Lattice Boltzmann Method for Spacecraft Propellant Slosh Simulation

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Microgravity propellant dynamics continue to offer a formidable modeling challenge for the computational fluid mechanics community.

- Analytical approaches to prediction of bulk behavior, e.g. tank forces and moments, degrades in accuracy below $Bo \approx 10$; small perturbations only.

- Flows dominated by surface tension; curved interfaces; fluid-wall contact angles approximately zero.

- Many semi-analytical or empirical methods that correlate well with theory rely on quasi-steady-state parameters and cannot accurately predict effects of transient flows, e.g. throttling, thruster pulses.

- Momentum transfer due to fluid must be computed accurately for simulation-based verification.

Our research explores the applicability of the lattice Boltzmann method (LBM) to modeling of cryogenic propellant dynamics in microgravity.
The lattice Boltzmann method (LBM) is an emerging approach to CFM using an explicit temporal and spatial discretization of the continuous Boltzmann equation:

$$\frac{\partial f}{\partial t} + \xi^T \nabla_x f + \mathbf{a}^T \nabla_x f = \Omega(f)$$

- Describes evolution of particle distribution functions, e.g. density distribution
- Regular Cartesian discretization of a 2×D position-velocity phase space on a lattice
- In discrete form, the lattice Boltzmann equation is given by

$$f(x_k + \mathbf{e}_x \delta t, t_0 + \delta t) = f(x_k, t_0) - \mathbf{A} (f(x_k, t_0) - f^\text{eq}(x_k, u_k, \rho(x_k))) \delta t$$

**D2Q9 Model**

**Conserved Moments**

$$\rho(x_k) = \sum_i f_i(x_k)$$

$$\rho(x_k) \mathbf{u}_k = \sum_i \mathbf{e}_i f_i(x_k)$$
The fluid dynamics are propagated in two steps over multiple layers:
1. Advection (copy fluid density to adjacent cell: “streaming”)
2. Collision (simulate collisions by relaxing toward Maxwell equilibrium: “relaxation”)

Proper choice of units (time=space=1) and periodic lattice: no actual data copy
- The streaming step is done using pointer arithmetic: fast
- Data locality (only need knowledge of adjacent cells): parallelization

Limitations:
- Constant (wall) temperature: isothermal flow
- Effective speed of sound is related to the lattice physical parameters
  - Compressibility error increases as $M > 0.1$
  - Incompressible flow approximation is valid only for steady flow at low velocities
- Stability decreases as timestep decreases at a fixed kinematic viscosity
Wall boundary conditions are straightforward to implement
- So-called “bounce back rule”: invert velocity distributions at boundary
- Reconstruct unknown distributions by storing in boundary for one timestep
- Not a hydrodynamically accurate BC, but simulates no-slip wall
- More accurate BCs are required for free slip, walls with high curvature, inlet flow, etc.

Relaxation operation and body forces
- Body forces implemented using Kupershtokh exact difference method (EDM)
- Shift equilibrium distribution under action of force such that lattice remains in equilibrium
- Relaxation operation uses multiple relaxation time (MRT) scheme accounting for variation in kinematic viscosity with optional subgrid turbulence model
LBE models allow incorporation of multiple phases uniformly in the lattice
- Phase separation explicitly depends on temperature and a real gas EoS
- We use the Carnahan-Starling EoS corrected for the target conditions (LO₂ @ 94K) in a Shan-Chen like pseudopotential model

\[ p = \rho RT \frac{1 + \frac{b\rho}{4} + \left(\frac{b\rho}{4}\right)^2 - \left(\frac{b\rho}{4}\right)^3}{\left(1 - \frac{b\rho}{4}\right)^3} - a\rho^2 \]

- Phase segregation approximately obeys Maxwell construction (“mechanical stability”)

Parametric wall wetting model allows tuning of free surface contact angle
The behavior of droplets in microgravity is dominated by surface tension

- Droplet dynamics provide a useful verification case due to analytical solutions
- Oscillation of the free surface can be predicted by Lamb’s equation
- Effective surface tension can be determined from frequency

\[
\omega^2 = \frac{l(l - 1)(l + 2)}{r^3 \rho_L \sigma}
\]

Droplet Modes*

<table>
<thead>
<tr>
<th>Mode</th>
<th>Frequency</th>
<th>Droplet Radius</th>
<th>Surface Tension</th>
</tr>
</thead>
<tbody>
<tr>
<td>l=2</td>
<td>~1.3 Hz</td>
<td>(~1.3 Hz)</td>
<td></td>
</tr>
<tr>
<td>l=6</td>
<td>~9.3 Hz</td>
<td>(~9.3 Hz)</td>
<td></td>
</tr>
</tbody>
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Propellant sloshing dynamics are of fundamental concern in spacecraft dynamics

- Analytical solutions exist for axisymmetric containers at high $Bo$
- Below $Bo=1000$ modified analytical models must be used
  - Stable flow only (continuous free surface) and small perturbations
- CFD solutions required for turbulent flow, transient phenomena, PMD simulation, etc.

LBE method verified using a flow regime near analytical limit

- 0.15 m cylindrical LO$_2$ tank with hemispherical ends @ 0.001 g ($Bo=20$)
- Lattice size = $346^2$ (4.1 MB)
- Free decay from initial condition with acceleration 15 degrees from symmetry axis
- First mode frequency matches analytical predictions very well ($f=0.055$ Hz)
LBM approach used for small domain simulation in microgravity

- 0.1m spherical LO$_2$ container in microgravity
- High-g initial condition (settled fluid) and 0g at t=0 (20% fill fraction)
- Random perturbing acceleration (-3 dB @ 0.2 Hz, $g_{RMS}$=0.00003)
- Lattice size = 266$^2$ (2.4 MB)
Some promising results have been obtained in the application of the LBE to propellant sloshing dynamics and related microgravity fluid phenomena

- The LBE method has promise for simulation of thermodynamically consistent multiphase flows in cryogenic propellants
- Fundamental stability limitations remain for very low kinematic viscosities (real fluids!)
- Recent progress includes stability enhancement via adaptive time-stepping and improvement in surface tension model using multirange pseudopotential
  - Overcomes some stability and surface tension limitations by improving isotropy

Production simulation of cryogenic flows will require incorporation of thermal effects

- Thermal LBE codes are emerging and show some promise
- Important to capture convective phenomena, for example, for modeling of long-term fluid circulation in propellant storage systems

Ongoing work extends the present proof-of-concept model to a 3D code

- Parallelization opportunities may allow simulation of CFD-in-the-loop with spacecraft GN&C 6-DoF simulations, for example, using GPU computing
- Possible validation opportunities using existing microgravity fluid experiment data collected aboard International Space Station (ISS)
- 3D code targeted for NASA Exploration Upper Stage (EUS) ullage settling and propellant management studies