Advanced Modeling & Simulation Seminar Series
NASA Ames Research Center
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C++ Parallel Algorithms for GPU Programming
A Case Study with the Lattice Boltzmann Method

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Outline

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- C++ Parallel algorithms and GPU programming
  - Since C++17, many algorithms can be parallelized.
  - Different backends, different forms of parallelism. We focus on massively multi-threaded platforms.
  - NVIDIA HPC SDK (`nvc++`) offers the `stdpar` backend for GPUs.
- Applying this formalism to scientific problems
  - Many STL algorithms are available but not for all types of problems.
  - Stencil operations ? Non-local memory accesses ?
  - Idea: combine `for_each` style algorithms with memory-access operations (pointer arithmetics).
- Computational fluid dynamics: a lattice Boltzmann implementation
  - The concept is applied to a lattice Boltzmann code.
  - Complex simulation problems solved with state-of-the-art performance.

Part I

C++ PARALLEL ALGORITHMS AND GPUS

C++ Parallel Algorithms

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```
vector<double> v = { 1, 2, 3, 4 }, w(4);
transform( execution::par, begin(v), end(v), begin(w),
           [](double const& element) { return 2. * element; } );
// w is {2, 4, 6, 8}
```

Execution policy

Read from v, write into w

Lambda function: defines the operation to be applied to elements of v.

```
#include <execution>
```

```
nvc++ -stdpar -o program program.cpp
```

List of parallel algorithms

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adjacent_difference
adjacent_find
all_of
any_of
copy
copy_n
count
count_if
equal
exclusive_scan
fill
fill_n
find

find_end
find_first_of
find_if
for_each
for_each_n
inclusive_scan
move
none_of
partition
reduce
remove
remove_if

reverse
reverse_copy
rotate
rotate_copy
search
search_n
sort
stable_sort
swap_ranges
transform
transform_exclusive_scan
transform_inclusive_scan
transform_reduce

Execution Policies

- seq — Traditional non-parallel execution model
- unseq — Execution may be vectorized within a single thread
- par — Allows parallel, multi-threaded execution
- par_unseq — Allows parallel, multi-threaded execution and vectorization within each thread

Available implementations

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Common formalism

C++ Parallel STL

Hardware-specific implementation

Nvidia stdpar

GPU

Intel Threading-Building Blocks

CPU

Heterogeneous (device/host) vs Homogeneous

CUDA Unified Memory

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Execution of Parallel STL model on heterogenous platforms is possible thanks to CUDA unified memory.

```
vector<double> v = { 0., 1., 2., 3., 4., 5. };
for_each(begin(v), end(v), [](double& x) { x = sin(x / N * M_PI); });

for_each( execution::par_unseq, begin(v), end(v),
          [](double& x) { x = sqrt(x);  } );
```

Executed on host

Executed on device

In between, data is automatically transferred from host to device. Be aware of the performance cost!

WARNINGS

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- Transfer from and to device is automatic, the performance cost is easily overlooked.
- `nvc++` compiler needs to see the definition of all functions called on the device.
- With CUDA Unified memory, only heap data is managed automatically, stack data is not.

No pointers to data on the stack !

```
void multiply_with(vector<double>& v, double a) {
    for_each( execution::par_unseq, v.begin(), v.end(),
              [&](double& x) { x = a * x; } );
}
```

Problem: `a` is captured by reference.

```
void multiply_with(vector<double>& v, double a) {
    for_each( execution::par_unseq, v.begin(), v.end(),
              [=](double& x) { x = a * x; } )
}
```

OK: `a` is captured by value.

Thread safety

- Race conditions
  – The C++ Standard allows implementations to assume that user-provided functions are free of data races.
  – In the heat equation (the example in Part 2), absence of data race is enforced by working with two arrays, one that's read-only and one that's write-only .
  – In the flow solver (the example in Part 3), a smart in-place algorithm is used: read and write operations are carried out on identical memory addresses.
- Synchronization
  – Synchronization of threads takes place between subsequent STL algorithm calls.
  – Similar to OpenMP's fork-join model.

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Part II

EXAMPLE: SOLVING A SCIENTIFIC PROBLEM WITH STDPAR

2D Heat Equation

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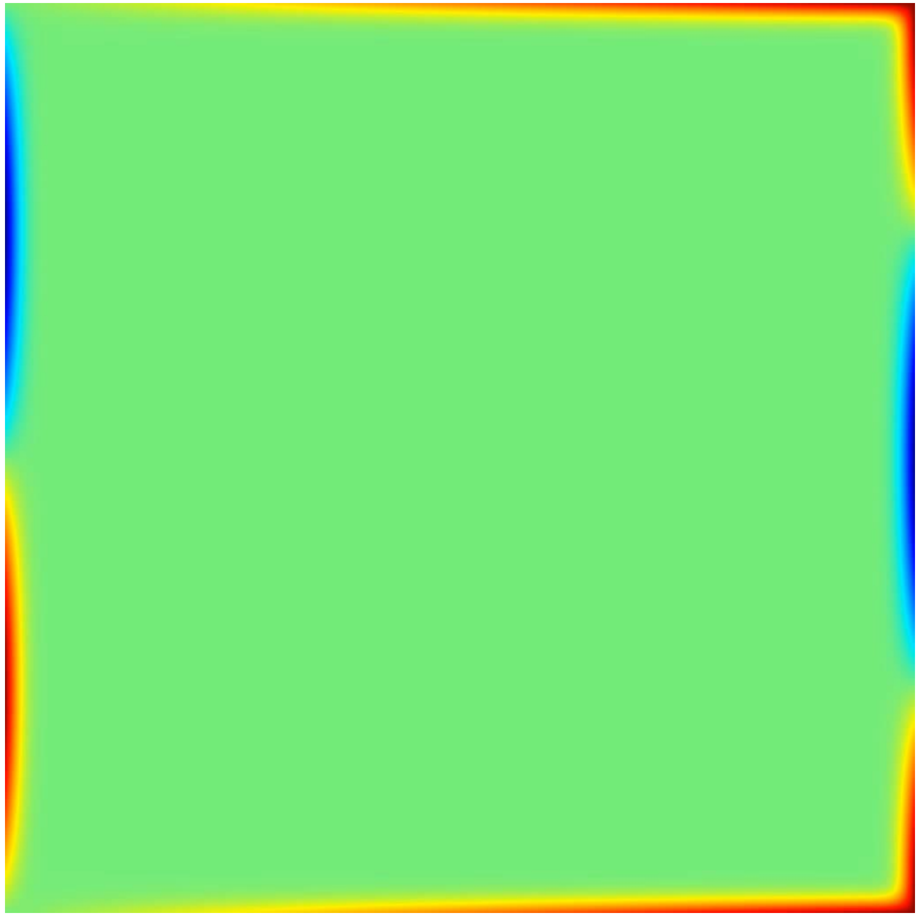
Time-dependent parabolic PDE

We apply a fixed temperature profile on boundaries

Without heat sources: convergence to stationary state



2D Heat Equation

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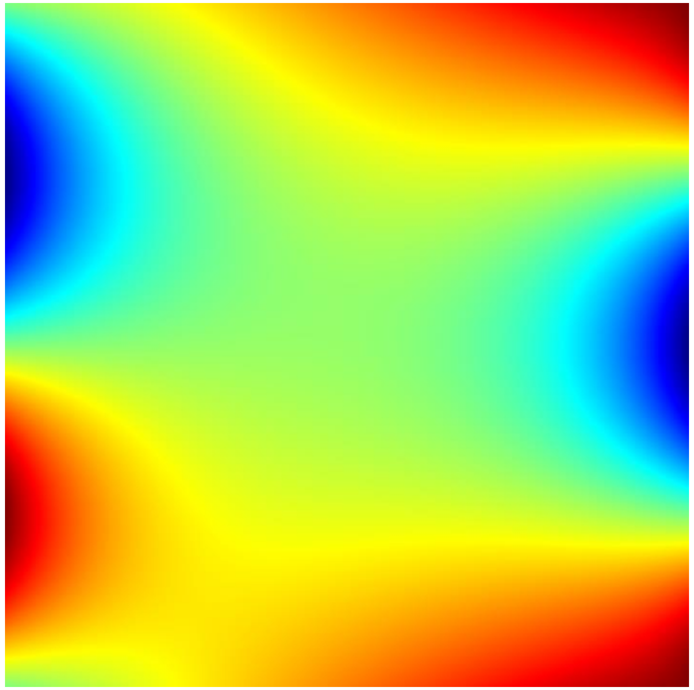
$$\frac{\partial u}{\partial t} = D\left(\frac{\partial^2}{\partial x^2}u(x,y) + \frac{\partial^2}{\partial y^2}u(x,y)\right)$$

$$\frac{u(t+\Delta t) - u(t)}{\Delta t}$$

Time:
Forward Euler

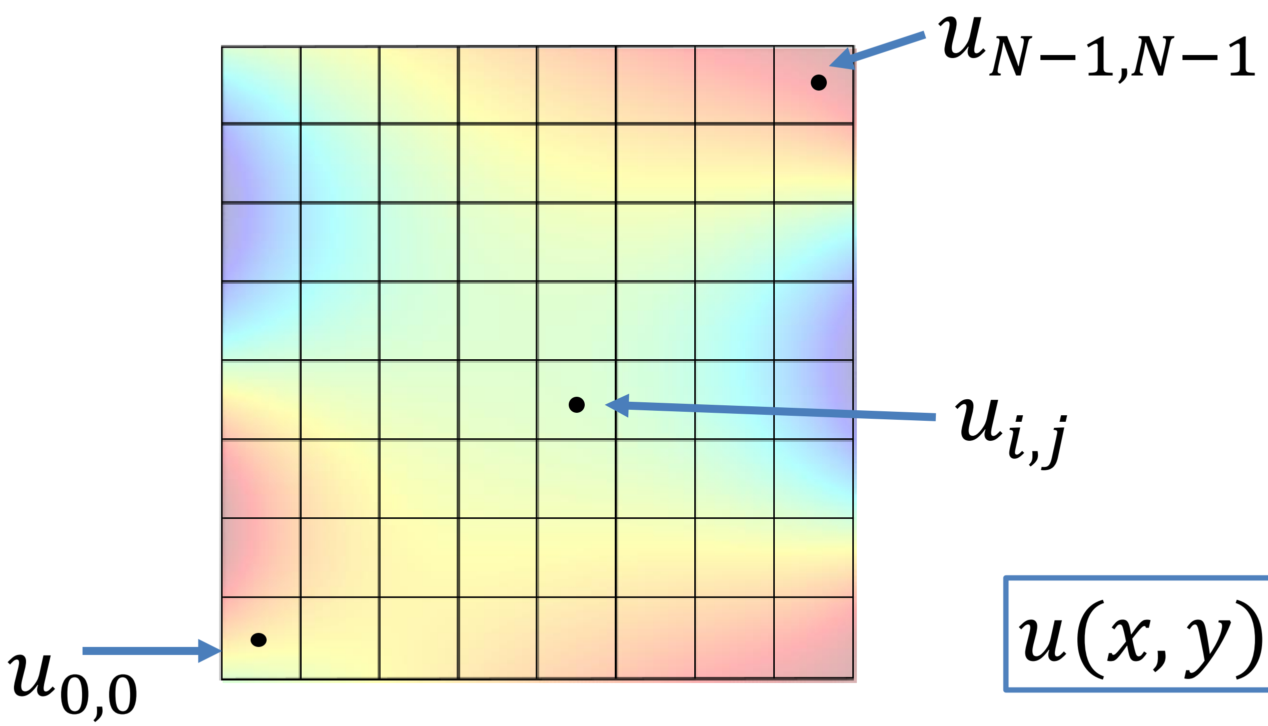
$$\frac{u(x+\Delta x,y) + u(x-\Delta x,y) - 2 * u(x,y)}{\Delta x^2}$$

Central differences (2nd order)



2D Heat Equation

$$u(t+\Delta t) = \left(1 - 4D\frac{\Delta t}{\Delta x^2}\right)u(t) + D\frac{\Delta t}{\Delta x^2}\big(u(x+\Delta x, y) + u(x-\Delta x, y) + u(x, y+\Delta x) + u(x, y-\Delta x)\big)$$



$$\boxed{u(x,y) \equiv u_{i,j}}$$

An implementation with algorithms

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```
double iterate(vector<double>& u, vector<double>& utmp, int N) {
    double l2 = transform_reduce (
        execution::par,
        begin(u), end(u), begin(utmp),
        0., plus<double>(),
        [Dconst](double const& u_from, double& u_to) {
            u_to = u_from * (1. - 4. * Dconst)
                    + Dconst * ( u[i-1] ... );
                return sqr(u_to - u_from);
            }
        } );
    return l2;
}
```

