GPU Implementation of Lattice Boltzmann Method with Immersed Boundary: observations and results

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The Oxford e-Research Centre Many-Core Seminar Series
5th June 2013

The University of Manchester
Acknowledgements

- Colleagues contributing to this work
  - Mr. Mark Mawson (PhD student @ Univ. Manchester)
  - Dr. Julien Favier (Univ. Marseilles)
  - Pr. Alfredo Pinelli (City Univ. London; prev. CIEMAT, Madrid)
  - Mr. Pedro Valero Lara PhD student @ CIEMAT)
  - Mr. George Leaver (Visualization, Univ. Manchester)

- Thanks to the UKCOMES community (UK Consortium Mesoscale Engineering Sciences), which led to this opportunity.
Overview of Seminar

• Lattice-Boltzmann method
  • An overview of the method
  • Some GPU-related optimizations
  • Validation / Results

• Immersed Boundary method
  • Overview of the method
  • Implementation of IB into LB
  • Some GPU optimisations
  • Results

• Realtime simulation
  • OpenGL tweaks
  • Live demos
Lattice Boltzmann Method: Introduction

The Lattice Boltzmann Method might be considered to be a ‘Mesoscale’ approach

- **Macroscale approaches:**
  - In the limit of low Knudsen number one can assume a ‘Continuum’.
  - The Navier Stokes equation can be applied to infinitesimal elements

- **Microscale approaches:**
  - In the limit of high Knudsen, one might resort to Molecular Dynamics
  - While this approach is impractical for macroscale applications

- **Mesoscale:**
  - Broadly, one can consider that Lattice Boltzmann Method operates between these constraints.
  - on one side it can be extended to macroscale problems, whilst retaining a strong underlying element of particle behaviour.
Lattice Boltzmann Method: Introduction

[Raabe, 2004, ]
Lattice Boltzmann Method: Introduction

- Focus on a *distribution* of particles $f(r, c, t)$
  - Characterises the particles without realising their individual dynamics
  - Instead considers the distribution of particle velocities
- For given equilibrium gas, one can obtain the Maxwell-Boltzmann distribution function:

$$f^{(eq)} = 4\pi \left( \frac{m}{2\pi kT} \right)^{\frac{3}{2}} c^2 e^{-\frac{mc^2}{2kT}}$$

- Macroscopic quantities recovered by integration
- Boltzmann equation describes the return of $f(r, c, t)$ to equilibrium conditions $f^{(eq)}(r, c, t)$
  - the cornerstone of the Lattice Boltzmann Method

$$f(r + cdt, c + Fdt, t + dt)drdc - f(r, c, t)drdc = \Omega(f)dcdt$$
Lattice Boltzmann Method: Introduction

- LBM has origins in Lattice Gas Cellular Automata
  - Hardy, Pomeau, de Pazzis [Hardy et al., 1973, ]
    - proposed a square lattice arrangement
    - though not rotationally invariant and produced ‘square vorticies’!
  - Frisch Hasslacher, Pomeau [Frisch et al., 1986, ]
    - proposed a hexagonal lattice; ensured realistic fluid dynamics
    - included a ‘random element’ and used look up tables.

- basic conservation laws applied
  - Particles can move only along one of the directions
  - Particles move only to next node in one timestep.
  - No particles at same site can move in same direction
Lattice Boltzmann Method: Introduction

- Boltzmann equation can be written as:

\[ \partial_t f + c \cdot \nabla_r f + F \cdot \nabla_c f = \Omega \]

- We use the BGK collision operator from [Bhatnagar et al., 1954, ] to approximate \( \Omega \)

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

- represents relaxation back to equilibrium distribution in timescale \( \tau \).

