simulate canonical 2D (e.g. TG, VC, oblique shock) and 3D (TG) test cases

• Validate and verify the implementation

• Benchmark against existing solvers (FUN3D, OVERFLOW)

• Determine scalability and performance using CPU MPI and NVIDIA’s CUDA

\textsuperscript{1}N. Frapolli, S. S. Chikatamarla, and I. V. Karlin, Phys. Rev. E 93, 063302 (2016).
The Entropic Compressible LBM relies on three primary components:

- Enlarged lattice and temperature dependent lattice weights
- Boltzmann’s $\mathcal{H}$-Theorem
- An additional set of populations ($g$) that represent rotational and vibrational energy to enable variable $\gamma$

Similarly to traditional LBM, this method uses a lattice. The standard method uses a DdQ7$^d$ lattice ($0, \pm 1, \pm 2, \pm 3$), or D2Q49 and D3Q343 for 2D and 3D respectively.

Lattice pruning can be used to reduce 3D lattice to D3Q39.

Method has the same structure and solution technique as traditional LBM:

$$f_i(x + \xi_i, t + 1) - f_i(x, t) = \Omega_f(f_i)$$
$$g_i(x + \xi_i, t + 1) - g_i(x, t) = \Omega_g(f_i)$$

$$\Omega_f(f_i) = \alpha \beta_1 (f_i^{eq} - f_i) + 2(\beta_1 - \beta_2)(f_i^* - f_i^{eq})$$
$$\Omega_g(f_i) = \alpha \beta_1 (g_i^{eq} - g_i) + 2(\beta_1 - \beta_2)(g_i^* - g_i^{eq})$$

Lattice

\[ w_0 = w_0(T) \]
\[ w_{\pm 1} = w_{\pm 1}(T) \]
\[ w_{\pm 2} = w_{\pm 2}(T) \]
\[ w_{\pm 3} = w_{\pm 3}(T) \]

\[ W_i(\xi_x, \xi_y, \xi_z, T) = w_{ix} w_{iy} w_{iz} \]

\[ \sum_{i=1}^{n} W_i = 1 \]

Discrete \( \mathcal{H} \)-Theorem

\[ \mathcal{H}(f) = \int f \ln f \ d^3\xi \rightarrow \mathcal{H}(f) = \sum_{i=1}^{n} f_i \ln f_i / W_i \]

Entropic Equilibrium (1)

\[ \rho = \sum_{i=1}^{n} f_i = \sum_{i=1}^{n} f_i^{eq} \]

\[ \rho u = \sum_{i=1}^{n} \xi_i f_i = \sum_{i=1}^{n} \xi_i f_i^{eq} \]

\[ 2\rho E^{tr} = 2\rho DT + \rho |u|^2 = \sum_{i=1}^{n} |\xi_i|^2 f_i = \sum_{i=1}^{n} |\xi_i|^2 f_i^{eq} \]

\[ 2\rho E = 2\rho C_v T + \rho |u|^2 = \sum_{i=1}^{n} |\xi_i|^2 f_i + \sum_{i=1}^{n} g_i = \sum_{i=1}^{n} |\xi_i|^2 f_i^{eq} + \sum_{i=1}^{n} g_i^{eq} \]

• Translational energy and total energy are both tracked

• Rotational energy is tracked using the separate distributions \( g_i \)

Entropic Equilibrium (2)

Minimize $\mathcal{H}$ using LM to enforce conservation to obtain $f_i^{eq}$:

$$
J(f_i^{eq}, \chi, \zeta, \lambda) = \sum_{i=1}^{n} f_i^{eq} \ln f_i^{eq} / W_i + \chi \left( \rho - \sum_{i=1}^{n} f_i^{eq} \right) + \zeta \cdot \left( \rho u - \sum_{i=1}^{n} \xi_i f_i^{eq} \right) + \lambda \left( 2\rho E^{tr} - \sum_{i=1}^{n} |\xi_i|^2 f_i^{eq} \right)
$$

$$
\frac{\partial J}{\partial f_i^{eq}} = 0 = \sum_{i=1}^{n} \left( \ln \frac{f_i^{eq}}{W_i} + 1 - \chi - \zeta \cdot \xi_i - \lambda |\xi_i|^2 \right)
$$

