Sailfish: Lattice Boltzmann Fluid Simulations with GPUs and Python

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Google

GTC 2012
My adventure with Computational Fluid Dynamics on GPUs

Let’s go back to 2009...

- Was working with stochastic differential equations on GPUs (google sdepy if you’re interested).

Some previous experience with Smoothed Particle Hydrodynamics on CPUs.

- No prior knowledge of the lattice Boltzmann method.

- Started with a simple implementation in C and quickly rewrote it in Python & CUDA.

credit: "Piled Higher and Deeper" by Jorge Cham, www.phdcomics.com
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![Procrastination diagram](https://www.phdcomics.com/comics/2014/08/29/procrastination.png)

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Why did I do that, how it worked out and can you do something similar?

... with some technical details ...
Fluid simulation

1. Macroscopic scale: continuum, velocity ($\vec{v}$), pressure ($p$), Navier-Stokes equation:

$$\rho \left( \frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \nabla \vec{v} \right) = -\nabla p + \mu \nabla^2 \vec{v} + \vec{f}$$

2. Mesoscopic scale: particle ensemble, the lattice Boltzmann method.

$$\frac{\partial f}{\partial t} + \frac{\partial f}{\partial \vec{x}} \cdot \vec{p} + \frac{\partial f}{\partial \vec{p}} \cdot \vec{F} = \frac{\partial f}{\partial t} \bigg|_{\text{coll}}$$

3. Microscopic scale: individual molecules and atoms, molecular dynamics.
Fluid simulation

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2 Mesoscopic scale: particle ensemble, the lattice Boltzmann method.

$$\frac{\partial f}{\partial t} + \frac{\partial f}{\partial \vec{x}} \cdot \frac{\vec{p}}{m} + \frac{\partial f}{\partial \vec{p}} \cdot \vec{F} = \frac{\partial f}{\partial t} \bigg|_{\text{coll}}$$

3 Microscopic scale: individual molecules and atoms, molecular dynamics.
Lattice Boltzmann: the basics

- Discrete, regular, Cartesian grid (\( i \) is a node index).
- Mass fractions: \( f_\alpha \):
  \[ f_C, f_E, f_W, f_S, f_N, f_{NE}, f_{NW}, f_{SE}, f_{SW} \]
- Macroscopic quantities:
  \[
  \rho_i = \sum_\alpha f_\alpha(\bar{x}_i, t) \\
  \rho_i \bar{v}_i = \sum_\alpha \bar{c}_\alpha f_\alpha(\bar{x}_i, t)
  \]
Lattice Boltzmann: the algorithm

Collision:

\[ f^*_\alpha(x_i, t) = f_\alpha(x_i, t) - \frac{f_\alpha(x_i, t) - f^{(eq)}_\alpha(\rho_i, \bar{v}_i)}{\tau} \]

Streaming:

\[ f_\alpha(x_i + c_\alpha, t + 1) = f^*_\alpha(x_i, t) \]
Lattice Boltzmann: the algorithm

1 Collision:

\[ f^*_\alpha(\vec{x}_i, t) = f_\alpha(\vec{x}_i, t) - \frac{f_\alpha(\vec{x}_i, t) - f^{(eq)}_\alpha(\rho_i, \vec{v}_i)}{\tau} \]

2 Streaming:

\[ f_\alpha(\vec{x}_i + \vec{c}_\alpha, t + 1) = f^*_\alpha(\vec{x}_i, t) \]
Lattice Boltzmann: the algorithm

1. **Collision:**

\[
f_\alpha^*(\vec{x}_i, t) = f_\alpha(\vec{x}_i, t) - \frac{f_\alpha(\vec{x}_i, t) - f_\alpha^{(eq)}(\rho_i, \vec{v}_i)}{\tau}
\]

2. **Streaming:**

\[
f_\alpha(\vec{x}_i + \vec{c}_\alpha, t + 1) = f_\alpha^*(\vec{x}_i, t)
\]
Why lattice Boltzmann?

- Applicable for low Mach number flows.
- Good for flows in complex domains (e.g. porous materials).
- Extremely well parallelizable (nearest-neighbour interactions).
- Easy to implement.

Image credit: EXA Corp.
Figure: Papers with "lattice Boltzmann" in the title (source: Scopus)
What is Sailfish?

