Dynaflow C.F.D. conference
Lattice Boltzmann Simulations and Application to Multiphase Flow

Sacha Jelic, Senior C.F.D. Thermal Engineer
Exa GmbH
January 13th 2011
Agenda

- Company Overview
- Current Applications Overview
- Lattice Boltzmann Background
- PowerFLOW Simulation Process
- Lattice-Boltzmann for Multiphase Flow
- Multiphase Applications
- Discussion
Agenda

- Company Overview
- Current Applications Overview
- Lattice Boltzmann Background
- PowerFLOW Simulation Process
- Lattice-Boltzmann for Multiphase Flow
- Multiphase Applications
- Discussion
About the Company

- Development of Lattice-Boltzmann based CFD Technology
  - Company founded in 1992
  - Based on research by founders at MIT

- Corporate Headquarters – Burlington, MA
  - 180 employees (90+ PhD)

- Worldwide Support Centers
  
  **USA:** Boston, Detroit, San Francisco
  **Europe:** Stuttgart, Paris, Munich, London, Torino
  **Asia:** Tokyo, Seoul

  - Current Sales Focus on Ground Transportation
Aerospace/Defense Customers
Agenda

- Company Overview
- **Current Applications Overview**
- Lattice Boltzmann Background
- PowerFLOW Simulation Process
- Lattice-Boltzmann for Multiphase Flow
- Multiphase Applications
- Discussion
Main Automotive Applications

- Aerodynamics
- Thermal
- Aeroacoustics
Aerodynamics

Drag History

Drag By Quadrants

Isosurfaces of Total Pressure

Soiling

Aerospace
Aeroacoustics: Wind Noise
Thermal Management

- Full 3D heat transfer analysis
  - *Radiation, Convection, Conduction*
  - *Heat exchanger model for 2D coolant calculation*

- General Flow Structure Around Vehicle

- Underhood Surface Temperature
- Radiator Air Recirculation
Fluid Structure interaction

- Aeroelastic response of a high-aspect ratio wing
  - High Lift
  - iteratively 2-way coupled
  - Results Published
Agenda

- Company Overview
- Current Applications Overview
- Lattice Boltzmann Background
- PowerFLOW Simulation Process
- Lattice-Boltzmann for Multiphase Flow
- Multiphase Applications
- Discussion
- *Space divided in cells, time is discrete.*
- *Microscopic model for fluid.*
- *Mass and momentum conserved during collision.*

Collision phase:

\[
t = 1
\]
- *Space divided in cells, time is discrete.*
- *Discrete microscopic model for fluid.*
- *Mass and momentum conserved during collision.*

- Particles are substituted by particle distribution functions $f(t, \bar{x}, \bar{e})$, to reduce noise.

\[
f_i(t + \Delta t, \bar{x} + \bar{e}_i \Delta t) - f_i(t, \bar{x}) = \Omega_i(f_i(t, \bar{x}))
\]

- Advection with constant $v$
- Collision Operator

$f(t, \bar{x}, \bar{e}_i)$ Particle distribution function
\[\bar{e}_i\] Microscopic velocity
\[\Omega(f)\] Collision operator
Lattice Boltzmann Background

Continues Boltzmann equation
\[
\frac{\partial}{\partial t} f(\bar{x}, \bar{v}, t) + \bar{v} \cdot \nabla f(\bar{x}, \bar{v}, t) = \Omega
\]

Lattice Boltzmann equation
\[
f_i(t + \Delta t, \bar{x} + \bar{e}_i \Delta t) - f_i(t, \bar{x}) = \Omega_i(f_i(t, \bar{x}))
\]

Navier Stokes equations
\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_\alpha}{\partial x_\alpha} = 0
\]
\[
\frac{\partial \rho u_\alpha}{\partial t} + \frac{\partial}{\partial x_\beta} (\rho u_\alpha u_\beta + D_{\alpha\beta}) = 0
\]
Collision operator: BGK approximation

