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

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Overview of Seminar

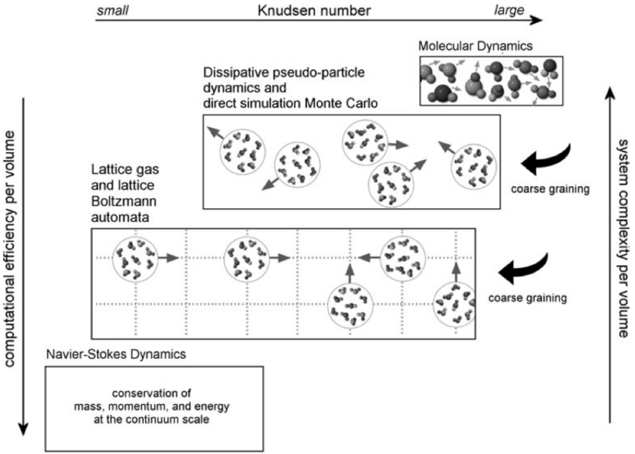
- Lattice-Boltzmann method
  - An overview of the method
  - Some GPU-related optimizations
  - Validation / Results
- Immersed Boundary method
  - Overview of the method
  - Implementation of IB into LB
  - Some GPU optimisations
  - Results
- Realtime simulation
  - OpenGL tweaks
  - Live demos

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

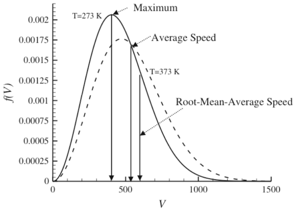


[Raabe, 2004,]

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 equilbrium 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 $f(\mathbf{r}, \mathbf{c}, t)$ to equilibrium conditions $f^{(eq)}(\mathbf{r}, \mathbf{c}, t)$
    - the cornerstone of the Lattice Boltzmann Method

$$f(\mathbf{r} + \mathbf{c}dt, \mathbf{c} + \mathbf{F}dt, t + dt)d\mathbf{r}d\mathbf{c} - f(\mathbf{r}, \mathbf{c}, t)d\mathbf{r}d\mathbf{c} = \Omega(f)d\mathbf{c}dt$$

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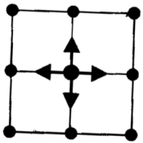
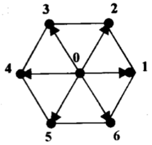
Lattice Boltzmann Method: Introduction

- 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 realisitic 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





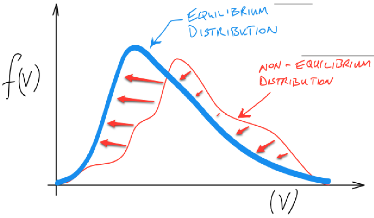
Lattice Boltzmann Method: Introduction

- 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 Ω

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



- represents relaxation back to equilibrium distribution in timescale τ.
  - And use expansion of $f^{(eq)}$ to be 2nd order accurate.

$$f^{(eq)} = \left(\frac{1}{2\pi c_s^2}\right) e^{\frac{-c^2}{2c_s^2}} \left[1 + \frac{\mathbf{c}\cdot\mathbf{u}}{c_s^2} + \frac{(\mathbf{c}\cdot\mathbf{u})^2}{2c_s^4} - \frac{u^2}{c_s^2}\right]$$

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,]:

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

  - 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,].

$$f^N(\mathbf{c}, \mathbf{c}, t) = \omega(c) = \sum_{n=0}^{N} \frac{1}{n} a^{(n)}, \qquad a^{(n)} = \int f \mathcal{H}^{(n)}(c) dc$$

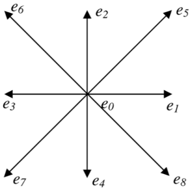
- Coefficients of the Hermite polynomial match the moments of the macroscopic variables

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

[Latt, 2013,]

