The Development of a Compressible Lattice Boltzmann Model for Turbomachine Applications

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Outline

1. Introduction
2. Statistic mechanics and Boltzmann equation
3. Lattice Boltzmann Method
4. Current LB model
5. Simulation of cascades and result
6. Parallel computing and result
7. Conclusion remarks
Introduction

- Lattice Boltzmann (LB) Method is a relatively new method for flow simulations.
- The start point of LB method is statistic mechanics and Boltzmann equation.
- The LB method tries to set up its model at molecular scale and simulate the flow at macroscopic scale.
In the last decade, the LB method has been successfully developed into a promising and complementary alternative to the traditional CFD method.
Statistic Mechanics

- Statistic mechanics views fluid as a collection of particles.
- The properties of the fluid are determined by the average properties of the particles in the collection.
1) Distribution Function

- A phase space consists of both location and velocity of particles is introduced.
- The distribution function is defined as the density of the number of particles at point \((x, \xi)\).
Assume that there is no external force and no collision between the particles, the velocity of the particles will not change.

The two domains have the same number of particles.

\[
f(x + \xi \Delta t, \xi, t + \Delta t) dx d\xi = f(x, \xi, t) dx d\xi
\]

\[
f(x + \xi \Delta t, \xi, t + \Delta t) = f(x, \xi, t)
\]
Collisions between particles change their velocities, and make them move in and out of the domain.

A collision term describes the net increase of the density of the number of particles in the domain due to the collision.

\[ f(x + \xi \Delta t, \xi, t + \Delta t) = f(x, \xi, t) + \Omega \Delta t \]
Boltzmann Equation

4) BGK Collision term

- One of the simplest collision models is the Bhatnagar, Gross and Krook (BGK) simplified collision model

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

- The BGK model is widely used in LB models
The Boltzmann equation in finite difference form:

\[ f\left(\tilde{x} + \xi \Delta t, \tilde{\xi}, t + \Delta t\right) = f\left(\tilde{x}, \tilde{\xi}, t\right) + \Omega \Delta t \]

By Taylor expansion, the above equation can be written in the differential form:

\[ \frac{\partial f}{\partial t} + \xi \cdot \nabla f = \Omega \]

This is the Boltzmann Equation
Boltzmann Equation

6) The Equilibrium Distribution Function

- The equilibrium distribution function for Boltzmann equation is the Maxwell-Boltzmann Distribution

\[
 f^{(eq)} = n \left( \frac{m}{2\pi k_B T} \right)^{D/2} \exp \left( - \frac{m(\vec{\xi} - \vec{v})^2}{2k_B T} \right)
\]

- The equilibrium distribution function is a function of macroscopic quantities and particle velocity.
The Macroscopic Properties

\[ Y(\bar{x}, t) = \frac{\int \eta(\bar{\xi}) f(\bar{x}, \bar{\xi}, t) d^3\xi}{\int f(\bar{x}, \bar{\xi}, t) d^3\xi} \]

- **Density**
  \[ \rho = m \int f(\bar{x}, \bar{\xi}, t) d^3\xi \]

- **Momentum**
  \[ \rho \bar{v} = m \int \bar{\xi} f(\bar{x}, \bar{\xi}, t) d^3\xi \]

- **Thermal Energy**
  \[ \rho \varepsilon = \frac{m}{2} \frac{D_f}{D} \int |\bar{\xi} - \bar{v}|^2 f(\bar{x}, \bar{\xi}, t) d^3\xi \]

- The Macroscopic properties are determined by the average value of properties of the particles.
The Enskog-Chapman Expansion

- It has been shown that the Euler equation and Navier-Stokes equation are the zeroth-order and first order approximations of the Boltzmann equation, respectively.
- That is to say, the Boltzmann equation describes the fluid phenomena in a more accurate way than tradition fluid dynamics does.
Lattice Boltzmann Method

- Lattice Boltzmann Method can be reviewed as a numerical method to solve the Boltzmann equation.
- In LB method, the phase space is discretized.
- In a LB model, the velocity of a particle can only be chosen from a velocity set, which has only a finite number of velocities.
Lattice Boltzmann Method
1) velocity set and grid