`transform_reduce` allows a reduction.

Reduction is a sum.

Lambda expression receives an element from `u` and one from `utmp` and returns a term for the sum.

Wait… how to access neighbors ?
We have access to the current element only.

Pointer arithmetics provides index

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```
double* u_ptr = &u[0];
…
[u_ptr, Dconst](double const& u_from, double& u_to) {
    size_t i = &u_from – u_ptr;
    u_to = u_from * (1. - 4. * Dconst)
               + Dconst * ( u_ptr[i-1] + u_ptr[i+1] +
                            u_ptr[i-N] + u_ptr[i+N] );
    return sqr(u_to - u_from);
} );
```

Capture a pointer to `u` heap data.

The address of `u_from` reveals the linear index.

The complete lambda expression

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```
[u_ptr, Dconst](double const& u_from, double& u_to) {
    size_t i = &u_from - u_ptr;
    size_t iX = i / N;
    size_t iY = i % N;
    bool on_boundary_x = iX == 0 || iX == N-1;
    bool on_boundary_y = iY == 0 || iY == N-1;
    if (on_boundary_x || on_boundary_y) {
        return 0.;
    }
    else {
        u_to = u_from * (1. - 4. * Dconst)
                   + Dconst * ( u_ptr[i-1] + u_ptr[IND(i+1)] +
                                u_ptr[i-N] + u_ptr[IND(i+N] );
        return sqr(u_to - u_from);
    }
} );
```

Exclude boundaries from computations.

Try it out:
www.gitlab.com/UnigeHPFS/paralg

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Part III

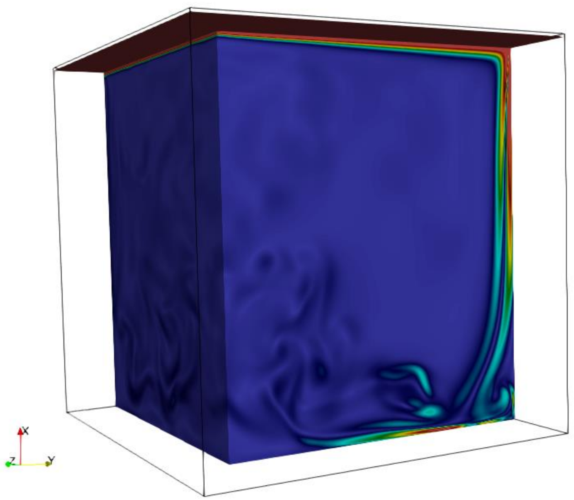
A COMPLETE EXAMPLE: COMPUTATIONAL FLUID DYNAMICS

The STLBM code

https://www.gitlab.com/UnigeHPFS/stlbm

- A collection of parallel-STL based code templates for fluid dynamics.
- Straightforward: a fully self-contained code in 600 lines.
- Approach: Lattice Boltzmann Method (LBM)