Difference Lattice models

D2Q9

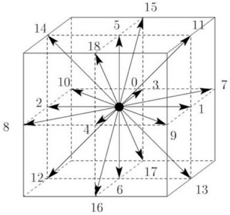


$$w_0 = \frac{4}{9}$$

$$w_{1-4} = \frac{1}{9}$$

$$w_{5-8} = \frac{1}{36}$$

D3Q19

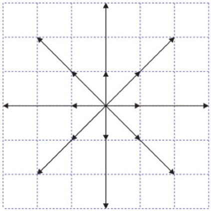


$$w_0 = \frac{12}{36}$$

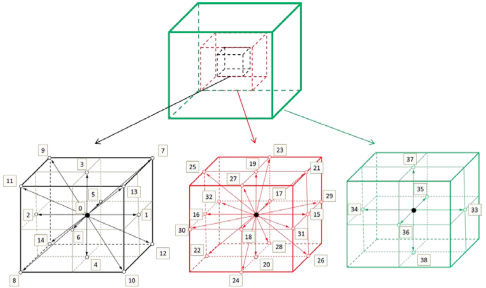
$$w_{1-6} = \frac{2}{36}$$

$$w_{7-18} = \frac{1}{36}$$

D2Q17

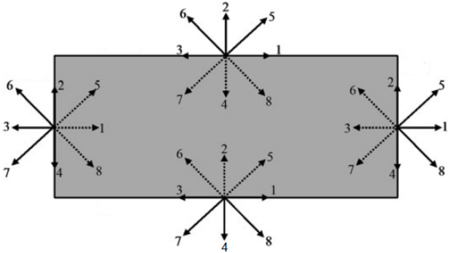


D3Q39[Nie and Chen, 2009,]



Boundary Conditions

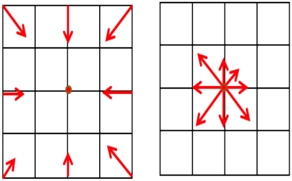
- 1st order bounce-back conditions are the most simple
- 2nd order Zou-He conditions have been implemented [Zou, 1997,]
- some ‘issues’ at corners and along edges where problem is ‘underdefined’



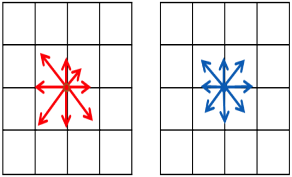
Lattice Boltzmann Method: Algorithm

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)



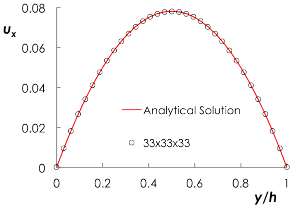
Collide(local)

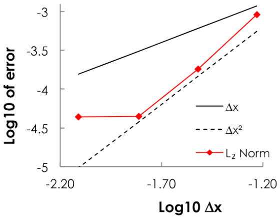


Validation of 3D solver & boundary conditions

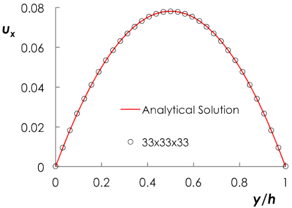
Poiseuille Flow

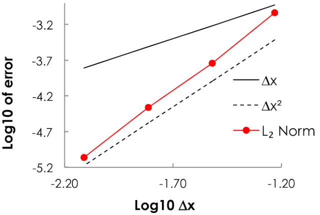
single precision





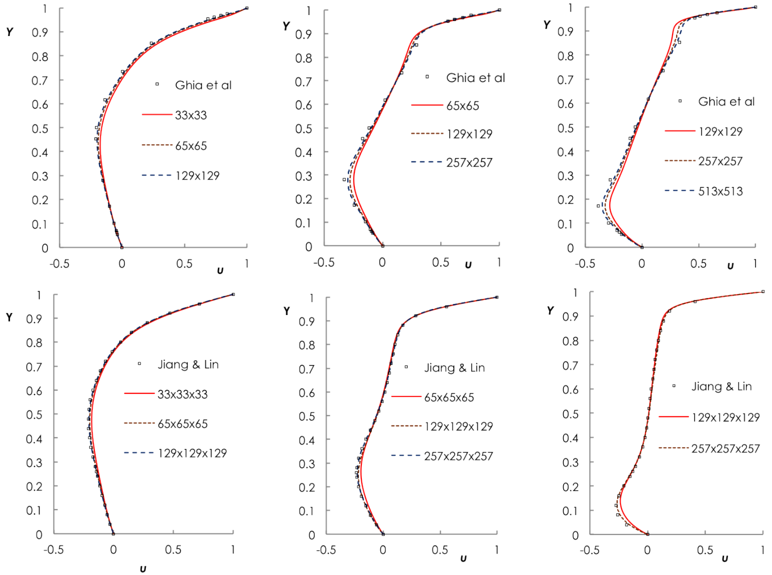
double precision





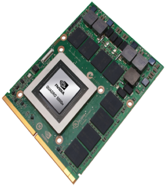
Validation of 3D solver & boundary conditions