- And use expansion of \( f^{(eq)} \) to be 2nd order accurate.

\[ f^{(eq)} = \left( \frac{1}{2\pi c_s^2} \right) e^{-\frac{c^2}{2c_s^2}} \left[ 1 + \frac{c \cdot u}{c_s^2} + \frac{(c \cdot u)^2}{2c_s^4} - \frac{u^2}{c_s^2} \right] \]
Lattice Boltzmann Method: Introduction

- Spatial discretization on lattice is provided by Gaussian Quadrature
- DnQm models used for n spatial dimensions and m discrete velocities
- Here we use D2Q9 and D3Q19
- Force term implemented following [Guo et al., 2002, ]:

\[ f_i(x+e_i, t+1) = f_i(x, t) - \frac{1}{\tau} (f_i(x, t) - f_i^{(0)}(x, t)) + \left( 1 - \frac{1}{2\tau} \omega_i \left( \frac{e_i - u}{c_s^2} + \frac{c_i \cdot u}{c_s^4} c_i \right) \right) \cdot f_{ib} \]

- \( f_{ib} \) eventually used for immersed boundary
Validity of LBM for different flows

- Based on 13-moment theory of [Grad, 1949, ] the distribution function may be expanded over velocity and space using orthonormal Hermite polynomials [Shan et al., 2006, ].

\[ f^N(c, c, t) = \omega(c) = \sum_{n=0}^{N} \frac{1}{n!} a^{(n)}, \quad a^{(n)} = \int f \mathcal{H}^{(n)}(c) dc \]

- Coefficients of the Hermite polynomial match the moments of the macroscopic variables

<table>
<thead>
<tr>
<th>H(n)</th>
<th>Resulting model</th>
<th>N-S momentum only</th>
<th>Burnett</th>
<th>N-S+Energy</th>
<th>Suitable physics</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>D2Q9 D3Q19</td>
<td>OK at small Ma</td>
<td>Not valid</td>
<td>Not valid</td>
<td>Incompressible non thermal flow</td>
</tr>
<tr>
<td>6</td>
<td>D2Q17 D3Q39</td>
<td>OK</td>
<td>OK at small Ma</td>
<td>OK at small temp variation</td>
<td>Supersonic regime</td>
</tr>
<tr>
<td>8</td>
<td>D2Q37 D3Q121</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>All !</td>
</tr>
</tbody>
</table>

[Grad, 1949, ]

[Shan et al., 2006, ]

[Latt, 2013, ]
Difference Lattice models

**D2Q9**

\[ w_0 = \frac{4}{9} \]
\[ w_{1-4} = \frac{1}{9} \]
\[ w_{5-8} = \frac{1}{36} \]

**D3Q19**

\[ w_0 = \frac{12}{36} \]
\[ w_{1-6} = \frac{2}{36} \]
\[ w_{7-18} = \frac{1}{36} \]

**D2Q17**

**D3Q39** [Nie and Chen, 2009, ]
Boundary Conditions

- 1st order bounce-back conditions are the most simple
- 2nd order Zou-He conditions have been implemented [Zou, 1997, ]
- some ‘issues’ at corners and along edges where problem is ‘underdefined’
Lattice Boltzmann Method: Algorithm

1. initialise
2. compute forces
3. compute equilibrium function
4. stream & collide
5. imposed boundary condition
6. compute macroscopic quantities
7. $\longrightarrow$ loop to 2

Stream (non-local)

Collide(local)
Validation of 3D solver & boundary conditions

Poiseuille Flow

single precision

double precision

Log10 of error vs. Log10 \( \Delta x \)

- \( \Delta x \)
- \( \Delta x^2 \)
- L_2 Norm

Analytical Solution

33x33x33
Validation of 3D solver & boundary conditions

Lid Driven Cavity 2D: [Ghia et al., 1982, ], 3D: [Jiang et al., 1994, ]
Implementation on GPU
## Hardware Tested

<table>
<thead>
<tr>
<th>Feature</th>
<th>FK104 : K5000M</th>
<th>GK110: K20c</th>
</tr>
</thead>
<tbody>
<tr>
<td>cores (SMX x cores/SMC)</td>
<td>1344 (7 x 192)</td>
<td>2496 (13 x 192)</td>
</tr>
<tr>
<td>regs / thread</td>
<td>63</td>
<td>255</td>
</tr>
<tr>
<td>DRAM</td>
<td>4GB</td>
<td>4.7GB</td>
</tr>
<tr>
<td>SP/DP ratio</td>
<td>24:1</td>
<td>3:1</td>
</tr>
<tr>
<td>Peak performance (single precision)</td>
<td>1.6 TFLOPS</td>
<td>3.5 TFLOPS</td>
</tr>
<tr>
<td>DRAM Bandwidth</td>
<td>66 GB/s (measured)</td>
<td>143 GB/s (measured)</td>
</tr>
</tbody>
</table>
Lattice Boltzmann Method: Algorithm

