CCDSC 2016

On a Novel Method for High Performance Computational Fluid Dynamics

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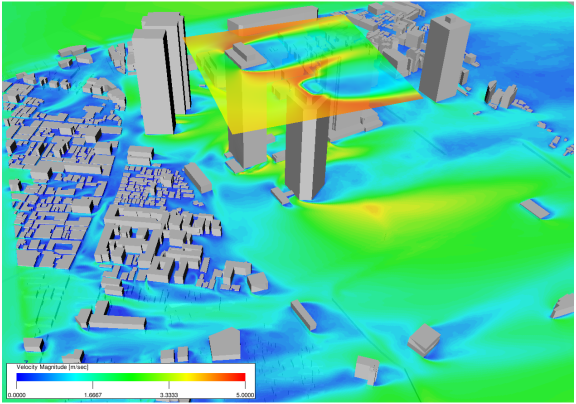
Outline

I – Motivation

Areas of interest: Urban physics



Margheri and Sagaut, 2014

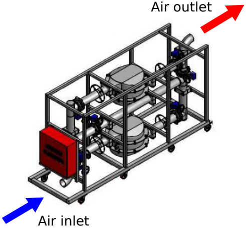
Urban micro-climate, pedestrian wind comfort, pollutant dispersion. . .

Areas of interest: Thermal energy storage

Shell and tube heat exchanger

Latent heat storage (phase change materials).

Zeolite beads



Sorption and/or chemical heat storage.

Computational Fluid Dynamics

The previous engineering applications rely heavily on CFD simulations.

- Multi-physics models.
- Complex geometries.
- $\mathcal{O}(10^9)$ fluid cells.
- Physically relevant simulation times.

Technical issues:

- Multi-physics commercial codes (e.g. Fluent) are expensive and do not scale over $\mathcal{O}(10^2)$ cores.
- Open CFD codes (e.g. code Saturne) are not designed for accelerators.

Unstructured vs Cartesian meshes

Unstructured

- Body fitting mesh.
- Time consuming generation process.
- Isotropy is an issue.
- Irregular data access pattern.

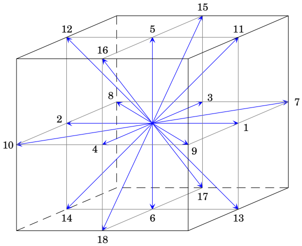
Cartesian

- Trivial meshing.
- GPU-friendly data layout.
- Hierarchical structure is often needed.

Lattice Boltzmann method

- Discretized version of the Boltzmann equation recovering the solutions of the Navier–Stokes equation.
- Regular Cartesian grid of mesh size δx with constant time step δt.
- Finite set of particular densities f_α associated to particular velocities $\boldsymbol{\xi}_\alpha$.
- Collision operator Ω (usually explicit).

$$\big|f_\alpha(\boldsymbol{x} + \delta t \boldsymbol{\xi}_\alpha, t + \delta t)\big\rangle - \big|f_\alpha(\boldsymbol{x},\, t)\big\rangle = \Omega \big|f_\alpha(\boldsymbol{x},\, t)\big\rangle$$



$$\rho = \sum_\alpha f_\alpha$$

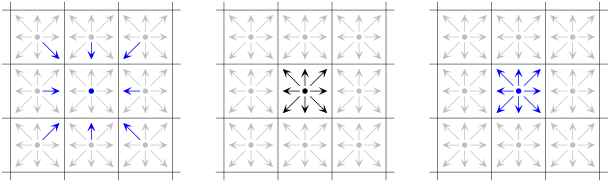
$$\rho \boldsymbol{u} = \sum_\alpha f_\alpha \boldsymbol{\xi}_\alpha$$