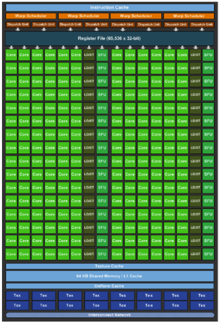
Lid Driven Cavity 2D: [Ghia et al., 1982,], 3D: [Jiang et al., 1994,]



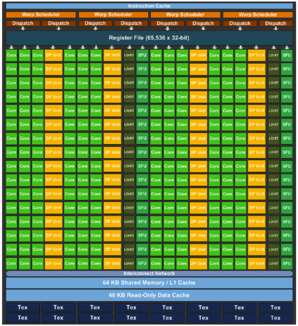
Implementation on GPU

Hardware Tested





(a) GK104



(b) GK110

Feature	FK104 :K5000M	GK110: K20c
cores (SMX x cores/SMC)	1344 (7 x 192)	2496 (13 x 192)
regs / thread	63	255
DRAM	4GB	4.7GB
SP/DP ratio	24:1	3:1
Peak performance (single precision)	1.6 TFLOPS	3.5 TFLOPS
DRAM Bandwidth	66 GB/s (measured)	143 GB/s (measured)

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

```
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

```
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

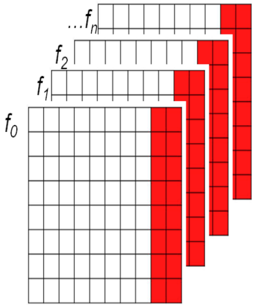
- Code is parallelized such that one thread will perform the complete LBM algorithm at one spatial location $f(x)_i$ in the fluid domain.
- Each thread stores values of $f(x)_i$ and an integer tag denoting boundary type. Density ρ and velocity u_i are only stored if output.
- All is stored in a struct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

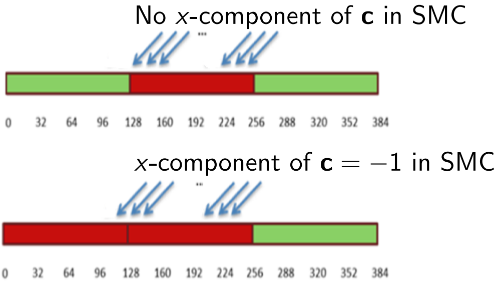
```
f[dir*Nx*Ny+Y*Nx+X]
```

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)





Maximising use of registers

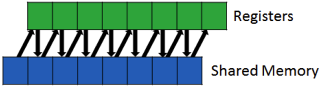
- maximum of 65536 registers and can host up to 2048 threads

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

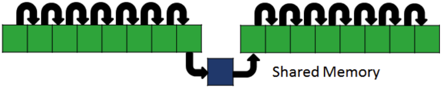
- in 3D we need 19 loads for $f(x)$ and 19 stores
    - we also need 1 integer (boundaries) and 4 macroscopic quantities
    - so total of 43 registers needed per thread
- for high registers/thread, large block sizes are impractical.
    - e.g block size of 1024 means only a single block would run
    - [Obrecht et al., 2013,] recommend maximum block size of 256