Flow in a lid-driven cavity

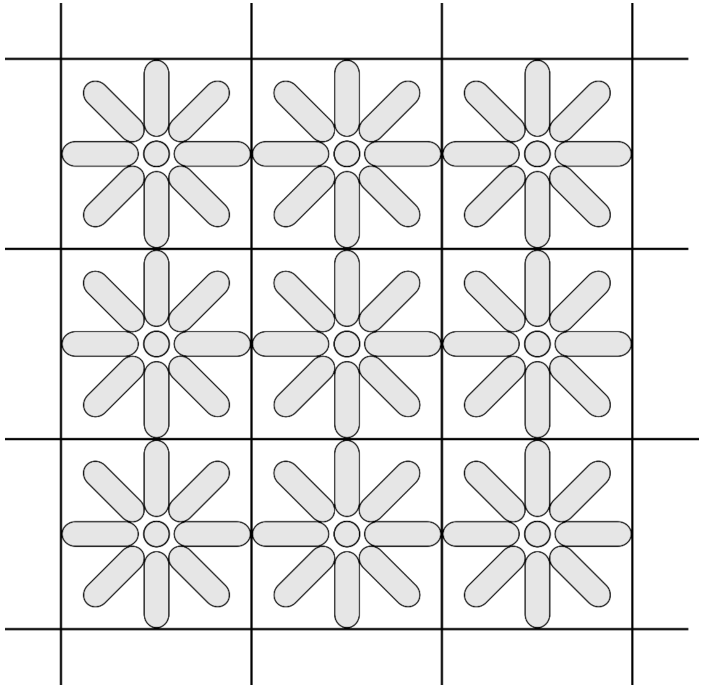


Porous media flow

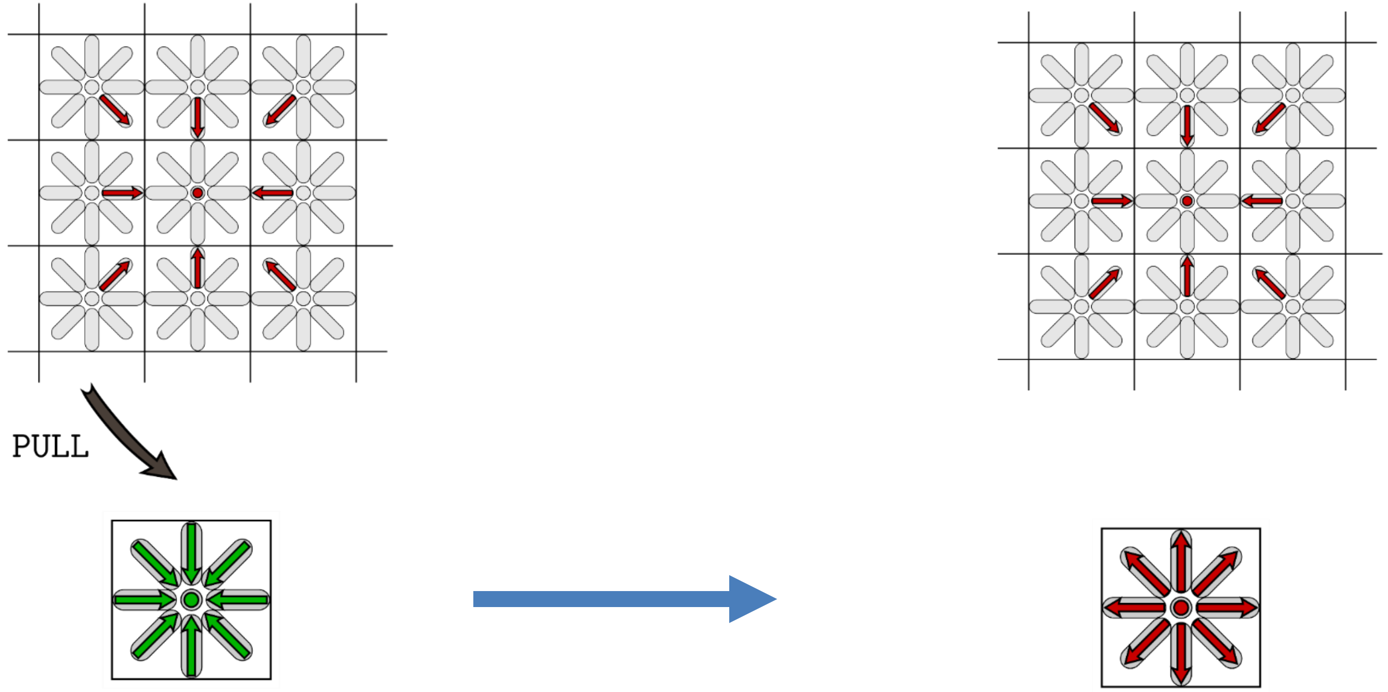
J. Latt, C. Coreixas, J. Beny,
Cross-platform programming model for many-core lattice Boltzmann simulations
arXiv preprint arXiv:2010.11751, 2020

Lattice Boltzmann scheme

- 9 variables per cell (2D), 19 or more variables per cell (3D).
- Similar to heat equation algorithm: nearest-neighbor cell access.
- Computations performed on every cell are more involved.
- Thread safety: we use in-place algorithm and select the memory access pattern carefully.



LBM: treatment of a single cell



Treatment of one cell: PULL - COMPUTE - PUSH

LBM: treatment of a single cell

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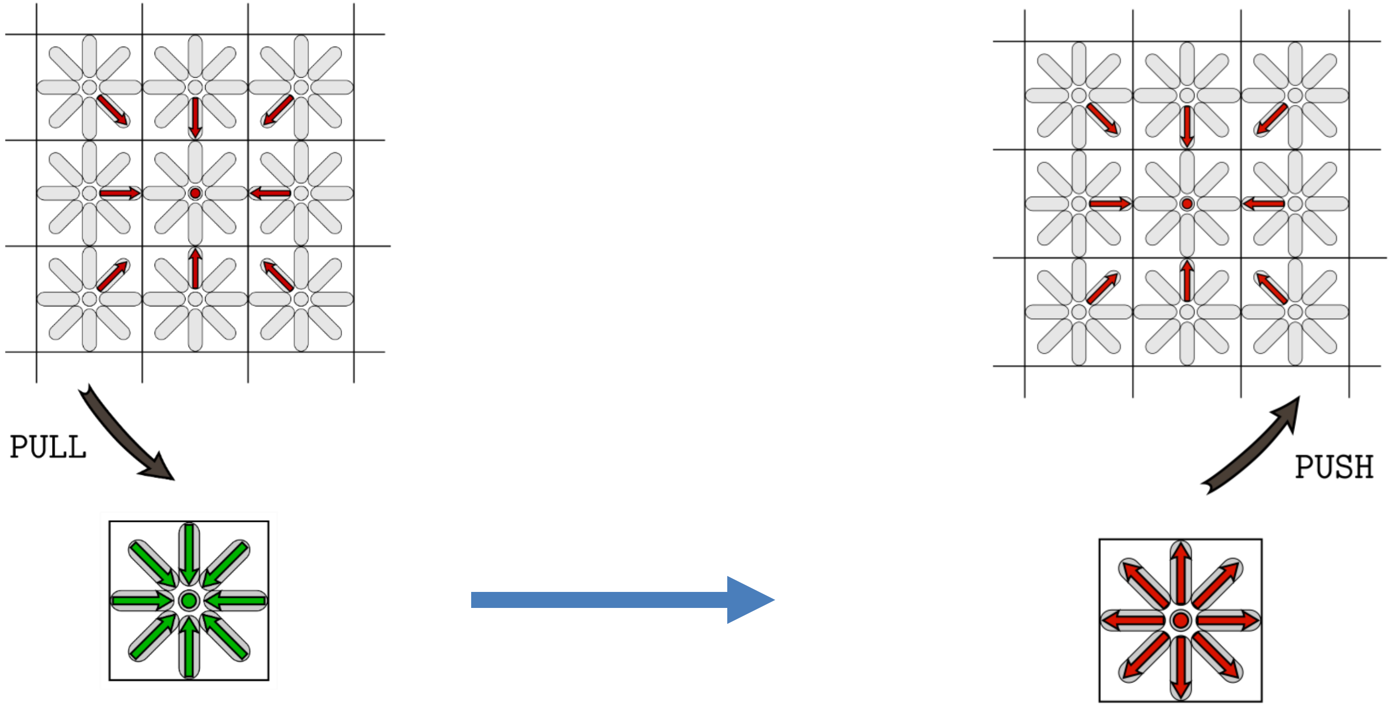


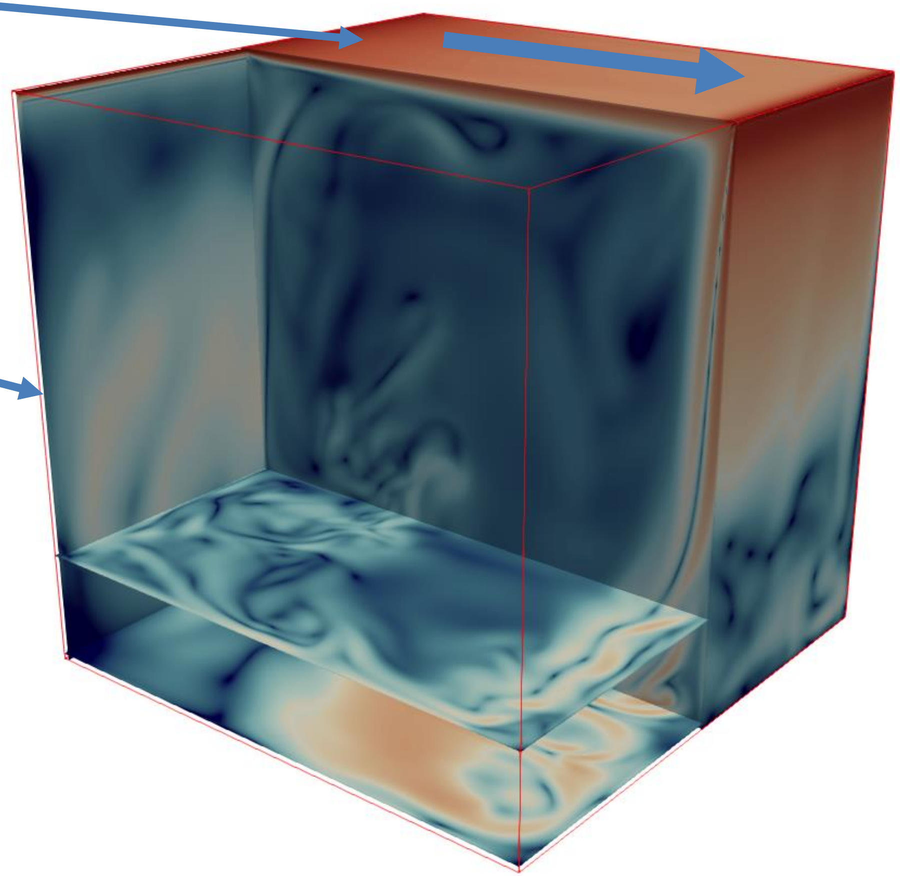
Thread safety: same data accessed at PULL and PUSH.