- GPU-based implementation of the lattice Boltzmann method.
- Open source (LGPL v3).
- Implemented using Python and CUDA C / OpenCL.
- Written from scratch.
- Under development for approximately 3 years.

http://sailfish.us.edu.pl
Why Python?

✔ Easy to understand.
✔ Very expressive (get stuff done quickly).
✔ Great support for GPU programming (via PyCUDA/PyOpenCL).
✔ Bindings with many system libraries.
✘ ... but also **too slow** for large-scale numerical work.
Python and GPUs

- "The boring stuff" (initialization, I/O, etc) becomes essentially free.
- Use metaprogramming ("programs which write other programs") to:
  - generate optimized code on a case-by-case basis,
  - explore parameter spaces to find optimal solutions,
  - provide isolation from hardware details.
- Possible realizations:
  - Abstract Syntax Trees.
  - Domain-specific languages.
  - Template-based code generation.
Metaprogramming one step further: computer algebra systems

- Numerical code initially described as formulas on paper.
- Computer code often repetitive.
- **Write formulas directly in your program and generate code automatically.**

New possibilities:
- Consistency checks at the level of mathematics.
- Code is documentation.
- Transform formulas prior to generating compilable code.
LBM as a framework

- Many lattice Boltzmann models which differ in:
  - lattice connectivity / dimension
  - collision operator
  - equilibrium function
  - turbulence models
  - ...

- Many formulas are independent of (some of) these details.
- RTCG makes it possible to easily experiment with all of these.
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BGK: \[
\left| f_i \right> - \left| f_i^{eq} \right> \over \tau
\]

- equilibrium function
- turbulence models
- ...

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MRT: \( M^{-1} S (M f_i - m_{eq}^i) \)

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- **RTCG makes it possible to easily experiment with all of these.**
Mako code:

```mako
${device_func}  inline void bounce_back(Dist *fi) 
{
    float t;

    %for i in sym.bb_swap_pairs(grid):
        t = fi->${grid.idx_name[i]};
        fi->${grid.idx_name[i]} = fi->${grid.idx_name[grid.idx_opposite[i]]};
        fi->${grid.idx_name[grid.idx_opposite[i]]} = t;
    %endfor
}
```
CUDA C code, D2Q9 grid:

```c
__device__ inline void bounce_back(Dist * fi)
{
    float t;
    t = fi->fE;
    fi->fE = fi->fW;
    fi->fW = t;
    t = fi->fN;
    fi->fN = fi->fS;
    fi->fS = t;
    t = fi->fNE;
    fi->fNE = fi->fSW;
    fi->fSW = t;
    t = fi->fNW;
    fi->fNW = fi->fSE;
    fi->fSE = t;
}
```
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    fi->fW = t;
    t = fi->fN;
    fi->fN = fi->fS;
    fi->fS = t;
    t = fi->fNE;
    fi->fNE = fi->fSW;
    fi->fSW = t;
    t = fi->fNW;
    fi->fNW = fi->fSE;
    fi->fSE = t;
}
```
CUDA C code, D3Q13 grid:

```c
__device__ inline void bounce_back(Dist * fi) {
    float t;
    t = fi->fNE;
    fi->fNE = fi->fSW;
    fi->fSW = t;
    t = fi->fSE;
    fi->fSE = fi->fNW;
    fi->fNW = t;
    t = fi->fTE;
    fi->fTE = fi->fBW;
    fi->fBW = t;
    t = fi->fBE;
    fi->fBE = fi->fTW;
    fi->fTW = t;
    ...}
```

```c
... t = fi->fTN;
    fi->fTN = fi->fBS;
    fi->fBS = t;
    t = fi->fBN;
    fi->fBN = fi->fTS;
    fi->fTS = t;
```
Collision step of the LB algorithm:

\[ f^*_\alpha(x_i, t) = f_\alpha(x_i, t) - \frac{f_\alpha(x_i, t) - f^{(eq)}_\alpha(\rho_i, \vec{v}_i)}{\tau} \]

with

\[ f^{(eq)}_\alpha(\rho_i, \vec{v}_i) = w_\alpha \rho \left( 1 + 3 \vec{c}_\alpha \cdot \vec{v}_i + \frac{9}{2} (\vec{c}_\alpha \cdot \vec{v}_i)^2 - \frac{3}{2} \vec{v}_i^2 \right) \]
Sailfish: symbolic run-time code generation example

\[
f^{(eq)}(\rho_i, \vec{v}_i) = w_\alpha \rho \left( 1 + 3 \vec{c}_\alpha \cdot \vec{v}_i + \frac{9}{2} (\vec{c}_\alpha \cdot \vec{v}_i)^2 - \frac{3}{2} \vec{v}_i^2 \right)
\]