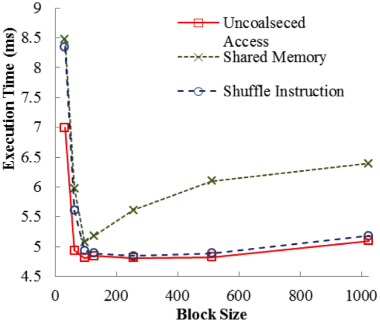
Shared mem shuffle operation on Keplers

Shared Mem

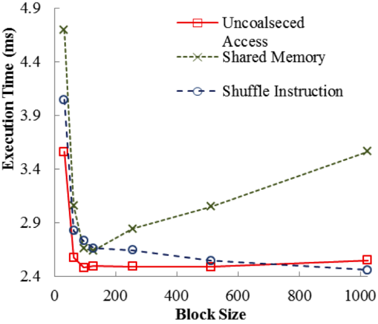


Shuffle



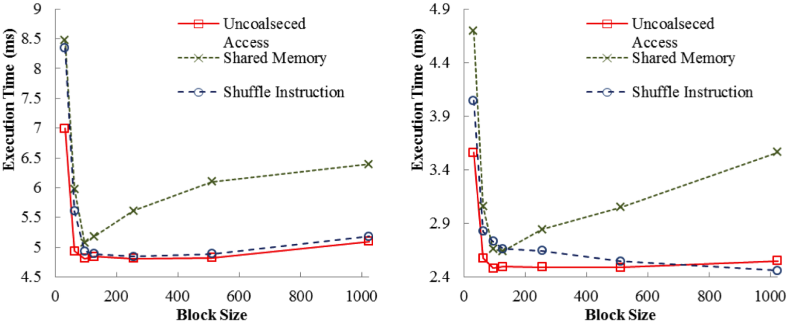


(a) K5000M



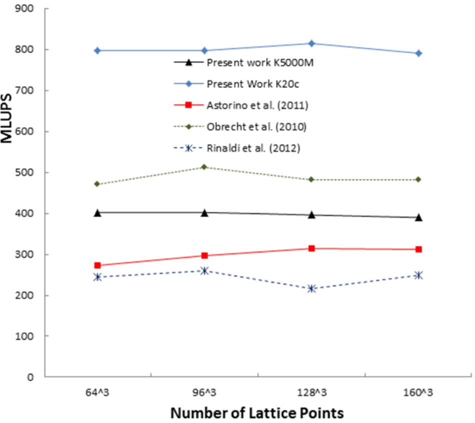
(b) K20c

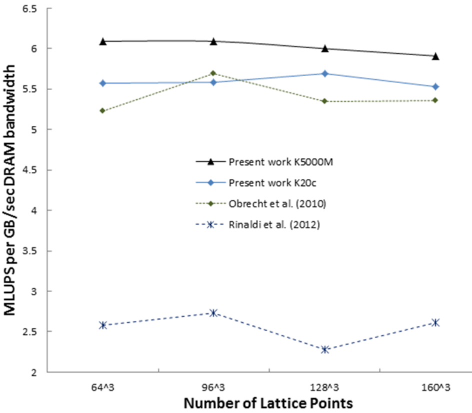
Shared mem shuffle operation on Keplers



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

Overall Performance





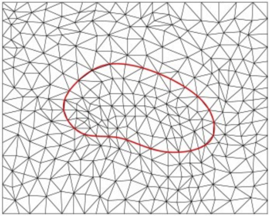
- Peak 814MLUPS and 402MLUPS for K20c and K5000M respectively
    - vs theoretical max of 892MLUPS and 412MLUPS based on measured bandwidth
- Compared well to other implementations (albeit on other h/w)
- [Rinaldi et al., 2012,] and [Astorino et al., 2011,] use Shared Mem.

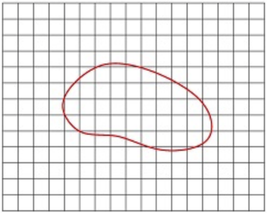
Immersed Boundary method

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.

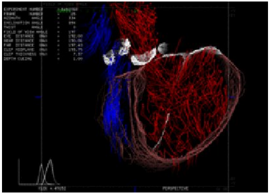
- Original Motivation of Charles Peskin [Peskin, 1977,]
  - Preserve efficient high order (Cartesian) solver
  - Define arbitrary mesh shape
- An alternative to body fitted mesh
  - Not a replacement, but a valuable tool





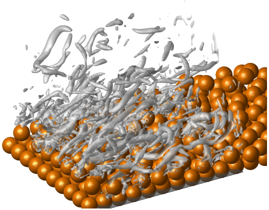
Original vs current approach

- [Peskin, 1977,]



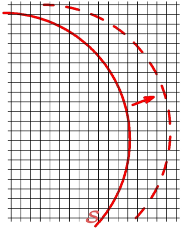
- Applied to a complete heart fluid system
- Peskin idea: model the boundary as a system of inextensible spring & dampers
- The *elastic* forces that restore the *true* and *actual* boundary position are supplied to the *rhs* of the momentum equations in terms of body forces.