An extremum is ensured with the following form of $f_i^{eq}$:

$$
f_i^{eq} = \rho W_i \exp(\chi + \zeta \cdot \xi_i + \lambda |\xi_i|^2) \quad \leftarrow \text{Positive-Definite}
$$

$$
g_i^{eq} = (2C_vT - D) f_i^{eq}
$$

$$
f^{eq}(\rho, u, \xi, \theta) = \frac{\rho}{(2\pi\theta)^{3/2}} \exp \left[ -\frac{(\xi - u)^2}{2\theta} \right] \quad \leftarrow \text{Continuous Velocity Space \nMaxwell-Boltzmann Distribution}
$$

Polynomial Equilibrium

5th order Hermite polynomial expansion

\[
\begin{align*}
   f_i^{eq} &= \rho W_i \left( 1 + \xi_i \cdot u + \frac{1}{2} [ (\xi_i \cdot u)^2 - u \cdot u ] + \frac{T - 1}{2} (\xi_i \cdot \xi_i - D) + \frac{\xi_i \cdot u}{6} [ (\xi_i \cdot u)^2 - 3u \cdot u ] \\
   &\quad + \frac{T - 1}{2} (\xi_i \cdot u)(\xi_i \cdot \xi_i - D - 2) + \frac{1}{24} [ (\xi_i \cdot u)^4 - 6(\xi_i \cdot u)^2(u \cdot u) + 3(u \cdot u)^2 ] \\
   &\quad + \frac{T - 1}{4} [ (\xi_i \cdot \xi_i - D - 2)(\xi_i \cdot u)^2 - u \cdot u ] - 2(\xi_i \cdot u)^2 ] \\
   &\quad - \frac{(T - 1)^2}{28} [ (\xi_i \cdot \xi_i)^2 - 2(D + 2)(\xi_i \cdot \xi_i) + D(D + 2) ] \\
   &\quad + \frac{\xi_i \cdot u}{120} [ (\xi_i \cdot u)^4 - 10(\xi_i \cdot u)^2(u \cdot u) + 15(u \cdot u)^2 ] \\
   &\quad - \frac{T - 1}{12} [ (\xi_i \cdot u)[ (\xi_i \cdot \xi_i - D - 4)((\xi_i \cdot u)^2 - 3(u \cdot u)) - 2(\xi_i \cdot u)^2 ] \\
   &\quad + \frac{(T - 1)^2}{8} [ (\xi_i \cdot \xi_i)^2 - D(D + 4)(\xi_i \cdot \xi_i) + (D + 2)(D + 4) ] \right)
\end{align*}
\]

[Fares, 2014]


\[
\mathcal{H}(f) = \mathcal{H}(f + \alpha(f^{eq} - f))
\]

- Entropic estimate \( \alpha \) is the non-trivial root of above constraint
- Entropy is guaranteed to remain the same or increase by construction
- For fully-resolved simulations, \( \alpha \) tends to 2 which is the BGK value

NACA0012 Airfoil\(^1\)

\( M_\infty = 1.4, Re = 3 \times 10^6 \)

Gas Properties

- Relaxation parameters are functions of dynamic viscosity and thermal conductivity (e.g. Sutherland law for viscosity and Prandtl number to compute thermal conductivity)

\[ \beta_1 = \frac{1}{\frac{2\mu}{\rho T} + 1} \]

\[ \beta_2 = \frac{1}{\frac{2\kappa}{\rho C_p T} + 1} \]

\[ \Omega_f(f_i) = \alpha \beta_1 (f_i^{eq} - f_i) + 2(\beta_1 - \beta_2)(f_i^* - f_i^{eq}) \]

\[ \Omega_g(f_i) = \alpha \beta_1 (g_i^{eq} - g_i) + 2(\beta_1 - \beta_2)(g_i^* - g_i^{eq}) \]

Quasi-Equilibrium

\[ f_i^* = f_i^{eq} + W_i \bar{Q} : R \]

\[ R = \frac{\xi_i \otimes \xi_i \otimes \xi_i - 3T\xi_i I}{6T^3} \]

\[ \bar{Q} = \sum_{i=1}^{n} f_i(\xi_i - u) \otimes (\xi_i - u) \otimes (\xi_i - u) \]

\[ g_i^* = g_i^{eq} + W_i \bar{q} \cdot r \]

\[ r = \frac{\xi_i}{T} \]

\[ \bar{q} = \sum_{i=1}^{n} g_i(\xi_i - u) \]

Chapman-Enskog expansion (1910~1920) is a popular approach and commonly used.

