Soft matter lattice Boltzmann simulations on Graphics Processing Units

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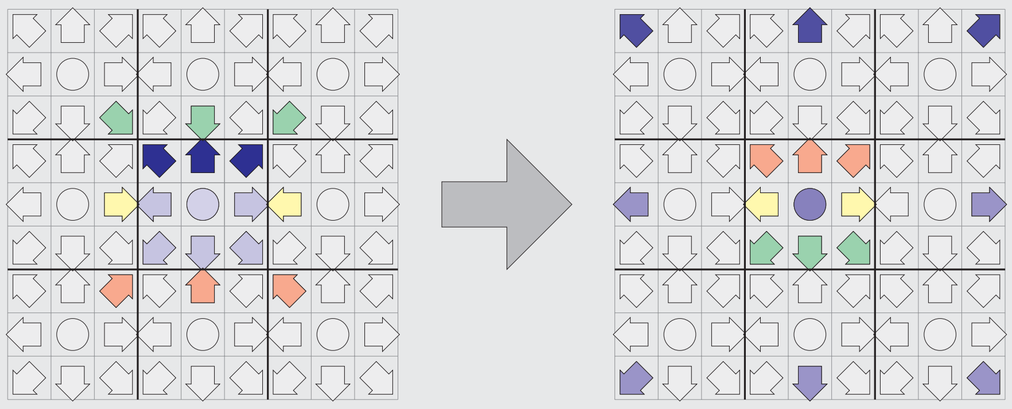
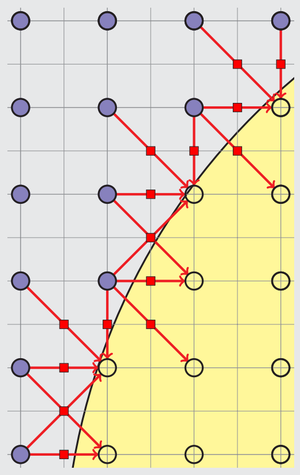
The Lattice Boltzmann Method



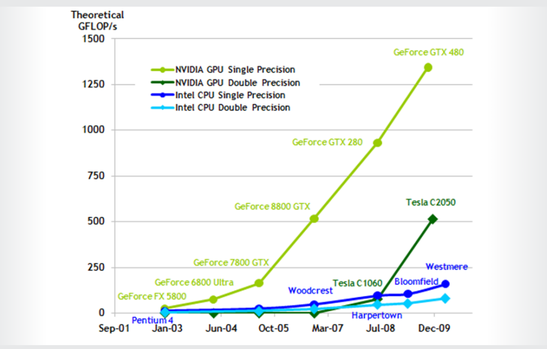
- Fluid described at the mesoscopic level by a set of velocity distributions f_α
- Density $\rho_i = \sum_\alpha f_\alpha(\vec{x}_i, t)$ and momentum $\rho_i \vec{v}_i = \sum_\alpha \vec{c}_\alpha f_\alpha(\vec{x}_i, t)$
- Basic algorithm (BGK approximation):

$$f_\alpha(\vec{x}_i + \vec{c}_\alpha, t+1) = f_\alpha(\vec{x}_i, t) - \frac{f_\alpha(\vec{x}_i, t) - f_\alpha^{(\mathrm{eq})}(\rho_i, \vec{v}_i)}{\tau}$$

- Particle-fluid coupling:
  - Moving mid-link bounce-back rules
  - Solid particles (no internal fluid)



The GPU Revolution



Courtesy of NVIDIA Inc.

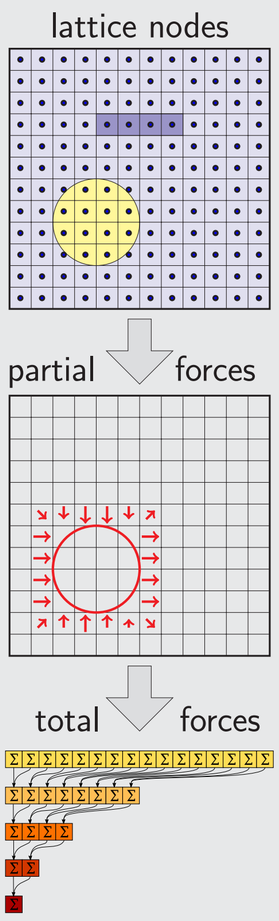
A single modern (NVIDIA) Graphics Processing Unit (GPU):