- [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)



Along $\mathcal{S}$ $u = u^{(d)}$

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

algorithm:

1. given f update position of Lagrangian markers (boundary shape)
2. advance momentum equation without boundary induced body forces (u^* on $\mathcal{S}$)
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)

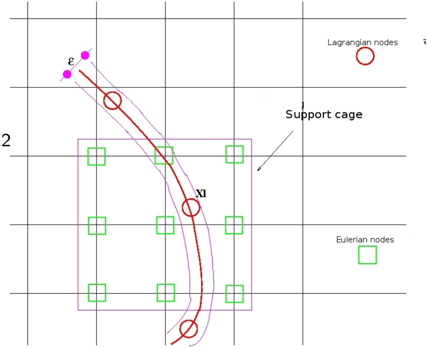
In discrete form in 2D

Interpolation

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

Spread (convolution)

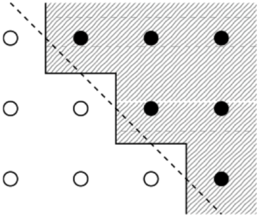
$$f(x_{i,j}) = \sum_{l\in\Omega_l} F(X_l)\delta_h(x_{i,j} - X_l)\epsilon\Delta l$$



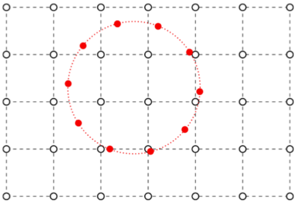
- Epsilon is the key to the accuracy
- it can be considered to represent the physical width of the surface.
- and it's computation guarantees that *interpolation*(*spread*(**F**))=**F**

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 ! $\longrightarrow$ 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

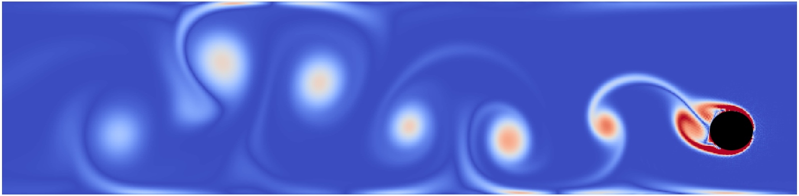
(see [Favier et al., 2013,] for full details)

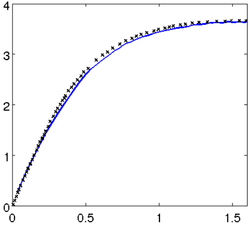
Rigid Particles: validation 1

Validation on finite-differences DNS [Uhlmann, 2005,]

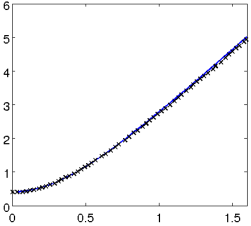
Falling particle under gravity $\rho_p/\rho_f = 8$, $Re = 165$

Starting at rest, no slip walls, gravity along x





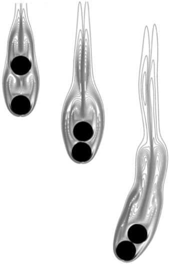
settling velocity

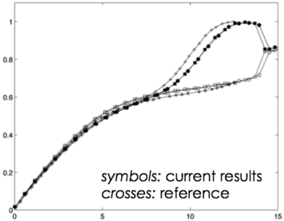


x-position

Rigid Particles: validation 2

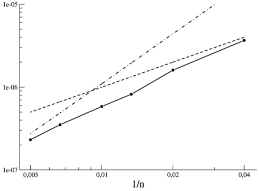
Kissing/Tumbing particles [Uhlmann, 2005,]

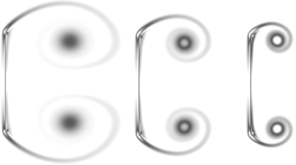


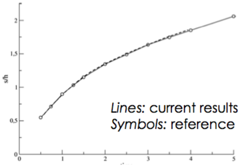


(a) u/U_{max} (parallel to gravity).