AA-Pattern: Bailey et al. *http://ieeexplore.ieee.org/document/5362489/*

Test case: 3D Lid-driven cavity

Moving top lid: constant velocity from left to right.

Cubic box with no-slip walls



Test case: 3D Lid-driven cavity

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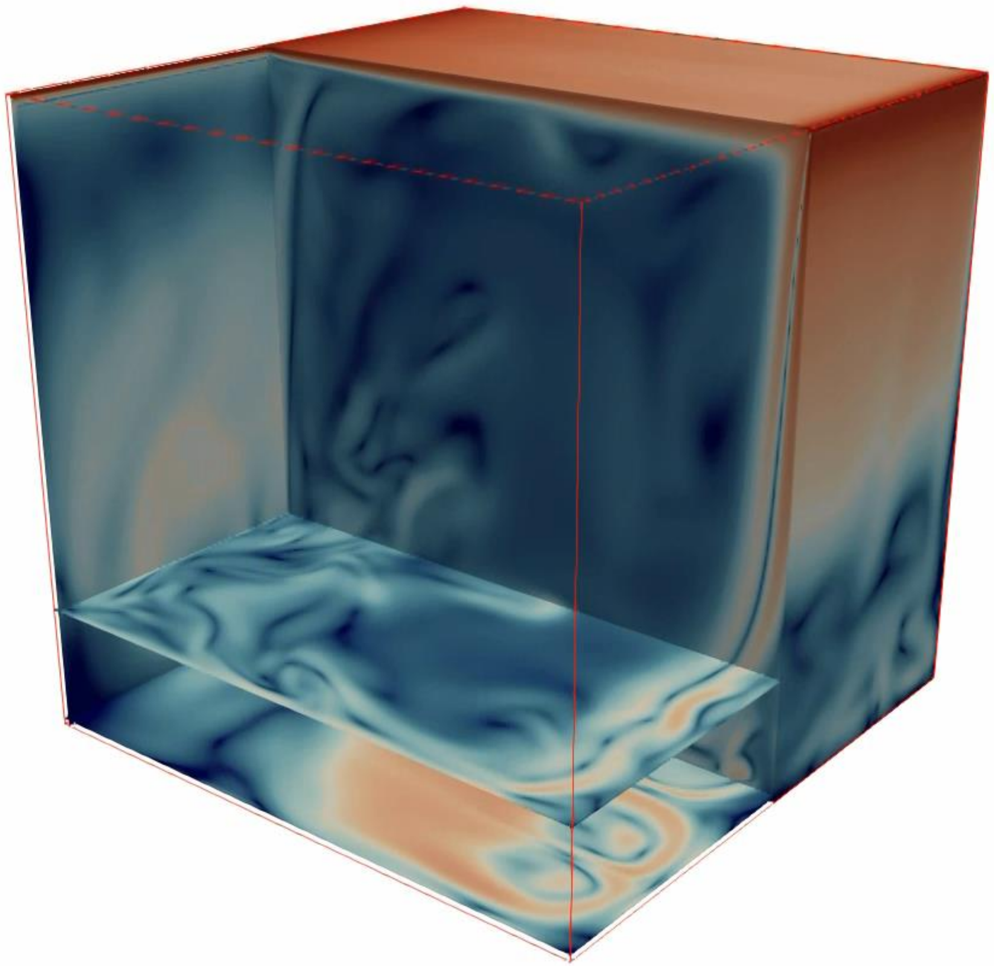
Reynolds: 10’000

LB model: D3Q19, Recursive-regularized with omega_bulk = 1, no subgrid-scale model.

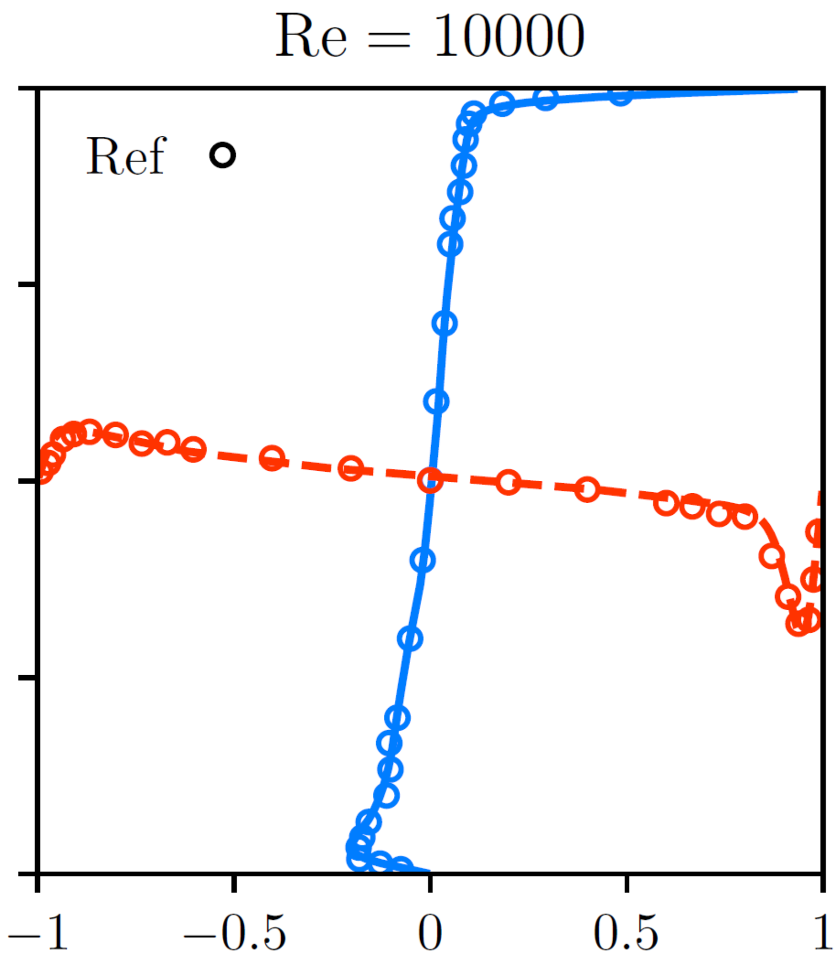
400 x 400 x 400 domain (homogeneous mesh)

560k iterations

2:40 hours on a A100



Validation: 3D cavity



400 x 400 x 400 domain
(Homogeneous mesh)

3 Million iterations

15 hours on a A100

Performance

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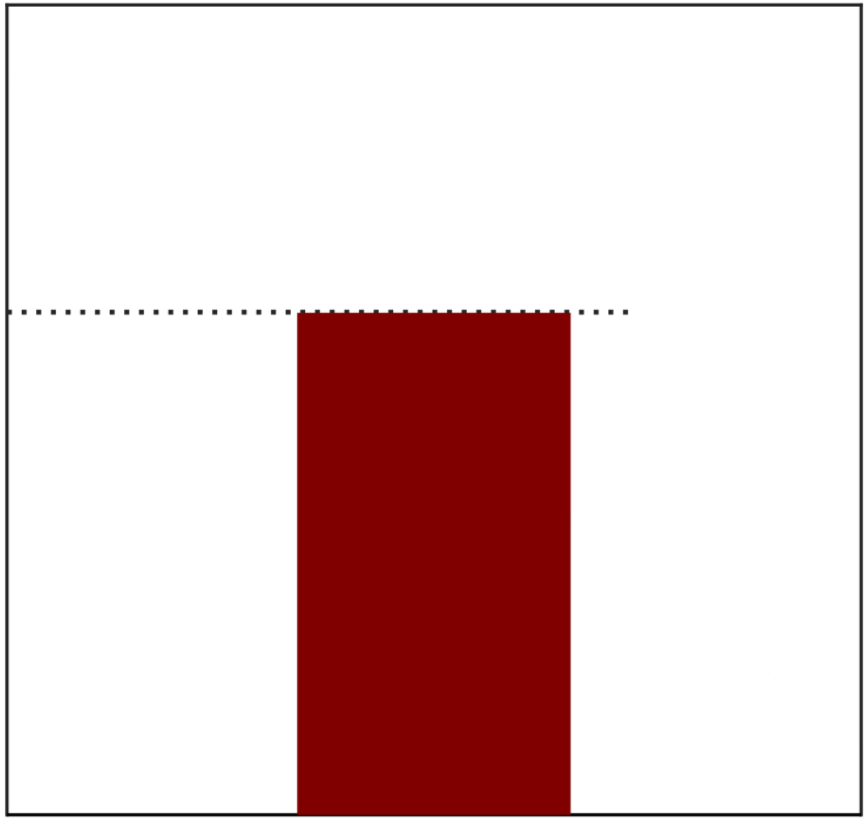
"Mega-LUPS":
Million lattice node updates per second