For the convenience of computation, the position space is discretized in such a way that the particles travel with one of the velocity in the velocity set will arrive at a correspondent node at next time step.
The Lattice Boltzmann Method

2) macroscopic properties

- In the LB method, the macroscopic properties are evaluated through the weight summation

\[ Y = \int n(\vec{\xi}) f^{(eq)}(\vec{x}, \vec{\xi}, t) d\vec{\xi} = \sum_{\alpha} W_\alpha n(\vec{\xi}_\alpha) f^{(eq)}(\vec{x}, \vec{\xi}_\alpha, t) \]

\[ \rho = m \sum_{\alpha} f^{(eq)}_\alpha \]

\[ \rho \vec{v} = m \sum_{\alpha} \vec{\xi}_\alpha f^{(eq)}_\alpha \]

\[ \rho \varepsilon = \frac{m}{2} \sum_{\alpha} |\vec{\xi}_\alpha - \vec{v}|^2 f^{(eq)}_\alpha \]

where

\[ f^{(eq)}_\alpha(\vec{x}, \vec{\xi}_\alpha, t) = W_\alpha f^{(eq)}(\vec{x}, \vec{\xi}_\alpha, t) \]
Lattice Boltzmann Method

3) Time evolution equation

- Boltzmann equation in finite difference form with the BGK collision term

\[
f(\tilde{x} + \tilde{\xi}_\alpha \Delta t, \tilde{\xi}_\alpha, t + \Delta t) = f(\tilde{x}, \tilde{\xi}_\alpha, t) - \frac{\Delta t}{\tau} (f(\tilde{x}, \tilde{\xi}_\alpha, t) - f^{(eq)}(\tilde{x}, \tilde{\xi}_\alpha, t))
\]

where \( \tilde{\xi}_\alpha \) is one of velocities in the velocity set

- Set \( \Delta t = \tau \)

\[
f(\tilde{x} + \tilde{\xi}_\alpha \Delta t, \tilde{\xi}_\alpha, t + \Delta t) = f^{(eq)}(\tilde{x}, \tilde{\xi}_\alpha, t)
\]
The Lattice Boltzmann Method

4) The calculation

\[ Y(\vec{x}, t) = \sum_{\alpha} \eta(\vec{x}_{\alpha}) f_{\alpha}^{(eq)}(\vec{x} - \vec{x}_{\alpha} \Delta t, \vec{x}_{\alpha}, t - \Delta t) = \sum_{\alpha} Y_{\alpha} (\vec{x} - \vec{x}_{\alpha} \Delta t, t - \Delta t) \]

- The calculation of LB method can be viewed as following steps
  1) a node dividing its macroscopic quantities into parts
  2) the node sending parts of the macroscopic quantities to corresponding nodes
  3) a node receiving the parts of the macroscopic quantities sent by nearby nodes, adding them together and obtaining the macroscopic quantities for next time step
Advantages of LB method

- Start from a clear and direct physical picture at molecular level;
- Algorithm is simple and straightforward;
- Natural parallel scheme;
- Easy to incorporate the physical phenomena at molecular level, possible of modeling fluid phenomena that can not be modeled with the traditional fluid mechanics.
Motivation

- There are very few reports about the successful LB simulations of the real life problems
- Successful extension of LB method to the simulation of turbomachinery can show the maturity of LB method and the promise of this method in the simulation of real life problem
- The parallel nature of LB method make it a possible high performance solver for turbomachine simulations
Challenges

1. Most of LB models can only simulate the flow with a small Mach number
2. Most of past LB simulations are laboratory type simulations with simple computational domain and boundary
3. The proper LB model for simulation should be developed and necessary techniques should be developed
The Current Work

- A compressible LB model has been chosen as the start point of this simulation.
- A boundary treatment has been successful introduced into the current model to implement the slip wall boundary conditions.
- A mesh has been devised for the irregular computational domain.
The Current Work

- Successful simulations have been carried out for three different cascades. It is the first time that turbomachines have been simulated by a LB model.
- The parallel performance of the LB model has been tested.
1) The Velocity Set

- A velocity in the velocity set consists of three parts.
- First the macroscopic velocity has been included explicitly into the microscopic velocity.
- Second, there is a set of diffusion velocity.
2) The diffusion velocity