**PUSH**
1. initialise
2. compute forces
3. compute $f^{(eq)}$
4. collide (local)
5. stream (non-local)
   - i.e. requires synchronisation
6. impose bcs.
7. compute macroscopic quantities

**PULL** (see [Rinaldi et al., 2012, ])
1. initialise
5. stream
   - i.e. read values from host into new location
6. impose bcs.
7. compute macroscopic quantities
2. compute forces
3. compute $f^{(eq)}$
4. collide
Lattice Boltzmann Method: GPU implementation

CPU implementation: push

```c
for(int dir = 0; dir < 9; ++dir) {
    Xnew=X+cx[dir]; // Stream x `PUSH'
    Ynew=Y+cy[dir]; // Stream y
    pop [dir][Xnew][Ynew] = pop_old[dir][X][Y] * (1 - omega)
    + pop_eq[dir] * omega + force_latt[dir]; // Collide
}
```

GPU implementation: pull

```c
int size=Nx*Ny;
for(dir = 0; dir < 9; ++dir) {
    Xnew=X-d_cx[dir]; // Stream x `PULL'
    Ynew=Y-d_cy[dir];
    pop_local[dir] = pop_old[dir*size+Ynew*Nx+Xnew];
}
```
Memory Arrangement

- Code is parallelized such that one thread will perform the complete LBM algorithm at one spatial location $f(x)_i$ in the fluid domain.
- Each thread stores values of $f(x)_i$ and an integer tag denoting boundary type. Density $\rho$ and velocity $u_i$ are only stored if output.
- All is stored in a struct within registers to minimise high latency access to DRAM once initially loaded.
- within DRAM it is common practise to ‘flatten’ multiple dimension

\[ f[\text{dir}\ast N_x\ast N_y\ast Y\ast N_x\ast X] \]
Instruction Level Parallelism

More ILP at expense of occupancy improves performance [Volkov, 2010, ]

- Operating on all indices of \( f \) in one thread helps to hide latency
- Use structs of arrays access to \( f \). Coalesced access therefore only depends on the \( x \) component of the discrete velocity direction (\( \mathbf{c} \))
- Cache hit rate is low as we don’t have repeat accesses (< 7% in L2)
- .. so instead maximise register use (which lowers occupancy)

No \( x \)-component of \( \mathbf{c} \) in SMC

\( x \)-component of \( \mathbf{c} = -1 \) in SMC
Maximising use of registers

- maximum of 65536 registers and can host up to 2048 threads

\[
\frac{\text{registers}}{\text{thread}} \times \frac{\text{threads}}{\text{block}} \times \frac{\text{blocks}}{\text{SMX}} \leq 65536
\]

- in 3D we need 19 loads for \( f(x) \) and 19 stores
  - we also need 1 integer (boundaries) and 4 macroscopic quantities
  - so total of 43 registers needed per thread

- for high registers/thread, large block sizes are impractical.
  - e.g. block size of 1024 means only a single block would run
  - [Obrecht et al., 2013, ] recommend maximum block size of 256
Shared mem shuffle operation on Keplers

Shared Mem

Shuffle

(a) K5000M

(b) K20c
Shared mem shuffle operation on Keplers

- ILP is more efficient than Shared memory or shuffle
- large block sizes are impractical for LBM
Overall Performance

- Peak 814 MLUPS and 402 MLUPS for K20c and K5000M respectively
  - vs theoretical max of 892 MLUPS and 412 MLUPS based on measured bandwidth
- Compared well to other implementations (albeit on other h/w)
- [Rinaldi et al., 2012, ] and [Astorino et al., 2011, ] use Shared Mem.
Immersed Boundary method
Immersed Boundaries (1977-)

Fluid equations solved on an Eulerian mesh. The geometrical complexity is embedded using an Lagrangian mesh via a system of singular forces.

