Sailfish: Lattice Boltzmann Fluid Simulations with GPUs and Python

Michał Januszewski

Institute of Physics
University of Silesia in Katowice, Poland

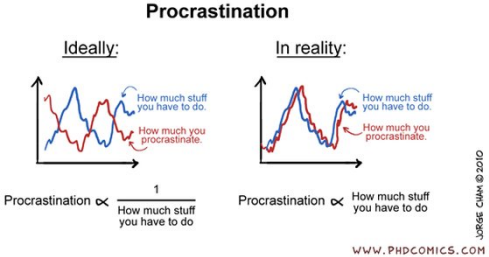
Google

GTC 2012

My adventure with Computational Fluid Dynamics on GPUs

Let's go back to 2009...

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



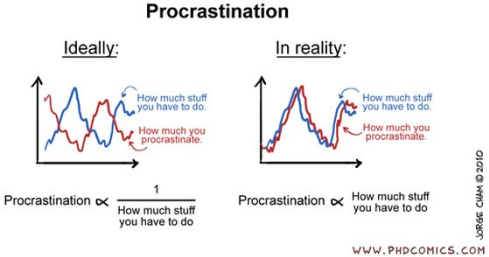
credit: "Piled Higher and Deeper" by Jorge Cham, www.phdcomics.com

- 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**.

My adventure with Computational Fluid Dynamics on GPUs

Let's go back to 2009...

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



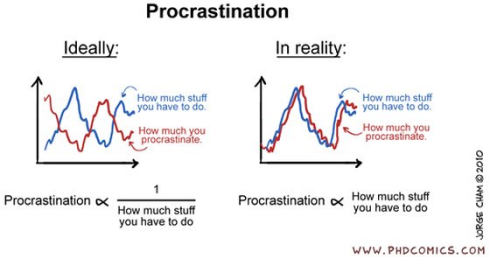
credit: "Piled Higher and Deeper" by Jorge Cham, www.phdcomics.com

- 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**.

My adventure with Computational Fluid Dynamics on GPUs

Let's go back to 2009...

- Was working with stochastic differental equations on GPUs (google `sdepy` if you're interested).



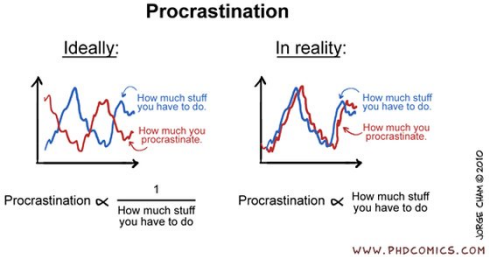
credit: "Piled Higher and Deeper" by Jorge Cham, www.phdcomics.com

- 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**.

My adventure with Computational Fluid Dynamics on GPUs

Let's go back to 2009...

- Was working with stochastic differental equations on GPUs (google `sdepy` if you're interested).



credit: "Piled Higher and Deeper" by Jorge Cham, www.phdcomics.com

- 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**

This talk

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

... with some technical details ...

Fluid simulation

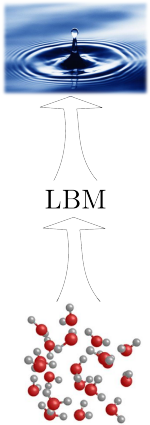
1. Macroscopic scale: continuum, velocity ($\vec{v}$), pressure (p), Navier-Stokes equation:

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

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

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

3. Microscopic scale: invidual molecules and atoms, molecular dynamics.



Fluid simulation

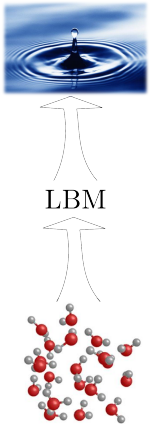
1. Macroscopic scale: continuum, velocity ($\vec{v}$), pressure (p), Navier-Stokes equation:

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

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

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

3. Microscopic scale: invidual molecules and atoms, molecular dynamics.



Fluid simulation

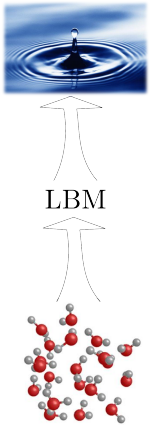
1. Macroscopic scale: continuum, velocity ($\vec{v}$), pressure (p), Navier-Stokes equation:

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

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

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

3. Microscopic scale: invidual molecules and atoms, molecular dynamics.

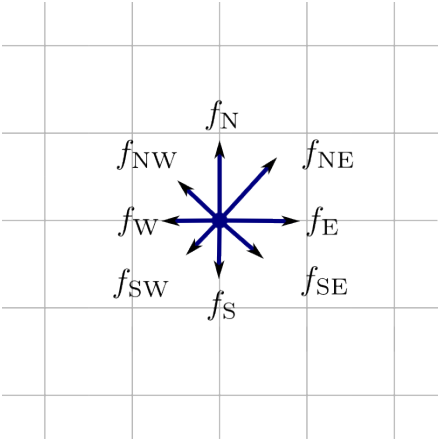


Lattice Boltzmann: the basics

- Discrete, regular, Cartesian grid (i is a node index).
- Mass fractions: f_α:
  $f_C, f_E, f_W, f_S, f_N, f_{NE}, f_{NW}, f_{SE}, f_{SW}$
- Macroscopic quantities:

$$\rho_i = \sum_\alpha f_\alpha(\vec{x}_i, t)$$

$$\rho_i \vec{v}_i = \sum_\alpha \vec{c}_\alpha f_\alpha(\vec{x}_i, t)$$



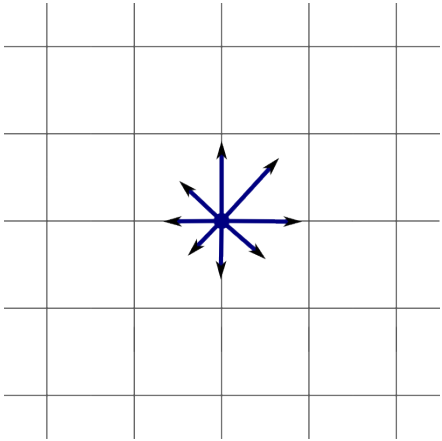
Lattice Boltzmann: the algorithm

1. Collision:

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

2. Streaming:

$$f_\alpha(\vec{x}_i + \vec{c}_\alpha, t+1) = f_\alpha^\star(\vec{x}_i, t)$$



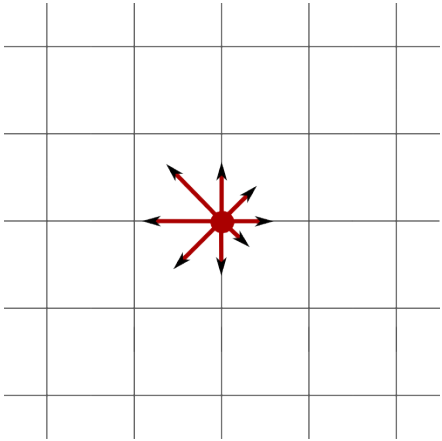
Lattice Boltzmann: the algorithm

1. Collision:

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

2. Streaming:

$$f_\alpha(\vec{x}_i + \vec{c}_\alpha, t+1) = f_\alpha^\star(\vec{x}_i, t)$$



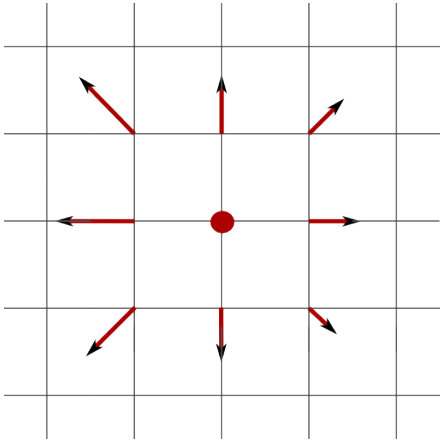
Lattice Boltzmann: the algorithm

1. Collision:

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

2. Streaming:

$$f_\alpha(\vec{x}_i + \vec{c}_\alpha, t+1) = f_\alpha^\star(\vec{x}_i, t)$$



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.**

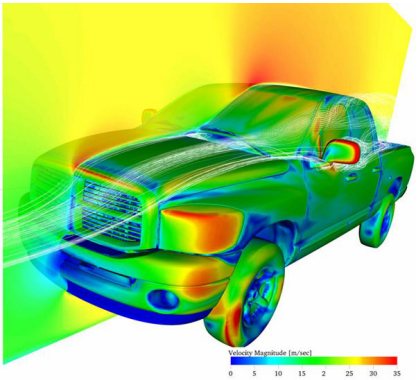


Image credit: EXA Corp.