Essentially a linearization of Boltzmann distribution based on the Knudsen number:

\[ Kn = \frac{\lambda}{L} \sim \epsilon \]

\[ f_i = f_{i}^{eq} + \epsilon f_{i}^{(1)} + \epsilon^2 f_{i}^{(2)} + \cdots \]

It can be shown that the method described thus far recovers the unsteady compressible Fourier-Navier-Stokes equations:

\[
\begin{align*}
\partial_t (\rho) + \partial_j (\rho u_j) &= 0 \\
\partial_t (\rho u_i) + \partial_j (\rho u_i u_j + \delta_{ij} p + \tau_{ij}) &= 0 \\
\partial_t (\rho E) + \partial_j ((\rho E + p)u_j + \tau_{ij} u_i + q_j) &= 0
\end{align*}
\]

Method Summary

- **Collision:**
  \[
  f_i'(x, t) = f_i(x, t) + \Omega_f(f_i(x, t)) \\
  g_i'(x, t) = g_i(x, t) + \Omega_g(g_i(x, t))
  \]

- **Streaming:**
  \[
  f_i(x + \xi_i, t + 1) = f_i'(x, t) \\
  g_i(x + \xi_i, t + 1) = g_i'(x, t)
  \]

Streaming step of Lattice Boltzmann for D2Q9 Lattice. The inner four cells are consistently colored to visualize the propagation.

LBM for Compressible Flow

Potential issues of the method:

- **Computational Efficiency. How does the method compare to existing methods?**
- Entropic methods add artificial viscosity in under-resolved areas similar to sub-grid scale (SGS) LES models.

Method requires at each node at each timestep:

- a multi-dimensional non-linear solve for equilibrium
- a scalar non-linear solve for entropic constant, $\alpha$

Our preliminary 2D results show that these non-linear solves are the bulk of the computational time.
Preliminary 2D Results

2D Taylor Green Vortex

Kinetic Energy Versus Time

Grid Convergence
Preliminary 2D Results

2D Inviscid Vortex Convection
($M = 0.5, 128^2$ Grids, 5L Distance)

VP = Vortex Preserving (AVC)
AD = Artificial Dissipation

| Method                | $|\omega_c|/|\omega_{c0}|$ (%) |
|-----------------------|------------------|
| Analytic              | 100%             |
| Roe-WENO5             | 99.8%            |
| ELBM 2nd Order        | 99.7%            |
| Roe-MUSCL 3rd Order   | 70.9%            |
| Roe-MUSCL 3rd Order VP| 99.0%            |
| Central+AD 4th Order  | 80.5%            |
| Central+AD 4th Order VP| 94.0%          |
Preliminary 2D Results

Double Shear Layer ($M = 0.35$ $Re = 30,000$)

$t_c = 0$  
$t_c = 1$

Mean Kinetic Energy Versus Time

- Reference
- ELBM 512$^2$
Preliminary 2D Results

Shock Tube (1024x1 Grid)

Density

\[ \rho \text{ [kg/m}^3\text{]} \]

\[ \rho_L = 1.0 \ \frac{kg}{m^3} \]

\[ \rho_R = 0.2 \ \frac{kg}{m^3} \]

Velocity

\[ u \text{ [m/s]} \]

\[ u_L = 0.0 \ \frac{m}{s} \]

\[ u_R = 0.0 \ \frac{m}{s} \]

Pressure

\[ P \text{ [kPa]} \]

\[ P_L = 50 \ \text{kPa} \]

\[ P_R = 10 \ \text{kPa} \]
Future Work

- Test transonic/supersonic cases
- Test 3D performance (3D TG/HIT/etc.)
- Extend implementation with Cartesian AMR framework:
  - Chombo
  - SAMRAI
  - AMReX
- Incorporate either wall-models or dual-mesh overset to enable complex geometry simulations

Temperature field of a flame computed with RNS, a block-structured AMR solver that uses AMReX as a basis for grid generation and data structures. [AMReX, 2018].

Dual-Mesh
(DoD CREATE-AV Kestrel/Helios)
OVERFLOW