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

\[ \begin{aligned}
    \tau \\
    f^{(eq)}
\end{aligned} \]

Single relaxation time

Solution for uniform gas, function of \( \rho(t, \vec{x}), u(t, \vec{x}), \ldots \)

Lattice Boltzmann equation:

\[ f_i(t + \Delta t, \vec{x} + \vec{e}_i \Delta t) = \]

\[ f_i(t, \vec{x}) - \frac{1}{\tau}(f_i(t, \vec{x}) - f_i^{(eq)}(t, \vec{x})) \]
Lattice Boltzmann Background

Macroscopic quantities

- Density:
  \[ \rho(t, \vec{x}) = \sum_i f_i(\vec{x}, t) \]

- Velocity
  \[ \vec{u}(t, \vec{x}) = \frac{1}{\rho(t, \vec{x})} \sum_i f_i(\vec{x}, t) \vec{e}_i \]

- Stress Tensor
  \[ D_{\alpha\beta}(t, \vec{x}) = \sum_i \vec{e}_{i\alpha} \cdot \vec{e}_{i\beta} f(t, \vec{x}) - \rho u_\alpha u_\beta \]
Lattice Boltzmann Background

Assuming: \( c = \Delta t = \Delta x = 1 \)

- **Speed of Sound**
  \[ c_s = \frac{1}{\sqrt{3}} c \]

- **Pressure**
  \[ p = \frac{1}{3} c^2 \rho \]

- **Viscosity**
  \[ \nu = c^2 \left( \frac{\tau}{3} - \frac{\Delta t}{6} \right) \]

**Stability:**

\( \nu > 0 \) or \( \tau > 1/2 \)
Macroscopic conservation equations

Mass: \( \psi_0 = 1 \)
Momentum: \((\psi_1, \psi_2, \psi_3) = \vec{e}_i \)
Energy: \( \psi_4 = \vec{e}_i^2 \)

\[ \sum_i \psi_i [f_i(t + \Delta t, \vec{x} + \vec{e}_i \Delta t) - f_i(t, \vec{x}) - \Omega_i(f_i(t, \vec{x}))] = 0 \]

- **Mass:**
  \[ \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_\alpha}{\partial x_\alpha} = 0 \]

- **Momentum:**
  \[ \frac{\partial \rho u_\alpha}{\partial t} + \frac{\partial}{\partial x_\beta} (\rho u_\alpha u_\beta + D_{\alpha\beta}) = 0 \]
Lattice Boltzmann Boundary Conditions

- Slip BC:

- No slip or bounce back BC:

- Periodic BC, inflow/outflow, Initial conditions.

- Wall model defines turbulent flow properties in 1st cell centre.

- *Cell-boundary intersections, curved surfaces* [Fillipova and Hänel, 1998]
PowerFLOW

- External / Internal aerodynamics
- DNS
- Heat transfer
- Porous media
- Newtonian fluid
- Instationary
- Turbulence Modeling (RNG k-ε)
- Grid refinement with VR-regions:
Postprocessing
Why Lattice Boltzmann?

- Highest level of accuracy
  - *Inherently transient*
  - *Low numerical dissipation*
- Ease of complex geometry handling
  - *No simplifications necessary*
  - *Guaranteed stability*
- Very fast turnaround times
  - *Days v. months*
  - *High scalability up to 1000 cores*
- Exa’s business model: strong partnerships
  - *Joint validation & Methodology*
Agenda

- Company Overview
- Current Applications Overview
- Lattice Boltzmann Background
- PowerFLOW Simulation Process
- Lattice-Boltzmann for Multiphase Flow
- Multiphase Applications
- Discussion
PowerFLOW 5G

- Next generation lattice Boltzmann solver
  - Higher order LB models
  - Multiphase
  - High Mach numbers
  - ....