Impulsively moved flat plate [Koumoutsakos and Shiels, 1996,]

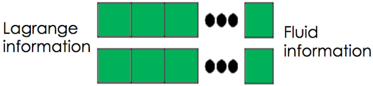




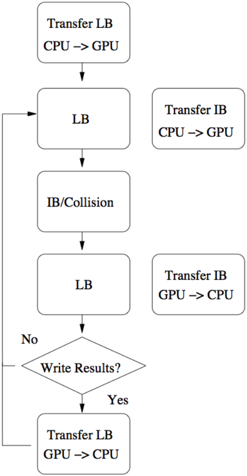


Immersed boundary + GPU

- 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.

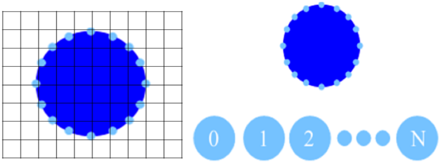


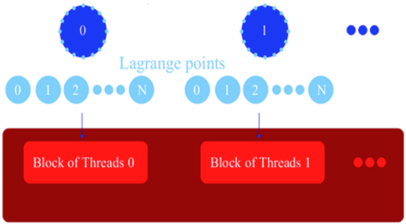
- Transfer from host to IBM kernel can be started simultaneously to hide latency
  - exploit capability to overlap memory transfers with executions
- spreading operation is a problem (atomic add)



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

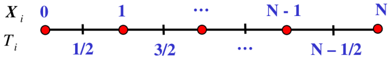
$$\begin{cases} \dfrac{\partial \mathbf{X}}{\partial t} = Interpol(\mathbf{u}) & \text{Kinematic condition} \\ \mathbf{F}_h = -Interpol(\mathbf{f}) & \text{Immersed boundary} \\ \rho \dfrac{\partial^2 \mathbf{X}}{\partial t^2} = \dfrac{\partial}{\partial s}(T \dfrac{\partial \mathbf{X}}{\partial s}) - \dfrac{\partial^2}{\partial s^2}(K_B \dfrac{\partial^2 \mathbf{X}}{\partial s^2}) + \rho \mathbf{g} - \mathbf{F}_h & \text{Solid momentum} \\ \nabla \cdot \mathbf{u} = 0 & \text{Incompressible condition} \\ \dfrac{\partial \mathbf{X}}{\partial s} \cdot \dfrac{\partial \mathbf{X}}{\partial s} = 1 & \text{Inextensibility condition} \end{cases}$$

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

- $\mathbf{f}$ 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 ($\mathbf{X}$ and T)



$$\frac{\mathbf{X}^{n+1} - 2\mathbf{X}^{n} + \mathbf{X}^{n-1}}{\Delta t^2} = [D_s(T^{n+1} D_s \mathbf{X}^{n+1})] + (F_b) + Fr\frac{\mathbf{g}}{g} - \mathbf{F}^n$$

$$D_s\mathbf{X}^{n+1} \cdot D_s\mathbf{X}^{n+1} = 1;$$

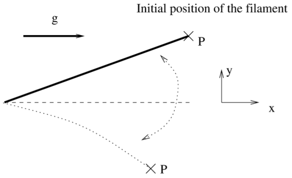
- Tension computed via iterative Newton-Raphson loop (by computing the exact Jacobian)
- For the initial guess, it's possible to derive a very good estimate for the tension, by incorporating the inextensibility condition in the momentum equations:

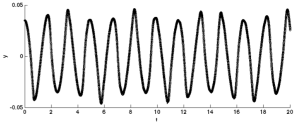
$$\frac{\partial^2 T^{n+1}}{\partial s^2} - \left(\frac{\partial^2 \mathbf{X}^n}{\partial s^2} \cdot \frac{\partial^2 \mathbf{X}^n}{\partial s^2}\right) T^{n+1} = -\frac{\partial \mathbf{X}^n}{\partial s} \cdot \frac{d\mathbf{F}_h^n}{ds} - \rho \frac{\partial \dot{\mathbf{X}}^n}{\partial s} \cdot \frac{\partial \dot{\mathbf{X}}^n}{\partial s} + \frac{\partial \mathbf{X}^n}{\partial s} \cdot \frac{\partial^3}{\partial s^3}\left(K_B \frac{\partial^2 \mathbf{X}^n}{\partial s^2}\right)$$

$$\Longrightarrow AT^{n+1} = rhs^n \quad \text{where A is a tridiagonal matrix}$$