- **Original Motivation of Charles Peskin** [Peskin, 1977, ]
  - Preserve efficient high order (Cartesian) solver
  - Define arbitrary mesh shape
- **An alternative to body fitted mesh**
  - Not a replacement, but a valuable tool
Original vs current approach

- [Peskin, 1977, ]

- Applied to a complete heart fluid system
- Peskin idea: model the boundary as a system of inextensible spring & dampers
- The *elastic* forces that restore the *true* and *actual* boundary position are supplied to the *rhs* of the momentum equations in terms of body forces.

- [Pinelli et al., 2010, ] (no springs) has been introduced and applied (CIEMAT): no *k* stiffness introduced

- Modified approach has some advantages:
  - Moving boundary
  - Deformable boundary
- Sharing a drawback:
  - pressure correction error
Immersed Boundary: basics (I)

\[ \frac{\partial u}{\partial t} = \text{rhs} + f, \quad f = \frac{u^{(d)} - u^n}{\Delta t} - \text{rhs} \quad \forall \vec{x} \in S \]

algorithm:

1. given $f$ update position of Lagrangian markers (boundary shape)
2. advance momentum equation without boundary induced body forces ($u^*$ on $S$)
3. compute $f$ as a function of the difference $u^{(d)} - u^*$
4. repeat momentum advancement with $f$
5. compute for pressure correction, project velocity field
6. goto 1.
Immersed Boundary: basics (II)

In discrete form in 2D

Interpolation

\[ U^*(x_l) = \sum_{i,j} u^*(x_{i,j}) \delta_h(x_{i,j} - X_l) \Delta x^2 \]

Spread (convolution)

\[ f(x_{i,j}) = \sum_{l \in \Omega_l} F(X_l) \delta_h(x_{i,j} - X_l) \epsilon \Delta l \]

- Epsilon is the key to the accuracy
- it can be considered to represent the physical width of the surface.
- and it’s computation guarantees that interpolation(spread(F)) = F
Coupling IB with LB

- Bounceback does not offer high accuracy
  - assumes ‘stair-step’ surface
  - and is problematic for moving/flexible boundaries

- Inherent suitability of LB to IB
  - Lattice already uniform Cartesian
  - Poisson-free! \( \rightarrow \) No pressure correction drawback
Lattice Boltzmann Method: Algorithm

1. initialise
2. set forces to zero
3. find velocity field in absence of object (call LBM)
4. compute support not required if not moving
5. find epsilon Costly, & also not required if not moving
6. interpolate fluid velocity onto Lagrangian marker
7. compute required force for object
8. spread force onto lattice
9. (solve other equations: collision, tension, bending, inextensibility)
10. find velocity field with object (call LBM again)
11. compute macroscopic quantities

(see [Favier et al., 2013, ] for full details)
Rigid Particles: validation 1

Validation on finite-differences DNS [Uhlmann, 2005, ]
Falling particle under gravity $\rho_p/\rho_f = 8$, $Re = 165$

Starting at rest, no slip walls, gravity along $x$
Rigid Particles: validation 2

Kissing/Tumbling particles [Uhlmann, 2005, ]

Impulsively moved flat plate [Koumoutsakos and Shiels, 1996, ]
Transactions for each point of the object are coalesced
  • each point only needs information about itself
Transactions moving data between fluid and boundary are random with much higher cache use.

Transfer from host to IBM kernel can be started simultaneously to hide latency
  • exploit capability to overlap memory transfers with executions
spreading operation is a problem (atomic add)
Small vs. large objects

- Objects are treated according to size; number of Lagrangian markers (nlag)
- For small objects ($nlag < 1024$) we assign one block per object
  - generally the case for 2D
- For large objects ($nlag > 1024$), we need to launch a kernel for each object
  - e.g. for a sphere radius $r = 20$ we need $nlag$ 4000
Flexible beating filament I