Pull formulation of the LBM

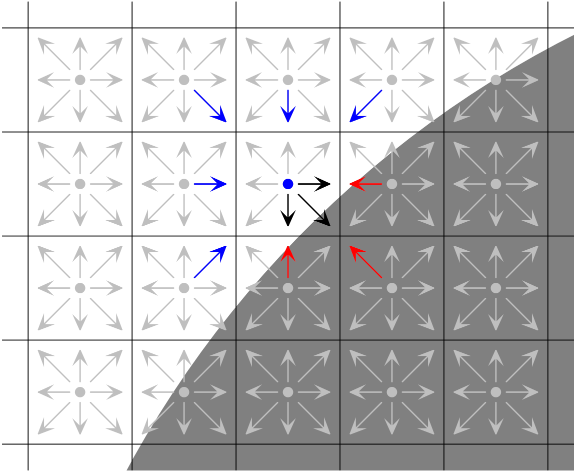
Two-step formulation of LBM: propagation (1) followed by collision (2).

$$\left|f_\alpha(\boldsymbol{x}, t+\delta t)\right\rangle = \left|f^*_\alpha(\boldsymbol{x}-\delta t\boldsymbol{\xi}_\alpha, t)\right\rangle \tag{1}$$

$$\left|f^*_\alpha(\boldsymbol{x}, t+\delta t)\right\rangle = \left|f_\alpha(\boldsymbol{x}, t+\delta t)\right\rangle + \Omega\left|f_\alpha(\boldsymbol{x}, t+\delta t)\right\rangle \tag{2}$$



Solid-fluid interface



Simple bounce-back boundary condition

LBM pros and cons

Pros

- Explicitness, algorithmic simplicity.
- Easy solid boundary processing.
- Well-suited to GPUs.

Cons

- Large memory consumption (19 scalars vs 4 hydrodynamic variables).
- Impact on performance in memory bound context.

II – Link-wise artificial compressibility method

Link-wise artificial compressibility method (LW-ACM)

- Novel formulation of the artificial compressibility method.
- Strong analogies with lattice Boltzmann schemes.

Updating rule:

$$f_\alpha(\boldsymbol{x},\, t+1) = f_\alpha^{(\mathrm{e})}(\boldsymbol{x}-\boldsymbol{\xi}_\alpha,\, t) + 2\left(\frac{\omega-1}{\omega}\right)\left(f_\alpha^{(\mathrm{e,o})}(\boldsymbol{x},\, t) - f_\alpha^{(\mathrm{e,o})}(\boldsymbol{x}-\boldsymbol{\xi}_\alpha,\, t)\right)$$

where $f_\alpha^{(\mathrm{e})}$ are local equilibria which only depend on local ρ and $\boldsymbol{u}$, and $f_\alpha^{(\mathrm{e,o})}$ are the odd parts of the equilibrium functions:

$$f_\alpha^{(\mathrm{e,o})}(\rho,\, \boldsymbol{u}) = \frac{1}{2}\left(f_\alpha^{(\mathrm{e})}(\rho,\, \boldsymbol{u}) - f_\alpha^{(\mathrm{e})}(\rho,\, -\boldsymbol{u})\right).$$

P. Asinari, T. Ohwada, E. Chiavazzo, and A. F. Di Rienzo.
Link-wise artificial compressibility method.
Journal of Computational Physics, 231(15), 5109–5143, 2012.

First GPU implementation: TheLMA*

Two-step updating rule:

$$f_\alpha(\boldsymbol{x},\ t+1) = f_\alpha^*(\boldsymbol{x} - \boldsymbol{\xi}_\alpha,\ t) + 2\left(\frac{\omega - 1}{\omega}\right) f_\alpha^{(\mathrm{e,o})}(\boldsymbol{x},\ t)$$

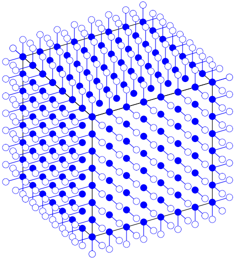
$$f_\alpha^*(\boldsymbol{x},\ t+1) = f_\alpha^{(\mathrm{e})}(\boldsymbol{x},\ t+1) - 2\left(\frac{\omega - 1}{\omega}\right) f_\alpha^{(\mathrm{e,o})}(\boldsymbol{x},\ t+1)$$