Lattice Boltzmann: History

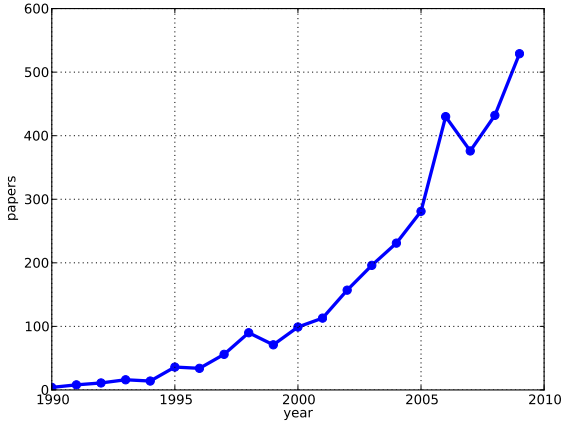


Figure: Papers with "lattice Boltzmann" in the title (source: Scopus)

What is Sailfish?

Image credit: Wikimedia

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

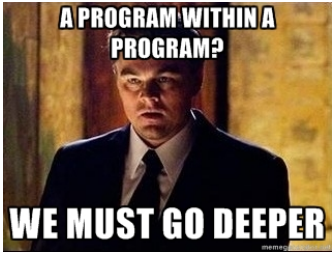
- GPU-based implementation of the lattice Boltzmann method.
- Open source (LGPL v3).
- Implemented using Python and CUDA C / OpenCL.
- Written from scratch.
- Under development for approximately 3 years.

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

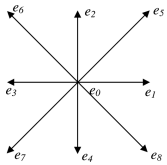
- Numerical code initially described as formulas on paper.
- Computer code often repetitive.
- **Write formulas directly in your program and generate code automatically.**

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

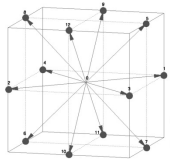


D2Q9

  - 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.**

LBM as a framework

- Many lattice Boltzmann models which differ in:
  - lattice connectivity / dimension

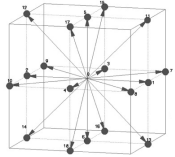


D3Q13

  - 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.**

LBM as a framework

- Many lattice Boltzmann models which differ in:
  - lattice connectivity / dimension



D3Q19

  - 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.**

LBM as a framework

- Many lattice Boltzmann models which differ in:
  - lattice connectivity / dimension
  - collision operator

    BGK: $\frac{|f_i\rangle - |f_i^{eq}\rangle}{\tau}$

  - equilibrium function
  - turbulence models
  - ...
- Many formulas are independent of (some of) these details.
- **RTCG makes it possible to easily experiment with all of these.**

LBM as a framework

- Many lattice Boltzmann models which differ in:
  - lattice connectivity / dimension
  - collision operator

    MRT: $M^{-1} S \left(M \left| f_i \right\rangle - \left| m_i^{eq} \right\rangle \right)$

  - equilibrium function
  - turbulence models
  - ...
- Many formulas are independent of (some of) these details.
- **RTCG makes it possible to easily experiment with all of these.**

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.**

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.**

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.**

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.**

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.**

Sailfish: Mako template example – bounceback rule

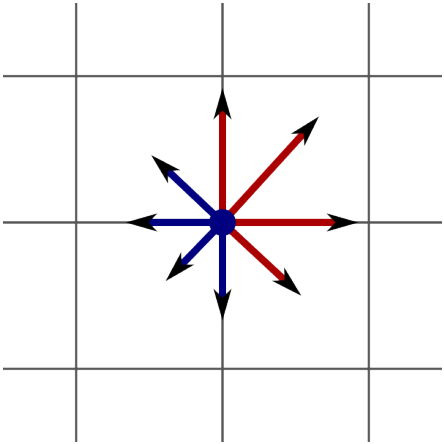
Mako code:

```
${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
}
```