- There are 3 levels of diffusion velocity in current model
- The module of the diffusion velocities are determined by macroscopic quantities

\[
\begin{align*}
\bar{c}_v' &= \begin{cases} 
0 & \text{for } \nu = 0 \\
\text{int} \left( \sqrt{D(\gamma - 1)pe/(\rho - b_0d_0)} \right) & \text{for } \nu = 1 \\
\text{int} \left( \sqrt{D(\gamma - 1)pe/(\rho - b_0d_0)} \right) + 1 & \text{for } \nu = 2
\end{cases}
\end{align*}
\]
3) The Velocity Set

A third set of velocities \( \vec{v}_k' \) is introduced to carry the particles to the nearest vertex nodes.

\[
\vec{r}_{jvk} = \vec{v} + \vec{c}_{jv} + \vec{v}_k'
\]
Current Model
4) The microscopic quantities

- Mass, only one species is considered, is a constant
  \[ m = 1 \]

- Velocity, consists of macroscopic velocity and a diffusion velocity
  \[ \vec{\xi}_{jv} = \vec{v} + \vec{c}_j' \]

- Total energy is the same for all particles
  \[ \zeta = \frac{1}{2} v^2 + e \]
Current Model

4) Modification of microscopic quantities

- For the purpose of recovering the correct Navier-Stokes equation, a correction term has been introduced.

\[ \chi_{jk}\tau = \frac{\rho}{\rho - b_0 d_0} \frac{D}{2 c_v'} \left( \mathbf{c}^{'}_j \cdot \mathbf{v}^{'}_k \right) \]

- Mass

\[ m_{jk}\tau = 1 - \lambda_{jk}\tau \]

- Velocity

\[ \xi_{jk}\tau = \mathbf{v} + \mathbf{c}^{'}_j - \lambda_{jk}\tau \mathbf{v} \]

- Total energy

\[ \zeta_{jk}\tau = \left( 1 - \lambda_{jk}\tau \right) \left( \frac{1}{2} v^2 + e \right) \]
Current Model
5) The equilibrium distribution function

\[ f_{jvk}^{(eq)} = f_{vk}^{(eq)} \]

\[ f_{vk}^{(eq)} = \alpha_k d_v \]

\[ d_1 = \frac{(\rho - b_0 d_0) c_2'^2 - D(\gamma - 1) pe}{b_1 (c_2'^2 - c_1'^2)} \]

\[ d_2 = \frac{D(\gamma - 1) pe - (\rho - b_0 d_0) c_1'^2}{b_2 (c_2'^2 - c_1'^2)} \]
The flow chart of computation

1. **Macroscopic properties**
   - Calculate the equilibrium distribution function
   - Calculate the microscopic velocities
   - The destination of particles
   - Calculate the macroscopic properties to be sent
   - Send
   - Receive
   - Calculate the macroscopic properties of new time step
Geometry of Cascade and Simulation domain

Inlet

Periodical boundary

wall

Periodical boundary

wall

Periodical boundary

Exit
Mesh
The mapping between coordinates and indexes

Mapping $XY$ To $MN$

Mapping $MN$ To $XY$

The coordinate of nodes

$(x, y)$

The index of array

$(m, n)$
Implement of boundary condition
1) wall boundary - auxiliary nodes

Auxiliary nodes were introduced to implement wall boundary conditions.
The macroscopic properties of auxiliary nodes are extrapolated from the computational domain.
Implement of boundary condition
3) periodical boundary
Wedge Cascade
Geometry

Ma = 2.0
Wedge Cascade
Result: Stream Line and Ma Contour
Wedge Cascade
Result: Static Pressure at Walls

\[ \frac{p}{p_0} \]

Present Result (upper wall)
Theoretical
Present Result (lower wall)
C3X Cascade
Geometry and inlet and outlet parameters

Stagger Angle 59.89°
Chord 14.49cm
Spacing 11.77cm
Solidity 1.23
Axial Chord 7.82cm

<table>
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<tr>
<th>Run Number</th>
<th>$\alpha_{in}$</th>
<th>$p_{t1}$ (Pa)</th>
<th>$T_{t1}$ (K)</th>
<th>$Ma_1$</th>
<th>$Re_1$</th>
<th>$p_2 / p_{t1}$</th>
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<td>7755</td>
<td>811</td>
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C3X Cascade RUN 143
Results