- Hundreds of computational cores programmable using CUDA C/OpenCL
- Computational power > 1 **TFLOPS**
- Several gigabytes of main memory (global memory)
- Tens of kilobytes of fast on-chip memory (shared memory)
- Programming model based on **kernels**, executed in **threads** grouped into **blocks**
- Inter-thread communication possible **within a single block** only

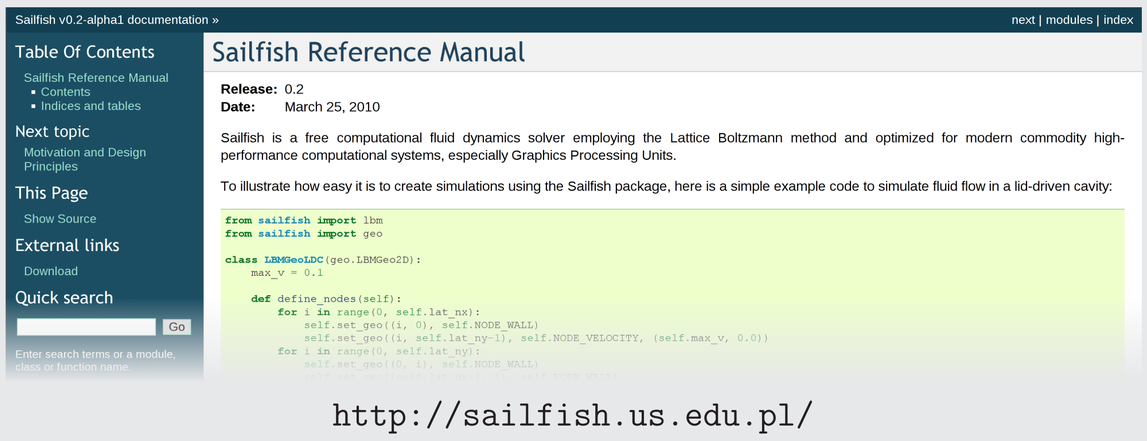
LB-Particle Models on GPUs

The A-B access pattern (two copies of the simulation domain) is used.

1. Collide and stream (1D blocks of several hundred nodes, 1 thread – 1 node).
   - 1.1 Apply boundary conditions if necessary.
   - 1.2 Apply the collision rule (BGK/MRT).
   - 1.3 For particle boundary nodes, save force and torque due to momentum transfer to a vector field in global memory.
   - 1.4 Use shared memory for the propagation step in the X dimension, propagate the remaining dimensions directly in global memory.
2. For every particle (in parallel, different kernels for different particles, 1 thread – 1 node):
   - 2.1 Parallel reductions to calculate the partial force and torque on a particle, coming from a smaller area of the simulation domain.
   - 2.2 Parallel reduction to sum these partial results and obtain the total force and torque.
3. Move the particles (1 thread – 1 particle).
4. For every particle (as in step 2):
   - 4.1 Update the geometry if necessary due to particle movement.
   - 4.2 Parallel reductions to obtain theh total force like in step 2.



The Sailfish Framework



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Sailfish Reference Manual

Release: 0.2
Date: March 25, 2010

Sailfish is a free computational fluid dynamics solver employing the Lattice Boltzmann method and optimized for modern commodity high-performance computational systems, especially Graphics Processing Units.

To illustrate how easy it is to create simulations using the Sailfish package, here is a simple example code to simulate fluid flow in a lid-driven cavity:

```
from sailfish import lbm
from sailfish import geo

class LBMGeoLDC(geo.LBMGeo2D):
    max_v = 0.1

    def define_nodes(self):
        for i in range(0, self.lat_nx):
            self.set_geo((i, 0), self.NODE_WALL)
            self.set_geo((i, self.lat_ny-1), self.NODE_VELOCITY, (self.max_v, 0.0))
        for i in range(0, self.lat_ny):
            self.set_geo((0, i), self.NODE_WALL)
```