Sailfish: Mako template example – bounceback rule

CUDA C code, D2Q9 grid:

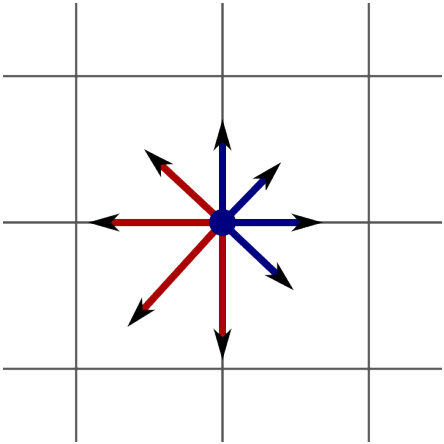
```
__device__ inline void bounce_back(Dist * fi)
{
        float t;
        t = fi->fE;
        fi->fE = fi->fW;
        fi->fW = t;
        t = fi->fN;
        fi->fN = fi->fS;
        fi->fS = t;
        t = fi->fNE;
        fi->fNE = fi->fSW;
        fi->fSW = t;
        t = fi->fNW;
        fi->fNW = fi->fSE;
        fi->fSE = t;
}
```



Sailfish: Mako template example – bounceback rule

CUDA C code, D2Q9 grid:

```
__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;
}
```



Sailfish: Mako template example – bounceback rule

CUDA C code, D3Q13 grid:

```
__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;
...
        t = fi->fTN;
        fi->fTN = fi->fBS;
        fi->fBS = t;
        t = fi->fBN;
        fi->fBN = fi->fTS;
        fi->fTS = t;
}
```

Sailfish: symbolic run-time code generation example

Collision step of the LB algorithm:

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

with

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

Sailfish: symbolic run-time code generation example

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

```
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
```

Sailfish: symbolic run-time code generation example

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

```
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
```

Sailfish: symbolic run-time code generation example

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

```
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
```

Sailfish: symbolic run-time code generation example

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

```
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
```

Sailfish: symbolic run-time code generation example

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

```
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
```

Sailfish: symbolic run-time code generation example

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

```
feq0.fC = 4 * rho / 9 + 4 * rho * (-3 * v0[0] * v0[0] / 2 - 3 * v0[1] * v0[1] / 2) / 9;
feq0.fE = rho / 9 + rho * (3 * v0[0] * (1 + v0[0]) - 3 * v0[1] * v0[1] / 2) / 9;
feq0.fN = rho / 9 + rho * (3 * v0[1] * (1 + v0[1]) - 3 * v0[0] * v0[0] / 2) / 9;
feq0.fW = rho / 9 + rho * (-3 * v0[0] * (1 - v0[0]) - 3 * v0[1] * v0[1] / 2) / 9;
feq0.fS = rho / 9 + rho * (-3 * v0[1] * (1 - v0[1]) - 3 * v0[0] * v0[0] / 2) / 9;
feq0.fNE = rho / 36 + rho * (3 * v0[0] * (1 + v0[0]) + 3 * v0[1] * (1 + v0[1] + 3 * v0[0])) / 36;
feq0.fNW = rho / 36 + rho * (-3 * v0[0] * (1 - v0[0]) + 3 * v0[1] * (1 + v0[1] - 3 * v0[0])) / 36;
feq0.fSW = rho / 36 + rho * (-3 * v0[0] * (1 - v0[0]) - 3 * v0[1] * (1 - v0[1] - 3 * v0[0])) / 36;
feq0.fSE = rho / 36 + rho * (-3 * v0[1] * (1 - v0[1] + 3 * v0[0]) + 3 * v0[0] * (1 + v0[0])) / 36;
```