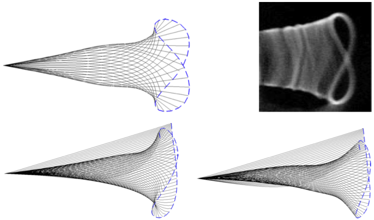
flexible filaments: validation 1

Without fluid (falling under its own weight)





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

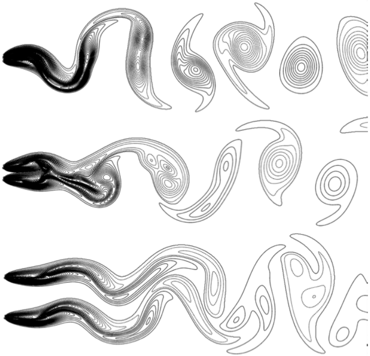


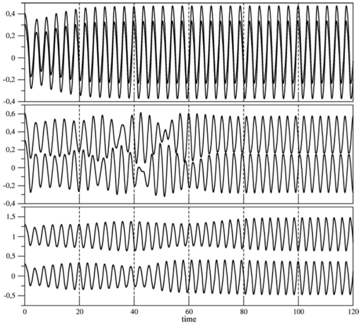
(a) Totally flexible filament ($K_B = 0$). (b) Rigid filament ($K_B = 0.001$).

(see [Favier et al., 2013,] for full details)

flexible filaments: validation 2

Filament interactions: 2 filaments



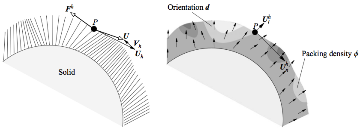


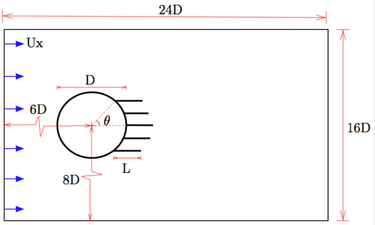
correct phase dependence on separation of filaments

(see [Favier et al., 2013,] for full details)

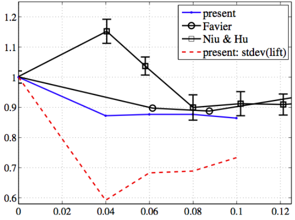
flexible filaments: investigation

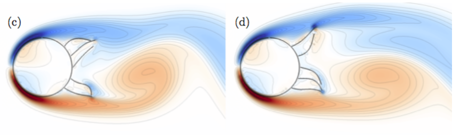
Cylinder coated with filaments: drag reduction [Revell et al., 2013,]





[Favier et al., 2009,]





EU funded project on this topic just started: PELSKIN

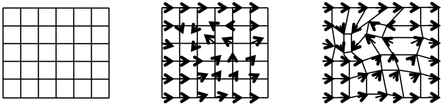
(temp web address : http://195.83.116.187/pelskin_web/)

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 α



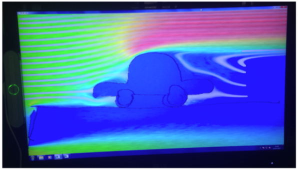
  - velocities used to displace mesh vertices using forwards integration
  - noise texture does not affect flow
  - mesh resolution may be coarser than lattice

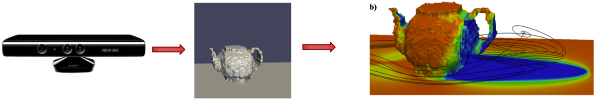
$$M_i(\mathbf{x}) = (1-\alpha)M_{i-1}\left(\mathbf{x} + \mathbf{u_i}\left(\mathbf{x}, t_i\right)\delta t\right) + \alpha N_i(\mathbf{x})$$

- Dye injection uses a similar method
  - can be more intuitive

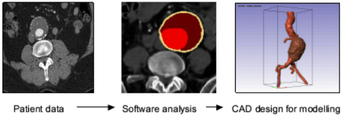
uses for Realtime?

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





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



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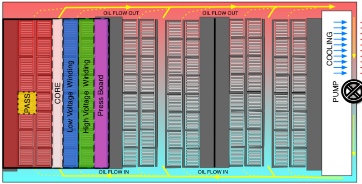

Conclusions

- 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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