Our stdpar implementation 3724 MLUPS



200x200x200 domain
Double-precision
A100 GPU

Performance vs. Peak performance

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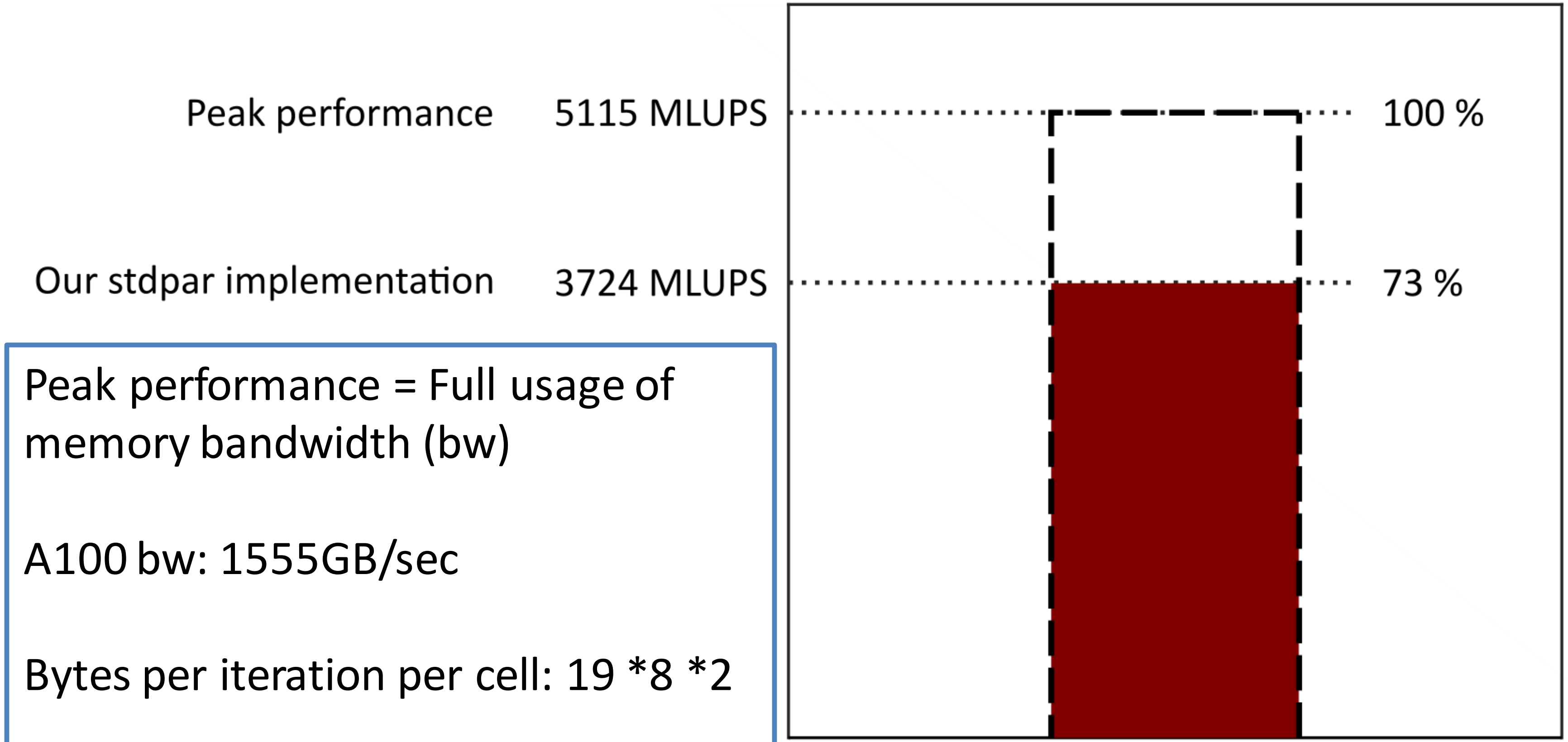
200x200x200 domain
Double-precision
A100 GPU



Peak performance = Full usage of memory bandwidth (bw)

A100 bw: 1555GB/sec

Bytes per iteration per cell: 19 *8 *2

Peak MLUPS = $1.555 * 10^6 / (19*8*2)$

Performance vs. Cuda code

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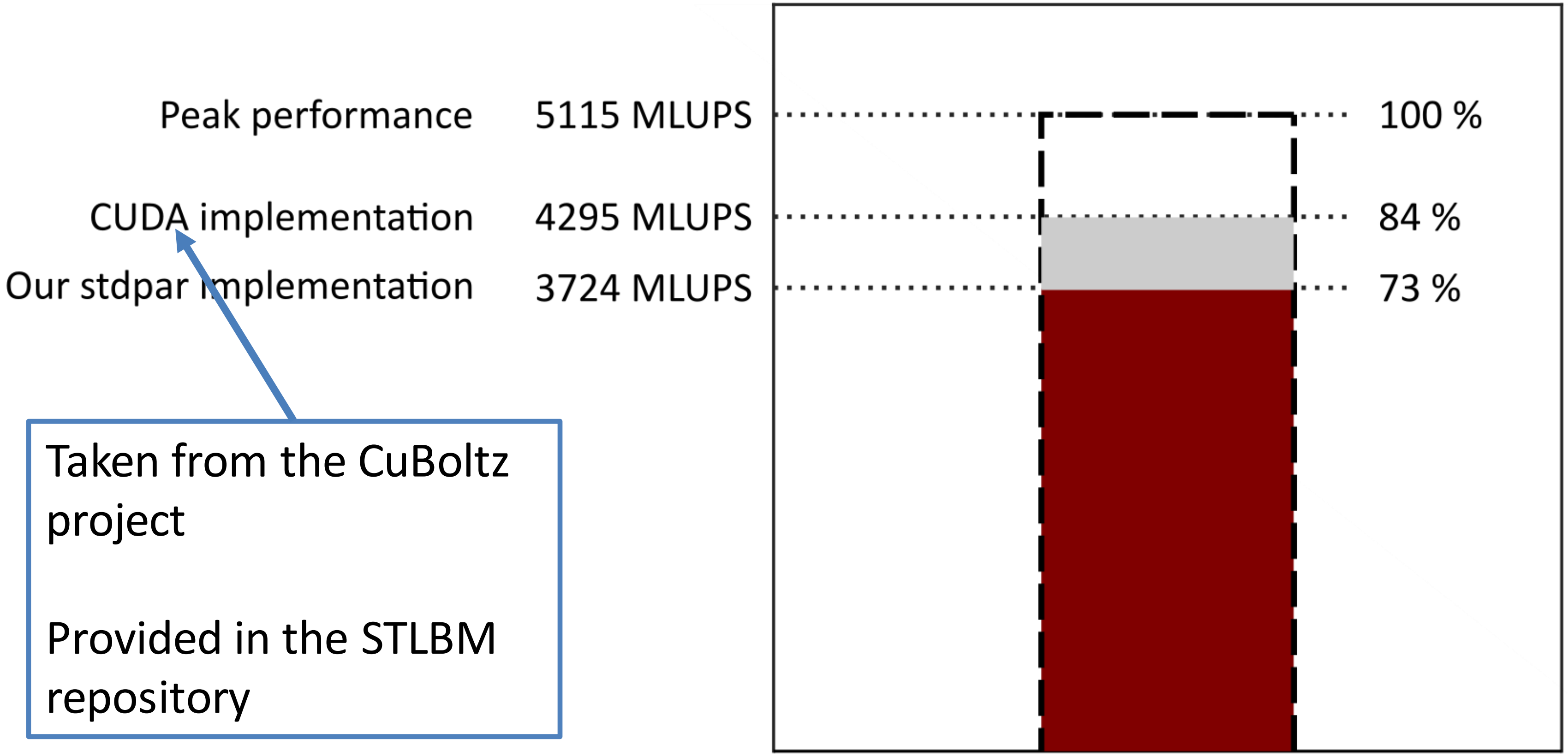
200x200x200 domain
Double-precision
A100 GPU