Sailfish: symbolic run-time code generation example

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

```
feq0.fC = rho / 3 + rho * (-3 * v0[0] * v0[0] / 2 - 3 * v0[1] * v0[1] / 2 - 3 * v0[2] * v0[2] / 2) / 3;
feq0.fE = rho / 18 + rho * (3 * v0[0] * (1 + v0[0]) - 3 * v0[1] * v0[1] / 2 - 3 * v0[2] * v0[2] / 2) / 18;
feq0.fW = rho / 18 + rho * (-3 * v0[0] * (1 - v0[0]) - 3 * v0[1] * v0[1] / 2 - 3 * v0[2] * v0[2] / 2) / 18;
feq0.fN = rho / 18 + rho * (3 * v0[1] * (1 + v0[1]) - 3 * v0[0] * v0[0] / 2 - 3 * v0[2] * v0[2] / 2) / 18;
feq0.fS = rho / 18 + rho * (-3 * v0[1] * (1 - v0[1]) - 3 * v0[0] * v0[0] / 2 - 3 * v0[2] * v0[2] / 2) / 18;
feq0.fT = rho / 18 + rho * (3 * v0[2] * (1 + v0[2]) - 3 * v0[0] * v0[0] / 2 - 3 * v0[1] * v0[1] / 2) / 18;
feq0.fB = rho / 18 + rho * (-3 * v0[2] * (1 - v0[2]) - 3 * v0[0] * v0[0] / 2 - 3 * v0[1] * v0[1] / 2) / 18;
feq0.fNE = rho / 36 + rho * (3 * v0[0] * (1 + v0[0]) + 3 * v0[1] * (1 + v0[1] + 3 * v0[0]) - 3 * v0[2] * v0[2] / 2) / 36;
feq0.fNW = rho / 36 + rho * (-3 * v0[0] * (1 - v0[0]) + 3 * v0[1] * (1 + v0[1] - 3 * v0[0]) - 3 * v0[2] * v0[2] / 2) / 36;
feq0.fSE = rho / 36 + rho * (-3 * v0[1] * (1 - v0[1] + 3 * v0[0]) + 3 * v0[0] * (1 + v0[0]) - 3 * v0[2] * v0[2] / 2) / 36;
feq0.fSW = rho / 36 + rho * (-3 * v0[0] * (1 - v0[0]) - 3 * v0[1] * (1 - v0[1] - 3 * v0[0]) - 3 * v0[2] * v0[2] / 2) / 36;
```

Sailfish: Run-Time Code Generation

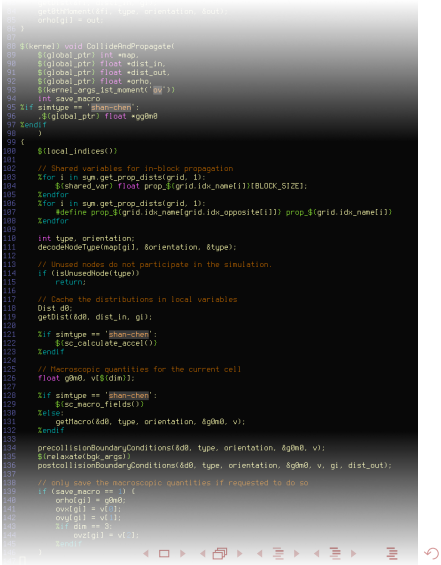
Sailfish uses template-based Run-Time Code Generation (RTCG).

- **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.

Sailfish: Summary of basic ideas

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.