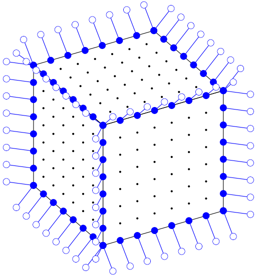
- LW-ACM very similar to LBM, with additional cost of loading and storing ρ and $\boldsymbol{u}$ at each time step.
- First GPU implementation of LW-ACM: slightly modified version of a TheLMA based single-GPU CUDA LBM solver.

C. Obrecht, F. Kuznik, B. Tourancheau, and J.-J. Roux.
The TheLMA project: Multi-GPU implementation of the lattice Boltzmann method.
International Journal of High Performance Computing Applications, 25(3):295–303, 2011.

Second GPU implementation: Louise

- Sufficient to have access to ρ and $\boldsymbol{u}$ at node $\boldsymbol{x}$ and its neighbours $\boldsymbol{x} - \boldsymbol{\xi}_\alpha$.
- Reduction of read redundancy: use CUDA blocks of $8 \times 8 \times 8$ threads, store ρ and $\boldsymbol{u}$ in an array of 10^3 `float4` structures in shared memory.





C. Obrecht, P. Asinari, F. Kuznik, and J.-J. Roux.
High-performance Implementations and Large-scale Validation of the Link-wise ACM.
Journal of Computational Physics, 275:143–153, 2014.

Data throughput and memory footprint

Louise data throughput per time step

- 992 `float4` structures read per CUDA block (41% of LBM).
- 512 written per block (21% of LBM).

Test hardware: GTX Titan Black (single precision)

- LBM: 38 million nodes (e.g. 320^3 cubic cavity).
- LW-ACM: 201 million nodes (e.g. 576^3 cubic cavity).

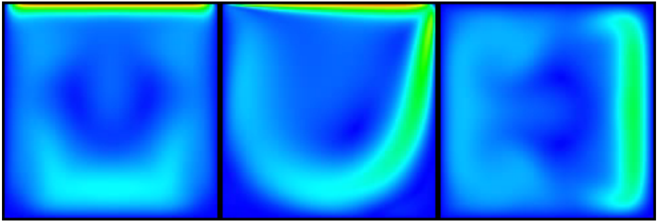
Local bounce-back boundary condition

- Bounce-back boundary condition: $f^*_\alpha(\boldsymbol{x} - \boldsymbol{\xi}_\alpha, t) = f_{\bar\alpha}(\boldsymbol{x}, t-1)$ where $\boldsymbol{x} - \boldsymbol{\xi}_\alpha$ is a wall node and $\bar\alpha$ is such that $\boldsymbol{\xi}_{\bar\alpha} = -\boldsymbol{\xi}_\alpha$.
- Louise does not keep f^*_α variables: finite difference boundary conditions (cumbersome for complex geometries).
- Louise* variant: *local* bounce-back $f^{(e)}_{\bar\alpha}(\boldsymbol{x},\ t) = f^{(e)}_\alpha(\rho, -\boldsymbol{u})$.

Updating rule at boundary node:

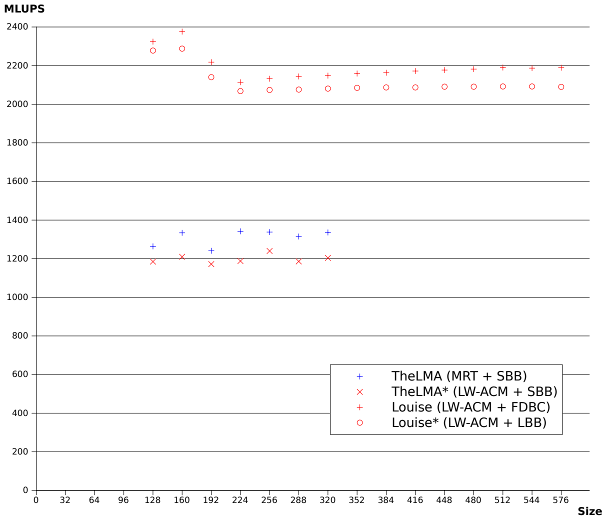
$$f_\alpha(\boldsymbol{x},\ t+1) = f^{(e)}_{\bar\alpha}(\boldsymbol{x},\ t) + 2\left(\frac{\omega-1}{\omega}\right)\left(f^{(e,o)}_\alpha(\boldsymbol{x},\ t) - f^{(e,o)}_{\bar\alpha}(\boldsymbol{x},\ t)\right).$$