Taken from the CuBoltz project

Provided in the STLBM repository

Performance on different platforms

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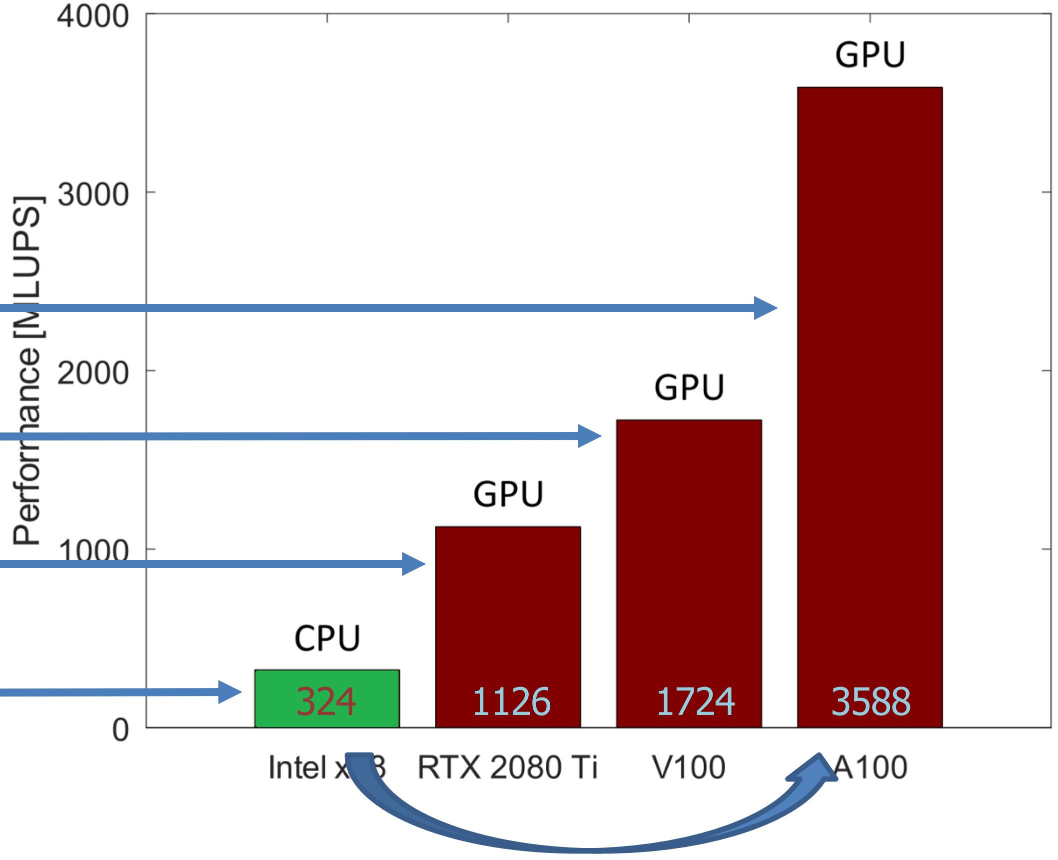
Nvidia A100 (Ampere)

NVidia V100 (Volta)

NVidia RTX 2080 Ti (Turing)

Intel Xeon Gold 6240R CPU, 48 cores



128 x 128 x 128
Double-precision

11-fold speedup

Collision models: low Reynolds

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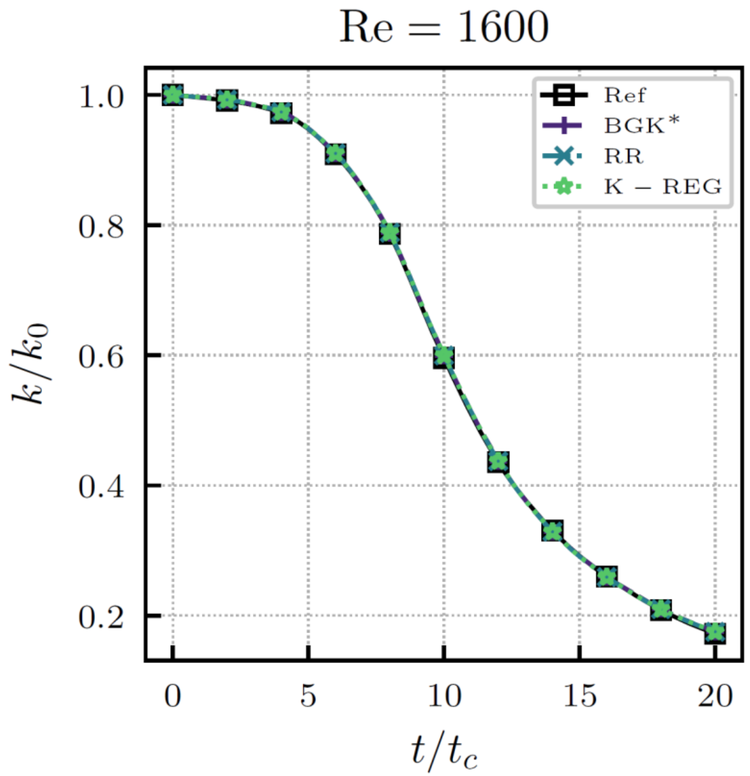
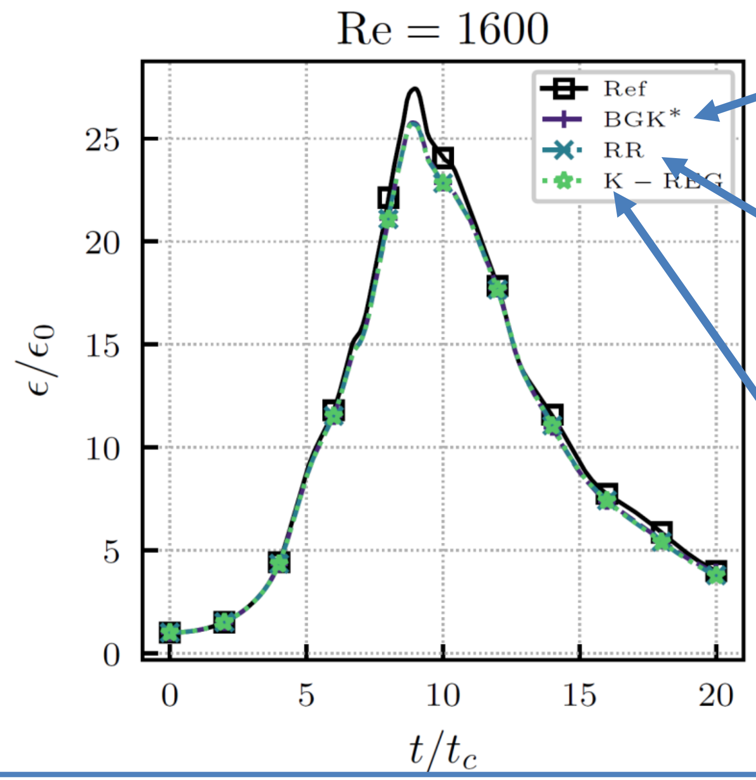
Decaying 3D Taylor-Green vortex

D3Q27, Re: 1600, Mach: 0.2, Resolution: 512 x 512 x 512





"Traditional" BGK model, but with extended equilibrium.

Recursive-regularized, a robust modern collision model (the one used for the cavity).

Cumulant approach with regularization of high-order moments: another robust choice.