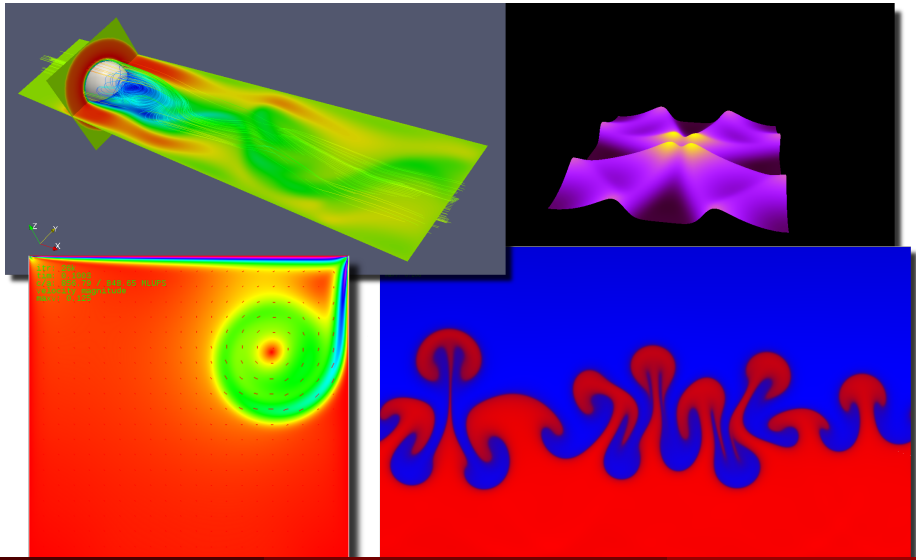


Sailfish: Results

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



How it all works: defining a simulation

```
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
```