RUN 143

p/p₀₁
1.00
0.95
0.89
0.84
0.79
0.73
0.68
0.63
0.57
0.52
0.46
0.41
0.36
0.30
0.25

Ma
1.30
1.22
1.14
1.05
0.97
0.89
0.81
0.73
0.64
0.56
0.48
0.40
0.31
0.23
0.15

RUN 143
C3X Cascade RUN 143
Results

RUN 143

\[ \frac{\rho}{\rho_0} \]

\[ 1.00 \]
\[ 0.96 \]
\[ 0.92 \]
\[ 0.88 \]
\[ 0.84 \]
\[ 0.80 \]
\[ 0.76 \]
\[ 0.73 \]
\[ 0.69 \]
\[ 0.65 \]
\[ 0.61 \]
\[ 0.57 \]
\[ 0.53 \]
\[ 0.49 \]
\[ 0.45 \]

RUN 143

\[ \frac{e}{e_1} \]

\[ 1.00 \]
\[ 0.98 \]
\[ 0.96 \]
\[ 0.94 \]
\[ 0.91 \]
\[ 0.89 \]
\[ 0.87 \]
\[ 0.85 \]
\[ 0.83 \]
\[ 0.81 \]
\[ 0.79 \]
\[ 0.76 \]
\[ 0.74 \]
\[ 0.72 \]
\[ 0.70 \]
C3X Cascade RUN 143
Results

p/p_{t1} vs. x/c_x

- Present Result
- Experiment Result
- Euler solution
- Navier-Stokes solution
C3X Cascade RUN 144
Results
C3X Cascade RUN 144
Results

\( \rho / \rho_0 \)

\( e / e_1 \)

RUN 144

RUN 144
C3X Cascade RUN 144
Results

$\frac{p}{p_{t1}}$

RUN 144
Present Result
 Experiment Result
 Euler solution
 Navier-Stokes solution

$x/c_x$

0 0.25 0.5 0.75 1

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
### VKI Cascade
Geometry and inlet and outlet parameters

- **Stagger Angle**: 55.0°
- **Chord**: 67.646 mm
- **Spacing**: 57.50 mm
- **Solidity**: 1.1765
- **Axial Chord**: 36.98 mm

### Run Parameters

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<tr>
<th>Run Number</th>
<th>( \alpha_{in} )</th>
<th>( P_{t1} ) (Pa)</th>
<th>( T_{t1} ) (K)</th>
<th>( Ma_1 )</th>
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VKI Cascade MUR 129
Results

\[
p/p_{01}
\]

\[
Ma
\]

MUR 129
VKI Cascade MUR 129

Results
VKI Cascade MUR 129 Results

$p/p_{t1}$ vs $s/c$

- Present Result
- Experiment Result

MUR 129

$p/p_{t1}$ vs $s/c$
Parallel Computing

- The LB method is a natural parallel method;
- The LB model is explicit in time;
- The area of dependent domain of a node is determined by the magnitude of velocity set, which is usually a small number.
Parallel computing
1) division of blocks

- The simulation of wedge cascade was parallelized to test the parallel performance of current LB model
Parallel computing
2) information exchange

Buffer Area

Computational Area

1
2
3
4
5
6
7
8
Parallel computing

3) Result

\[ \frac{nT(1)}{T(n)} \]

Speed Up

Number of Processor n

CPU Time

- 100%
- 80%
- 70%
Conclusion

1) A compressible LB model has been successfully developed for turbomachinery simulations.

2) Successful simulation of cascades has been carried out and it is the first successful turbomachinery simulation by a LB model.
Conclusion

3) A treatment of boundary condition in LB method has been introduced to the current compressible LB model.

4) A new mesh treatment method has been devised in order to use regular mesh on a irregular geometry.
Conclusion

5) The parallel efficiency of the new compressible LB model is studied. A linear efficiency has been demonstrated.

6) The theoretical basis of the current model is analyzed in detail.
Recommendation for future

1) A Navier-Stokes solver is expected
2) Incorporation of turbulence model
3) Development of non-uniform grid and curvilinear mesh in the LB model
4) Improvement for the parallel computing
5) Extension to 3D simulations
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