```python
def bgk_equilibrium(grid, rho=None):
    out = []
    if rho is None:
        rho = S.rho
    for i, ei in enumerate(grid.basis):
        t = (grid.weights[i] * rho * (1 + 3*ei.dot(grid.v) +
                       Rational(9, 2) * (ei.dot(grid.v))**2 -
                       Rational(3, 2) * grid.v.dot(grid.v)))
        out.append(t)
    return out
```
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M. Januszewski (IoP, US)
\[ f^{(eq)}_{\alpha}(\rho_i, \vec{v}_i) = w_{\alpha}\rho \left( 1 + 3 \vec{c}_{\alpha} \cdot \vec{v}_i + \frac{9}{2} (\vec{c}_{\alpha} \cdot \vec{v}_i)^2 - \frac{3}{2} \vec{v}_i^2 \right) \]

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```

M. Januszewski (IoP, US)  Sailfish: LBM with GPUs and Python  GTC 2012  15 / 26
\[
\begin{align*}
 f^{(eq)}_{\alpha}(\rho, \vec{v}_i) &= w_{\alpha}\rho \left( 1 + 3 \vec{c}_\alpha \cdot \vec{v}_i + \frac{9}{2}(\vec{c}_\alpha \cdot \vec{v}_i)^2 - \frac{3}{2}v_i^2 \right) \\
\text{feq0.fC} &= 4 \times \rho / 9 + 4 \times \rho \times (-3 \times v0[0] \times v0[0] / 2 - 3 \times v0[1] \times v0[1] / 2) / 9; \\
\text{feq0.fE} &= \rho / 9 + \rho \times (3 \times v0[0] \times (1 + v0[0]) - 3 \times v0[1] \times v0[1] / 2) / 9; \\
\text{feq0.fN} &= \rho / 9 + \rho \times (3 \times v0[1] \times (1 + v0[1]) - 3 \times v0[0] \times v0[0] / 2) / 9; \\
\text{feq0.fW} &= \rho / 9 + \rho \times (-3 \times v0[0] \times (1 - v0[0]) - 3 \times v0[1] \times v0[1] / 2) / 9; \\
\text{feq0.fS} &= \rho / 9 + \rho \times (-3 \times v0[1] \times (1 - v0[1]) - 3 \times v0[0] \times v0[0] / 2) / 9; \\
\text{feq0.fNE} &= \rho / 36 + \rho \times (3 \times v0[0] \times (1 + v0[0]) + 3 \times v0[1] \times (1 + v0[1] + 3 \times v0[0])) / 36; \\
\text{feq0.fNW} &= \rho / 36 + \rho \times (-3 \times v0[0] \times (1 - v0[0]) + 3 \times v0[1] \times (1 + v0[1] - 3 \times v0[0])) / 36; \\
\text{feq0.fSW} &= \rho / 36 + \rho \times (-3 \times v0[0] \times (1 - v0[0]) - 3 \times v0[1] \times (1 - v0[1] - 3 \times v0[0])) / 36; \\
\text{feq0.fSE} &= \rho / 36 + \rho \times (-3 \times v0[1] \times (1 - v0[1] + 3 \times v0[0]) + 3 \times v0[0] \times (1 + v0[0])) / 36;
\end{align*}
\]
\[ f^{(\text{eq})}(\rho_i, \vec{v}_i) = w_\alpha \rho \left( 1 + 3 \vec{c}_\alpha \cdot \vec{v}_i + \frac{9}{2} (\vec{c}_\alpha \cdot \vec{v}_i)^2 - \frac{3}{2} \vec{v}_i^2 \right) \]
Sailfish uses template-based Run-Time Code Generation (RTCG).

- **Code is readable (education!)**
- Code is optimized for specific simulation cases.
- Many formulas stored in symbolic form (SymPy expressions) instead of executable code.
  - Prevents developers from making silly mistakes.
  - Easier to read.
  - Automated consistency checks.
- Possibility to auto-tune.
- Think: flexibility of Mathematica with the performance of C.
Primary ideas of the project:

- Use Run-Time Code Generation to automatically generate optimized code.
- Allow for fast calculations using Python (no performance compromises!)
- Encourage experimentation.
- Eliminate sources of error.
- Minimize the use of programmer time.
Sailfish currently supports:

- **Distributed multi-GPU** simulations.
- Single and double precision calculations.
- **Multiple LB models** (2D, 3D; BGK, MRT, entropic; single fluid, binary fluids, . . .)
- Multiple output formats (NumPy, MatLab, VTK, . . .)
- CUDA and OpenCL backends.
Sample simulations

Sailfish: LBM with GPUs and Python
class RayleighTaylorDomain(Subdomain2D):
    def boundary_conditions(self, hx, hy):
        self.set_node(np.logical_or(hy == 0, hy == self.gy - 1), self.NODE_WALL)

    def initial_conditions(self, sim, hx, hy):
        sim.rho[:] = np.random.rand(*sim.rho.shape) / 100.0
