A LATTICE BOLTZMANN METHOD FOR TURBOMACHINEY SIMULATIONS

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Outline

- Lattice Boltzmann Method
- Objectives
- Current LB model
- Simulation of cascades and result
- Parallel computing and result
- Conclusion remarks

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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.
- LBM has been applied to mostly incompressible flows and simple geometry.

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.
**Boltzmann Equation**

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 $(x, \xi)$.

\[ dN = f(x, \xi, t)dxd\xi \]

Phase space for 1D problem

2) Time Evolution Of Distribution Function

- Assume that there is no external force and no collision between the particles, the velocity of the particles will not change.

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

The two domain have the same number of particles

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

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

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

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

The BGK model is widely used in LB models.
5) Boltzmann Equation

The Boltzmann equation in finite difference form:

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

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

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

This is the Boltzmann Equation

The Macroscopic Properties

The Macroscopic properties are determined by the average value of properties of the particles

- density
  \[\rho = m \int f(\tilde{x}, \tilde{\xi}, t) d^3 \xi\]
- momentum
  \[\rho \tilde{v} = m \int \tilde{\xi} f(\tilde{x}, \tilde{\xi}, t) d^3 \xi\]
- thermal energy
  \[\rho \varepsilon = \frac{m}{2} \frac{D_f}{D} \int |\tilde{\xi} - \tilde{v}|^2 f(\tilde{x}, \tilde{\xi}, t) d^3 \xi\]
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

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

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

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

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

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

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

where \( \xi_\alpha \) is one of velocities in the velocity set

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

\[ f\left(\tilde{x} + \xi_\alpha \Delta t, \xi_\alpha, t + \Delta t\right) = f^{(eq)}\left(\tilde{x}, \xi_\alpha, t\right) \]

The Lattice Boltzmann Method

4) The Calculation

\[ Y\left(\tilde{x}, t\right) = \sum_\alpha \eta\left(\xi_\alpha\right) f^{(eq)}\left(\tilde{x} - \xi_\alpha \Delta t, \xi_\alpha, t - \Delta t\right) = \sum_\alpha Y_\alpha \left(\tilde{x} - \xi_\alpha \Delta t, t - \Delta t\right) \]

- 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

- Develop a compressible LB model.
- Introduce a boundary condition that allows accurate turbine blade simulation
- Develop mesh treatment for the irregular computational domain
The Current Work

- Simulations 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

Current Model

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
Current Model

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

\[ c'_v = \begin{cases} 
0 & \text{for } \nu = 0 \\
\text{int} \left( \sqrt{D(y-1)\rho e/(\rho - b_0 d_0)} \right) & \text{for } \nu = 1 \\
\text{int} \left( \sqrt{D(y-1)\rho e/(\rho - b_0 d_0)} \right) + 1 & \text{for } \nu = 2 
\end{cases} \]

Current Model

3) The Velocity Set

- A third set of velocities is introduced to carry the particles to the nearest vertex nodes

\[ \vec{r}_{jk} = \vec{v} + \vec{c}'_{jv} + \vec{v}'_k \]
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
  \[ \xi_{jv} = \bar{v} + \tilde{c}_{jv} \]

- 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
  \[ \chi_{jvk} = \frac{\rho}{\rho - b_0 d_0 c_v^2} D \left( \tilde{c}_{jv} \cdot \bar{V}_k \right) \]

- Mass
  \[ m_{jvk} = 1 - \lambda_{jvk} \]

- Velocity
  \[ \xi_{jvk} = \bar{v} + \tilde{c}_{jv} - \lambda_{jvk} \bar{v} \]

- Total energy
  \[ \zeta_{jvk} = \left( 1 - \lambda_{jvk} \right) \left( \frac{1}{2} v^2 + e \right) \]
5) The Equilibrium Distribution Function