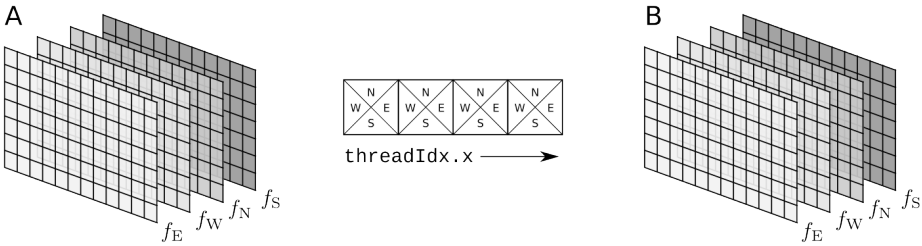
...

```
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

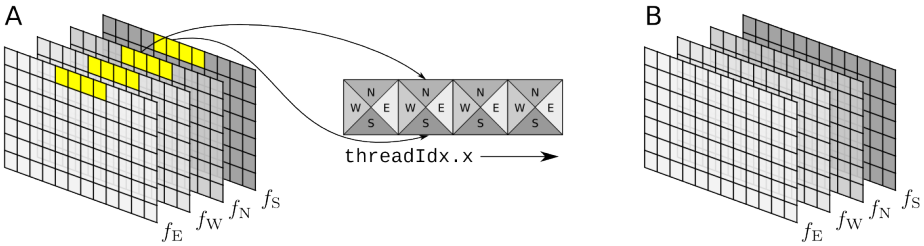
1. Start a **controller** process.
2. Decompose domain into subdomains (cuboids).
3. Start a **master** process on each computational node.
4. Start **subdomain handlers** on each computational node (one process per domain).
5. Each handler:
   - sets initial conditions via macroscopic fields (numpy 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



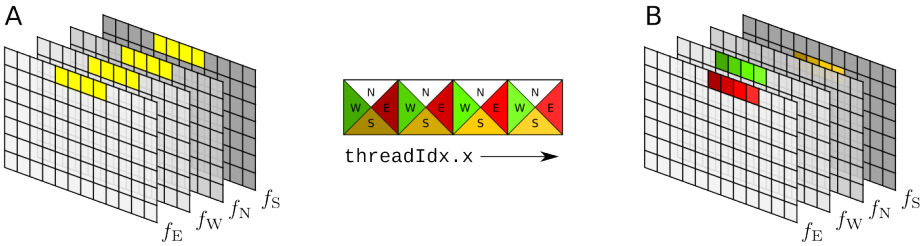
- Store mass fractions in a structure of arrays in global memory. Two lattices (A and B).
- 1 node – 1 GPU thread, arranged in 1D block:
  - Aligned memory access as mass fractions are loaded into registers from lattice A.
  - Relaxation fully local using registers.
  - Write data to lattice B in global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

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.

How it all works: LBM implementation on the GPU

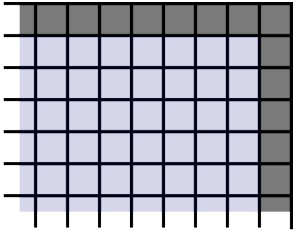


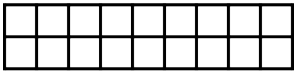
- Store mass fractions in a structure of arrays in global memory. Two lattices (A and B).
- 1 node – 1 GPU thread, arranged in 1D block:
  - Aligned memory access as mass fractions are loaded into registers from lattice A.
  - Relaxation fully local using registers.
  - Write data to lattice B in global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

How it all works: main loop

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.



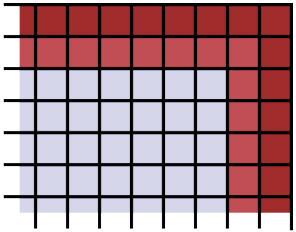


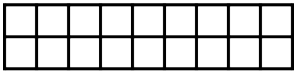
GPU buffer in global mem.

How it all works: main loop

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.



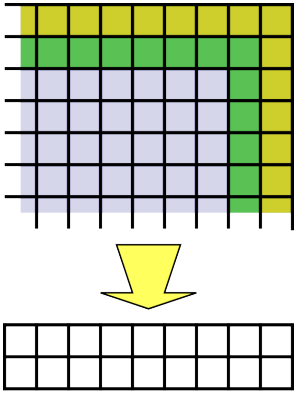


GPU buffer in global mem.

How it all works: main loop

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.

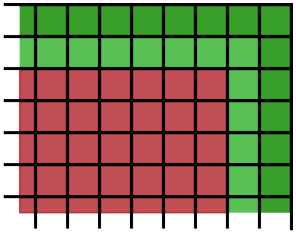


GPU buffer in global mem.

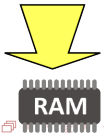
How it all works: main loop

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.



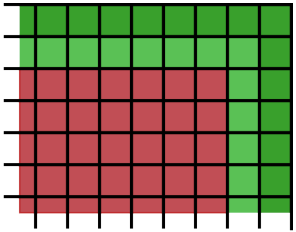
GPU buffer in global mem.



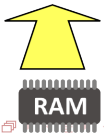
How it all works: main loop

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.



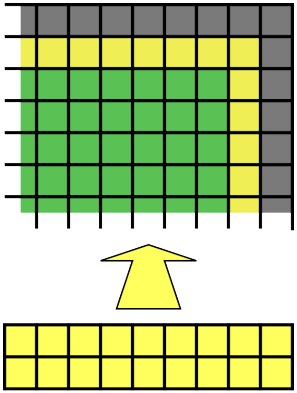
GPU buffer in global mem.



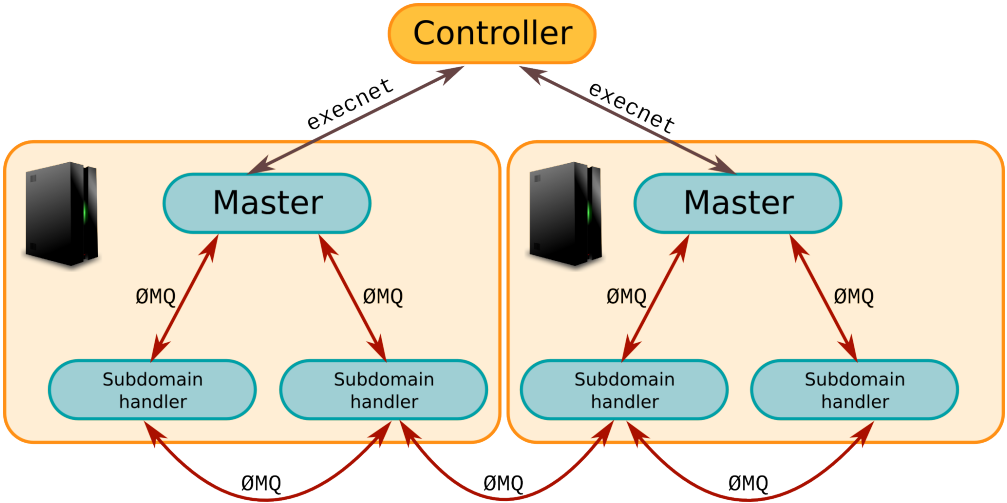
How it all works: main loop

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.



How it all works: node-node communication



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.

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.

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.

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.

Thanks

Thanks for your attention. Questions?