- Current status
  - Prototype has been completed
  - Looking for industrial partners to guide further development
Key Principle: Modeling Physics – not Phenomena

- Multiphase is natural extension of discrete particle approach
  - Physics of phase interaction can be modeled more intuitively
  - Both at the boundary and in the bulk of the fluid

- Key advantage over Navier-Stokes based methods: no requirement to track interface front
  - Interface fronts emerge from particle interactions
Multiphase Lattice Boltzmann

- Multiphase Model in PowerFLOW: Model interaction force (Shan-Chen* Model)
  - Model phase transitions through non ideal gas
    - single distribution function, van der Waals theory
  - Enables very large density ratios
  - Any number of components can be modeled

- Each component is represented by its own distribution function

\[ f_i^\sigma (t + \Delta t, \bar{x} + \bar{e}_i^\sigma \Delta t) - f_i^\sigma (t, \bar{x}) = \Omega_i^\sigma (f_i^\sigma (t, \bar{x})) \]

- Interaction force between particles and neighboring sites of different species

* Hudong Chen: Chief Scientist, Exa Corp.
  Xiaowen Shan: Director Advanced Physics, Exa Corp.
Interaction modeling

- Define interaction force between molecules at \( x \) and \( x' \):

\[
F(x, x') = -G \psi(x) \psi(x')(x' - x)
\]

- Increment momentum in collision:

\[
\rho \Delta u = \tau F
\]

- Macroscopic level: non-ideal gas
  
Equation of State:

\[
p = \rho \theta + \frac{G \psi^2(\rho)}{2}
\]
Capabilities & Limitations

- Capabilities
  - Multi-phase
  - Multi-component
  - Phase transitions
    - Cavitation, condensation, evaporation, ...
  - Chemical reactions

- Current limitations
  - Low Reynolds number
  - Heat transfer
Agenda

- Company Overview
- Current Applications Overview
- Lattice Boltzmann Background
- PowerFLOW Simulation Process
- Lattice-Boltzmann for Multiphase Flow
- Multiphase Applications
- Discussion
Application Examples

- Fuel cells
- Pumps
  - Multi-phase
  - Rotating geometry
- Rock physics
  - Absolute & relative permeabilities, capillary pressures
- Chemical processing
  - Separation and filtration
  - Mixers
- Pipeline Flows
- Tribology
- Droplet flows
- ....
Simulation of water in gas diffusion layer

- Geometry: Scan of teflon-coated paper
- Simulation conditions
  - Frictionless side walls and periodic inlet-outlet boundaries condition
  - The density ratio water/air is order 1000
  - The Re number based on the porous structure height and averaged terminal velocity of the water phase is 30
  - The Ca number is 0.2
Multiphase Application Example: Dam Break

High Wettability

Low Wettability
Dam Break: Comparison to Experiments

- Height of leading edge v. time
- Location of leading edge v. time
Multiphase Application Example: Droplet Breakup

- Simulation of water droplets in continuous haxedecane phase
  - *Density ratio* ~ 1
  - *Kinematic viscosity ratio* 0.05 – 1.0
- Experiments show that generation of daughter droplets can be controlled through passive breakup
  - *Depends on extension and capillary number*
Droplet Breakup: Comparison to Experiment

- Similar trend for splitting/no-splitting regions
- Critical Ca number is different
  - *Maybe due to difference in density and dynamic viscosity ratios (kinematic viscosity ratio was matched)*
  - *Contact angle: droplets in simulation are non-wetting*
Chemical Reactions Application: Biosensors

- Application: microdevice to screen drugs inhibiting AI-2 synthesis
- Results shown in terms of Peclet and Damköhler nr.
  - *High Pe*: small conversion of reactants, high overall flux of products
  - *High Da*: fast saturation of conversion of reactants
  - Right tradeoff Pe v. Da depends on application

<table>
<thead>
<tr>
<th>Pe</th>
<th>33</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pe</td>
<td>230</td>
</tr>
</tbody>
</table>
Biosensor

Conversion of reactants as function of Pe

Conversion of reactants as function of Da

Production of new species at the wall