Apply inextensibility condition to the filament

\[
\frac{\partial \mathbf{X}}{\partial t} = \text{Interpol}(\mathbf{u}) \quad \text{Kinematic condition}
\]

\[
\mathbf{F}_h = -\text{Interpol}(\mathbf{f}) \quad \text{Immersed boundary}
\]

\[
\rho \frac{\partial^2 \mathbf{X}}{\partial t^2} = \frac{\partial}{\partial s} \left( T \frac{\partial \mathbf{X}}{\partial s} \right) - \frac{\partial^2}{\partial s^2} \left( K_B \frac{\partial^2 \mathbf{X}}{\partial s^2} \right) + \rho g - \mathbf{F}_h \quad \text{Solid momentum}
\]

\[
\nabla \cdot \mathbf{u} = 0 \quad \text{Incompressible condition}
\]

\[
\frac{\partial \mathbf{X}}{\partial s} \cdot \frac{\partial \mathbf{X}}{\partial s} = 1 \quad \text{Inextensibility condition}
\]

following method of [Huang et al., 2007, ]

- \(f\) is the force required by the fluid to verify the b.c
- \(\mathbf{F}_h\) is the hydrodynamic force resulting from having applied the b.c.
Flexible beating filament II

- Application to Lattice-Boltzmann solver
- Staggered discretization of the Lagrangian space ($X$ and $T$)

\[ \frac{X_{n+1} - 2X^n + X^{n-1}}{\Delta t^2} = [D_s(T_{n+1}D_sX^{n+1})] + (F_b) + Fr \frac{g}{g} - F^n \]

\[ D_sX^{n+1} \cdot D_sX^{n+1} = 1; \]

- Tension computed via iterative Newton-Raphson loop (by computing the exact Jacobian)
- For the initial guess, it’s possible to derive a very good estimate for the tension, by incorporating the inextensibility condition in the momentum equations:

\[ \frac{\partial^2 T^{n+1}}{\partial s^2} - \left( \frac{\partial^2 X^n}{\partial s^2} \cdot \frac{\partial^2 X^n}{\partial s^2} \right) T^{n+1} = - \frac{\partial X^n}{\partial s} \cdot \frac{dF^n}{ds} - \rho \frac{\partial \dot{X}^n}{\partial s} \cdot \frac{\partial X^n}{\partial s} + \frac{\partial X^n}{\partial s} \cdot \frac{\partial^3 (K_B \frac{\partial^2 X^n}{\partial s^2})}{\partial s^3} \]

\[ \Rightarrow AT^{n+1} = rhs^n \text{ where } A \text{ is a tridiagonal matrix} \]
flexible filaments: validation 1

Without fluid (falling under its own weight)

With fluid (for different rigidities we observe correct ‘kick’ of free end)

(a) Totally flexible filament ($K_B = 0$). (b) Rigid filament ($K_B = 0.001$).

(see [Favier et al., 2013, ] for full details)
Filament interactions: 2 filaments

Correct phase dependence on separation of filaments

(see [Favier et al., 2013, ] for full details)
**flexible filaments: investigation**

Cylinder coated with filaments: drag reduction [Revell et al., 2013, ]

EU funded project on this topic just started: PELSKIN

Realtime LBM
Realtime output

several OpenGL visualization techniques are implemented

- **Contour colour map** (for velocity magnitude) is stored on the device
- **Image Based Flow Visualization** (IBFV) simulates advection of particles through an unsteady vector field (macroscopic $u$ field)
  - instead of particle seeding which can be hit or miss
  - noise textures are used to represent dense set of particles, which are advected forwards using texture mapping
- previous frame $M$ is textured onto a distorted mesh and blended with random noise texture $N$ according to blending factor $\alpha$

\[
M_i(x) = (1 - \alpha)M_{i-1}(x + u_i(x, t_i) \delta t) + \alpha N_i(x)
\]

- velocities used to displace mesh vertices using forwards integration
- noise texture does not affect flow
- mesh resolution may be coarser than lattice

- **Dye injection** uses a similar method
  - can be more intuitive
uses for Realtime?

- Initially started out as a gimmick, used for teaching and open days

- Attracting increased attention in some areas
  - training for medical surgical procedure
  - for complex industrial applications where ‘intuition’ is missing
Conclusions

- LBM solver implemented on Kepler hardware with some optimizations
  - 814 MLUPS peak on K20c
- IB-LB solver validated for rigid and flexible geometry
  - various flow physics investigations underway
  - context of EU project PELSKIN
  - BBSRC project on ‘protein manufacturability’
- Realtime version of the solver available
  - with various visualization options
  - exploring potential applications
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