        sim.phi[:] = np.random.rand(*sim.phi.shape) / 100.0
        sim.rho[(hy <= self.gy / 2)] += 1.0
        sim.phi[(hy <= self.gy / 2)] = 1e-4
        sim.rho[(hy > self.gy / 2)] = 1e-4
        sim.phi[(hy > self.gy / 2)] += 1.0

class RayleighTaylorSCSim(LBBinaryFluidShanChen, LBForcedSim):
    subdomain = RayleighTaylorDomain

    @classmethod
    def update_defaults(cls, defaults):
        defaults.update({'lat_nx': 640,
                         'lat_ny': 400,
                         'grid': 'D2Q9',
                         'G': 1.2,
                         'visc': 1.0 / 6.0,
                         'periodic_x': True})

    @classmethod
    def modify_config(cls, config):
        config.tau_phi = sym.relaxation_time(config.visc)

    def __init__(self, config):
        super(RayleighTaylorSCSim, self).__init__(config)
        self.add_body_force((0.0, -0.15 / config.lat_ny), grid=1)

if __name__ == '__main__':
    ctrl = LBSimulationController(RayleighTaylorSCSim, LBGeometry2D)
    ctrl.run()
How it all works: simulation setup and code generation

1. Start a **controller** process.
2. Decompose domain into subdomains (cuboids).
3. Start a **master** process on each computational node.
4. Start **subdomain handlers** on each computational node (one process per domain).
5. Each handler:
   - sets initial conditions via macroscopic fields (numpy arrays),
   - generates CUDA code based on the features used in its subdomain,
   - executes the main loop.
How it all works: LBM implementation on the GPU

- Store mass fractions in a structure of arrays in global memory. Two lattices (A and B).
- 1 node – 1 GPU thread, arranged in 1D block:
  - Aligned memory access as mass fractions are loaded into registers from lattice A.
  - Relaxation fully local using registers.
  - Write data to lattice B in global memory.
- In the next iteration the role of A and B is reversed.
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In the next iteration the role of A and B is reversed.
Idea: Overlap network I/O and GPU computation.

- Split domain into **boundary** and **bulk**.
- Run simulation in the boundary first.
- Run kernels to collect data into a continuous memory block.
- Run simulation in the bulk area.
  - Copy data to be transferred from the GPU to the host.
  - Send data to remote nodes.
  - Receive data from remote nodes.
  - Copy data from the host to the GPU.
- Run kernels to distribute data from remote nodes to the correct locations in global memory.
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How it all works: node-node communication

Controller

execnet

OMQ

OMQ

OMQ

OMQ

OMQ

OMQ

Master

Subdomain handler

Subdomain handler

Master

Subdomain handler

Subdomain handler
Use the right tool for the job: Python + GPUs.

- RTCG based on symbolic expressions is a powerful tool for building code quickly and reliably.
- Programmer time more important than computer time.
- With GPUs this does not necessarily mean a need to compromise on performance.
Summary

- Use the right tool for the job: Python + GPUs.
- RTCG based on symbolic expressions is a powerful tool for building code quickly and reliably.
- Programmer time more important than computer time.
- With GPUs this does not necessarily mean a need to compromise on performance.
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Programmer time more important than computer time.

With GPUs this does not necessarily mean a need to compromise on performance.
Use the right tool for the job: Python + GPUs.

RTCG based on symbolic expressions is a powerful tool for building code quickly and reliably.

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Thanks for your attention. Questions?