Runtime video (Louise)



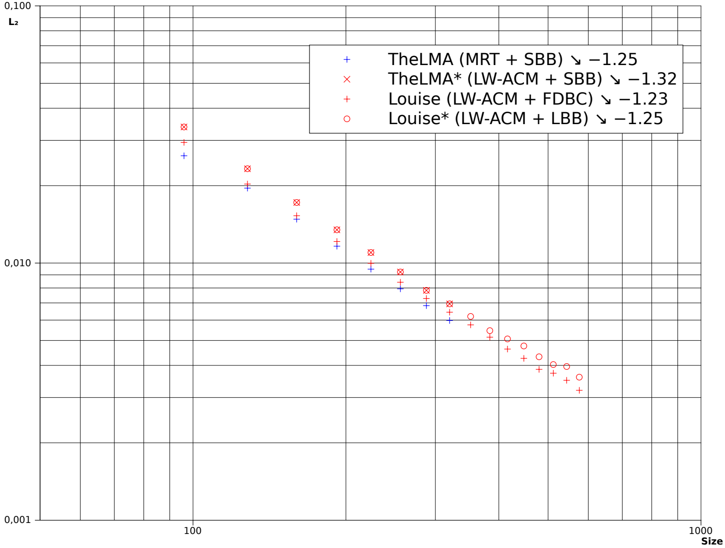
Lid-driven cubic cavity at $\mathrm{Re} = 1000$, $160^3 \approx 4.1$ million nodes, 20320 time steps, computation time 37.1 s on the GTX Titan, 2259 MLUPS.

Performance comparison: lid-driven cavity in single precision



GPU start temperature: 60 °C, runtime per resolution ≈ 30 s. For long term computations, performance is about 15% less.

Velocity discrepancy with respect to spectral element data



III – Work in progress

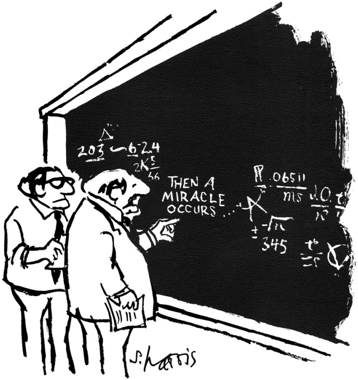
OpenCL Link-wise ACM on Many-core Processors (OpenCLAMP)

- OpenCLAMP: newly developed OpenCL program based on the same principles as Louise*.
- Performance portability: execution parameters specified in a JSON configuration file loaded at runtime.
- Performance on GTX Titan Black: similar than for Louise* code, i.e. higher than 2000 MLUPS, using $8 \times 8 \times 8$ work-groups.
- Performance on octocore Xeon (E5-2687W v2 at 3.40GHz): up to 40 MLUPS using $32 \times 1 \times 1$ work-groups.

Conclusions

- LW-ACM promising approach for CFD on GPUs.
- Device memory consumption divided by up to 5.25 with respect to LBM.
- Performance on Kepler GPUs increased by $1.8\times$.
- OpenCLAMP: to be released soon as a free software.
- Future work: extension to thermal flows, MPI-based multi-device.

Thank you for listening!



"I THINK YOU SHOULD BE MORE EXPLICIT HERE IN STEP TWO."