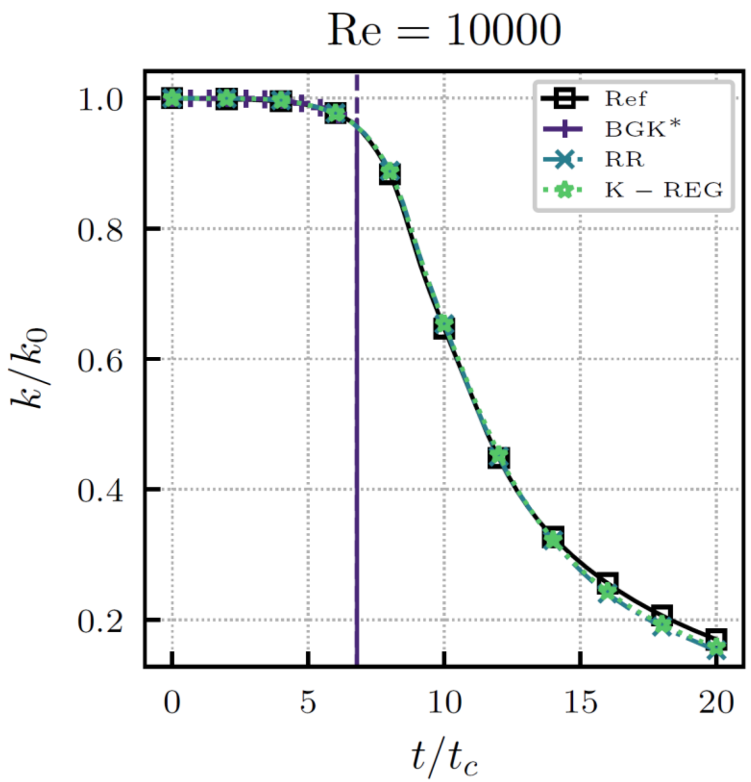
Laizet et al., *3D Taylor-Green vortex Direct Numerical Simulation statistics from Re=1250 to Re=20000,* Zenodo, 2019

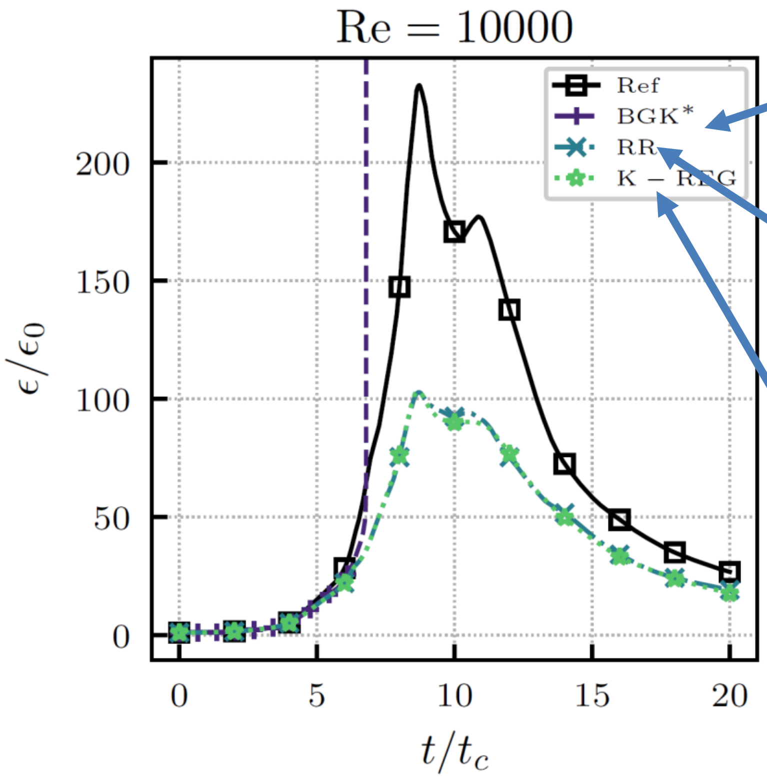
Coreixas, Chopard & Latt. *Comprehensive comparison of collision models…* Phys. Rev. E, 2019, 100, 033305.
Coreixas, Wissocq, Chopard & Latt. *Impact of collision models on the physical properties…* Phil. Trans. R. Soc. A, 2020, 378, 20190397.

Collision models: high Reynolds

Decaying 3D Taylor-Green vortex

D3Q27, Re: 10’000, Mach: 0.2, Resolution: 512 x 512 x 512





“Traditional” BGK model, but with extended equilibrium.

Recursive-regularized, a robust modern collision model (the one used for the cavity).

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Laizet et al., *3D Taylor-Green vortex Direct Numerical Simulation statistics from Re=1250 to Re=20000,* Zenodo, 2019

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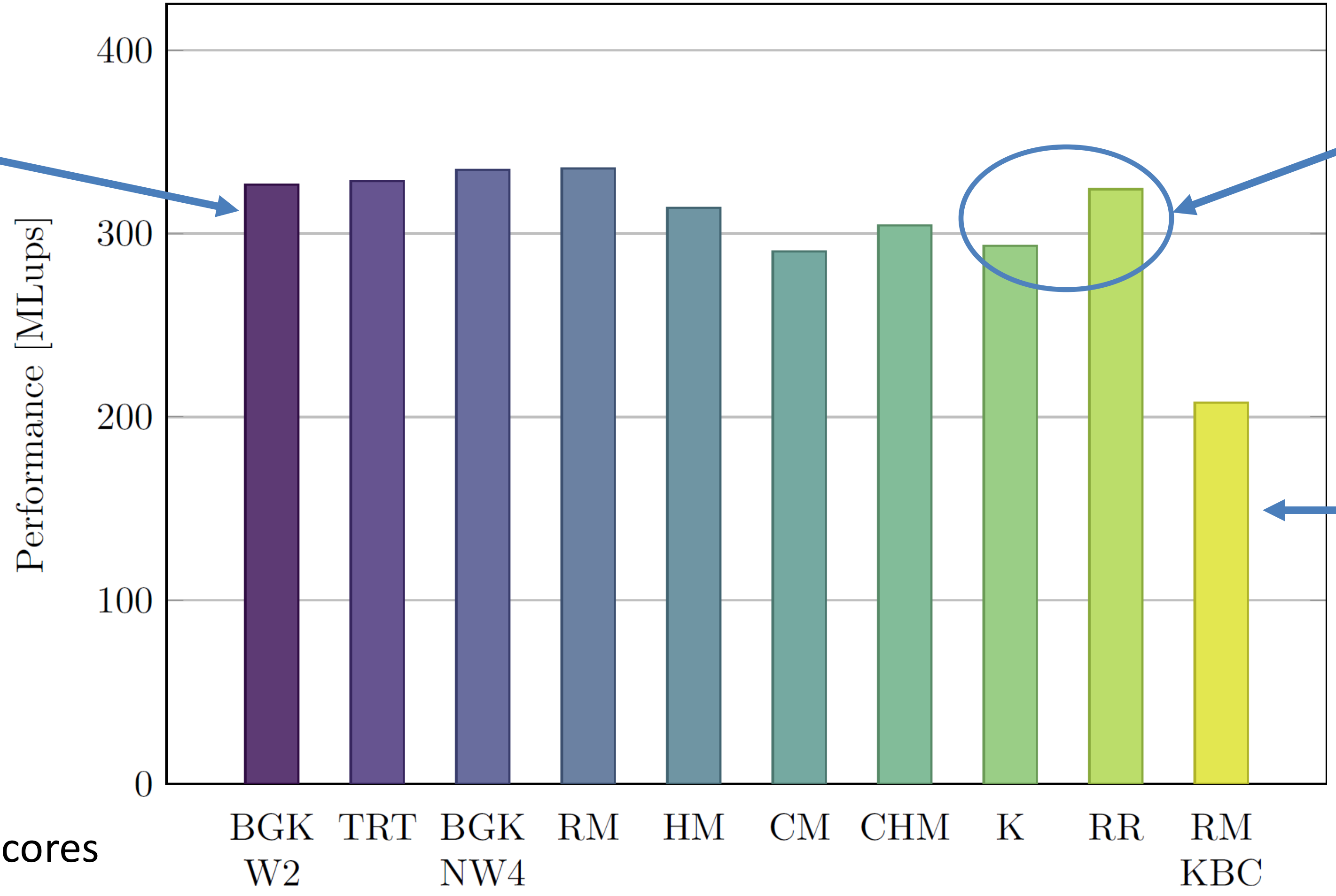
Performance of collision models: CPU

The most standard, BGK model



The more robust alternatives from the previous slides.

KBC: another one, also used in the literature.