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

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

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

\[ d_2 = \frac{D(\gamma - 1) \rho e - (\rho - b_0 d_0) c_1'^2}{b_2 (c_2^2 - c_1^2)} \]

\[ \alpha_1 = |u_3'v_3'| \quad \alpha_2 = |u_4'v_4'| \]

\[ \alpha_3 = |u_1'v_1'| \quad \alpha_4 = |u_2'v_2'| \]

The Flow Chart Of Computation

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
The Mapping Between Coordinates and Indexes

The coordinate of nodes

Mapping XY To MN

Mapping MN To XY

The index of array

Implement of Boundary Condition
1) Wall Boundary - Auxiliary Nodes

Auxiliary nodes were introduced to implement wall boundary conditions

Computational domain

Auxiliary nodes

Boundary
Implement of Boundary Condition

2) Wall Boundary - Extrapolation

The macroscopic properties of auxiliary nodes are extrapolated from the computational domain.

Implement of Boundary Condition

3) Periodical Boundary

Periodical Boundary

Original Destination

Modified Destination
Wedge Cascade
Geometry

Ma = 2.0

Result: Stream Line and Ma Contour

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**Wedge Cascade**

Result: Static Pressure at Walls

![Graph showing static pressure at walls](image)

- Present Result (lower wall)
- Present Result (upper wall)
- Theoretical

**C3X Cascade**

Geometry and Inlet and Outlet Parameters

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

<table>
<thead>
<tr>
<th>Run Number</th>
<th>$\alpha_{in}$</th>
<th>$P_{in}$ (Pa)</th>
<th>$T_{i1}$ (K)</th>
<th>$Ma_1$</th>
<th>$Re_1$</th>
<th>$p_2/p_{in}$</th>
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C3X Cascade RUN 143

Results

\[ \frac{p}{p_{t1}} \]

\[ \frac{p}{p_{01}} \]

Ma

RUN 143

Present Result

Experiment Result

Euler solution

Navier-Stokes solution

RUN 144

Ma

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C3X Cascade RUN 144
Results

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

- 1.00
- 0.97
- 0.94
- 0.90
- 0.87
- 0.84
- 0.81
- 0.78
- 0.74
- 0.71
- 0.68
- 0.65
- 0.61
- 0.58
- 0.55

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

- 1.00
- 0.99
- 0.97
- 0.96
- 0.94
- 0.93
- 0.91
- 0.90
- 0.89
- 0.88
- 0.86
- 0.84
- 0.83
- 0.81
- 0.80

C3X Cascade RUN 144
Results

\[ \frac{p}{p_{tl}} \]

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

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### 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

<table>
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<th>$T_{r1}$ (K)</th>
<th>$Ma_1$</th>
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<td>0.84</td>
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</table>

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### VKI Cascade MUR 129
Results

- **$p/p_{01}$**
  - 1.00
  - 0.96
  - 0.93
  - 0.89
  - 0.86
  - 0.82
  - 0.79
  - 0.75
  - 0.71
  - 0.68
  - 0.64
  - 0.61
  - 0.57
  - 0.54
  - 0.50

- **Ma**
  - 1.00
  - 0.93
  - 0.86
  - 0.82
  - 0.79
  - 0.71
  - 0.64
  - 0.57
  - 0.50
  - 0.43
  - 0.36
  - 0.29
  - 0.21
  - 0.14
  - 0.07
  - 0.00

MUR 129

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VKI Cascade MUR 129

$\rho/\rho_0$
- 1.00
- 0.97
- 0.94
- 0.91
- 0.89
- 0.86
- 0.83
- 0.80
- 0.77
- 0.74
- 0.71
- 0.69
- 0.66
- 0.63
- 0.60

$e/e_1$
- 1.00
- 0.99
- 0.97
- 0.96
- 0.95
- 0.94
- 0.92
- 0.91
- 0.90
- 0.88
- 0.87
- 0.86
- 0.85
- 0.83
- 0.82

Experiment Result
Present Result

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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.

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

3) Result

Parallel computing

Speed Up

nT(1) / T(n)

Number of Processor n

0 100 200 300 400 500

0 100 200 300 400 500

- 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.

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 an 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 detailed.