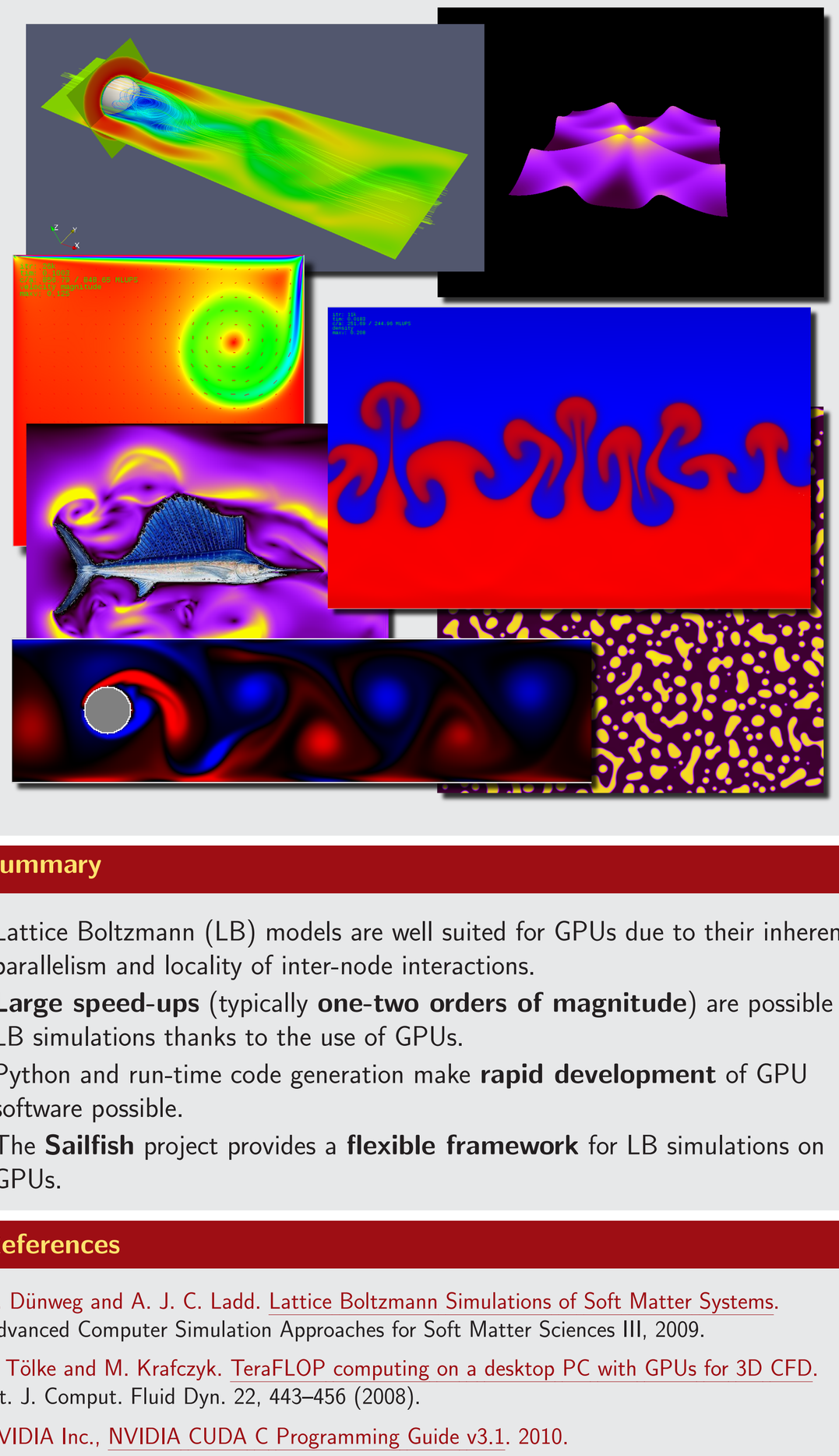
http://sailfish.us.edu.pl/

Sailfish is an open source lattice Boltzmann simulation framework written in Python. It employs **run-time code generation** and **symbolic calculation** techniques to automatically generate code for the GPU. The code is generated from Mako templates, and dynamically compiled using PyCUDA/PyOpenCL.

Key features:

- Generated code is automatically optimized
- CUDA and OpenCL backends
- BGK and MRT models in 2D and 3D
- Single and double precision calculations
- Single and binary fluid models
- Built-in on-line visualization modules
- Fluid-structure interactions using the moving boundary method

Sample Simulations



Summary

- Lattice Boltzmann (LB) models are well suited for GPUs due to their inherent parallelism and locality of inter-node interactions.
- **Large speed-ups** (typically **one-two orders of magnitude**) are possible in LB simulations thanks to the use of GPUs.
- Python and run-time code generation make **rapid development** of GPU software possible.
- The **Sailfish** project provides a **flexible framework** for LB simulations on GPUs.

References

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- J. Tölke and M. Krafczyk. TeraFLOP computing on a desktop PC with GPUs for 3D CFD. Int. J. Comput. Fluid Dyn. 22, 443–456 (2008).
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