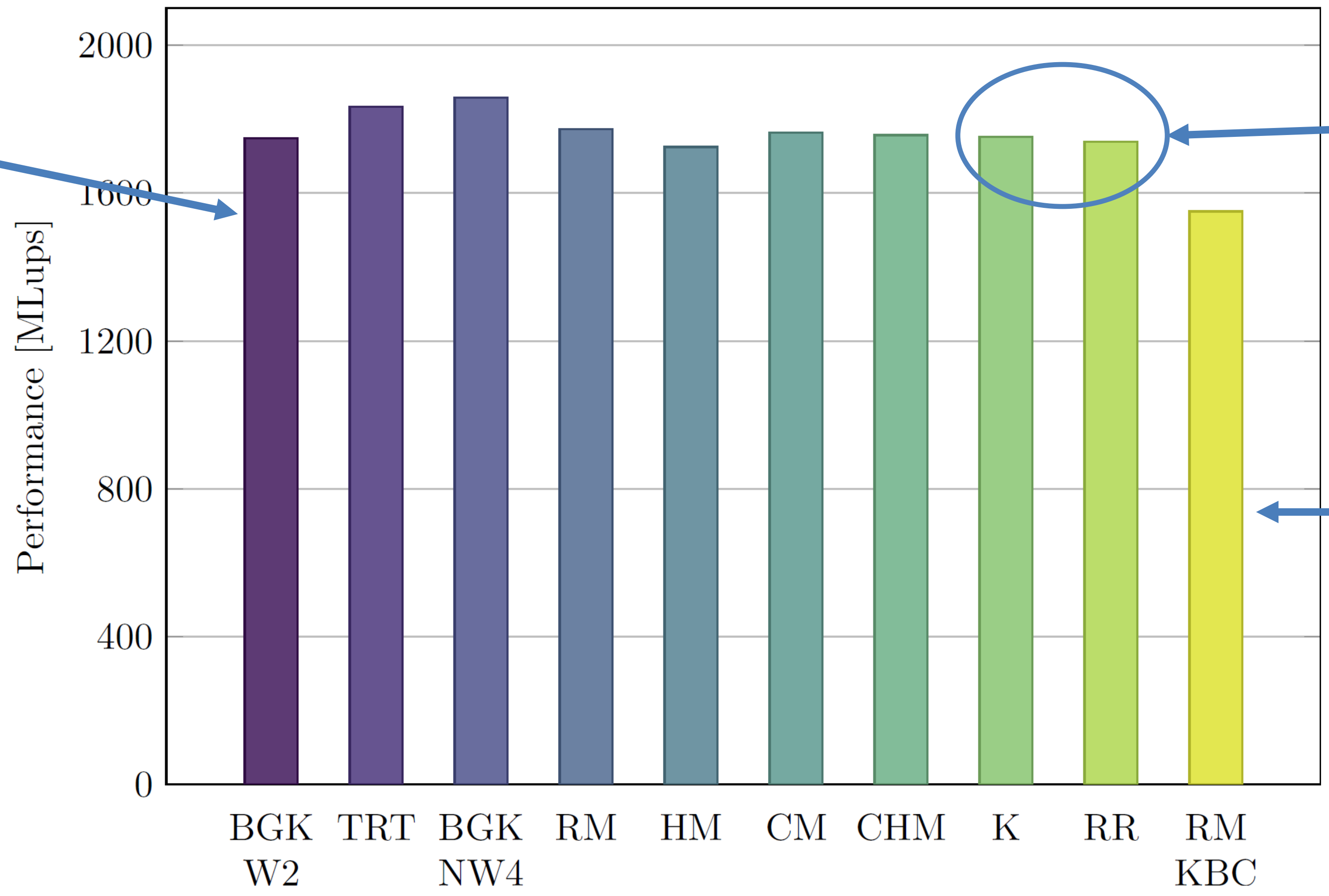
Resolution: 128 x 128 x 128

Lattice: D3Q19

CPU: Xeon Gold 48 cores

Performance of collision models: GPU

The most standard, BGK model



The more robust alternatives from the previous slides.

KBC: another one, also used in the literature.

Resolution:
128 x 128 x 128

Lattice: D3Q19

GPU: V100

Conclusion

- Parallel STL: allows parallelization of numerical algorithms in a fully hardware agnostic way.
- For some algorithms, the performance on GPUs is almost the same as in an “optimal” code.
- A few hundred lines of code, without hardware-specific knowledge, achieve cluster-level performance.
- Performance varies little from one collision model to another: robust, modern collision models should be preferred (code can be copy-pasted from the STLBM project).

Outlook

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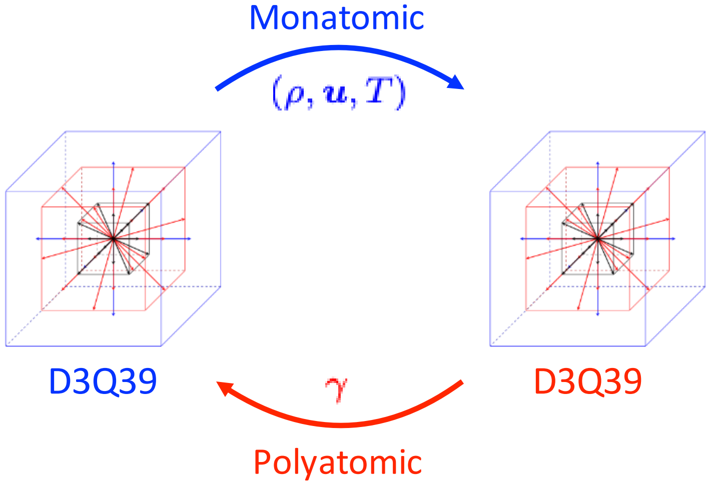
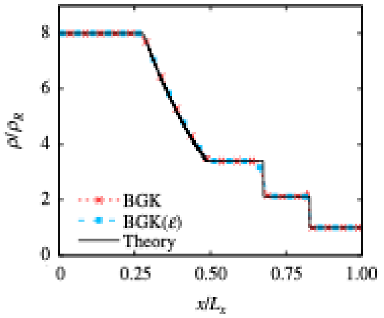
Compressible LBMs

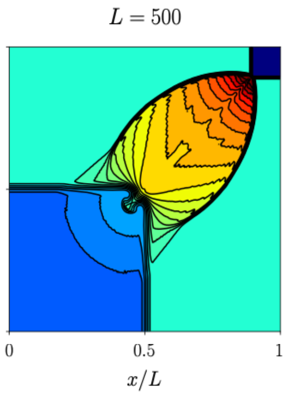


Performance (D3Q39Q39)

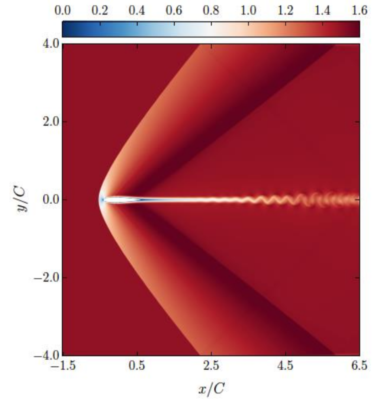
Hardware	i7-8700 (3.2 GHz)	Volta 100	Ampere 100
MLUPS	0.67	30	~ 60
μs/pt/it	1.49	0.033	~ 0.016

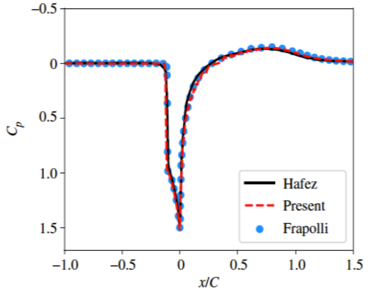
Riemann problems



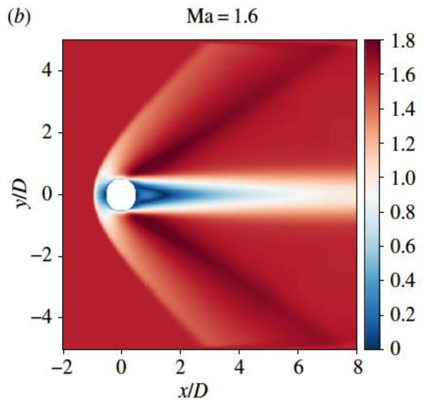


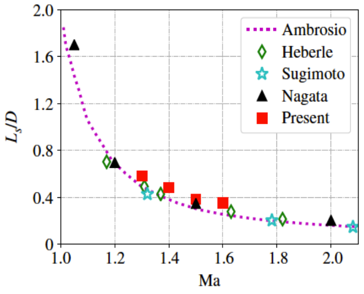
Flow past NACA0012





Flow past sphere





Latt et al., Efficient supersonic flow simulations using lattice Boltzmann methods based on numerical equilibria , *Phil. Trans. R. Soc. A*, **2020**.
Coreixas & Latt, Compressible lattice Boltzmann methods with adaptive velocity stencils: An interpolation-free formulation, *Phys. Fluids*, **2020**

Thank you for your attention

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High Performance Fluid Simulation Group:
www.unige.ch/hpfs/

Example codes from this presentation:
www.gitlab.com/UnigeHPFS/paralg

STLBM source code:
www.gitlab.com/UnigeHPFS/stlbm

We thankfully acknowledge
- The Swiss PASC project for funding.
- The NVIDIA HPC Software and Compiler teams for access to a A100.

Results – Sod Shock Tube

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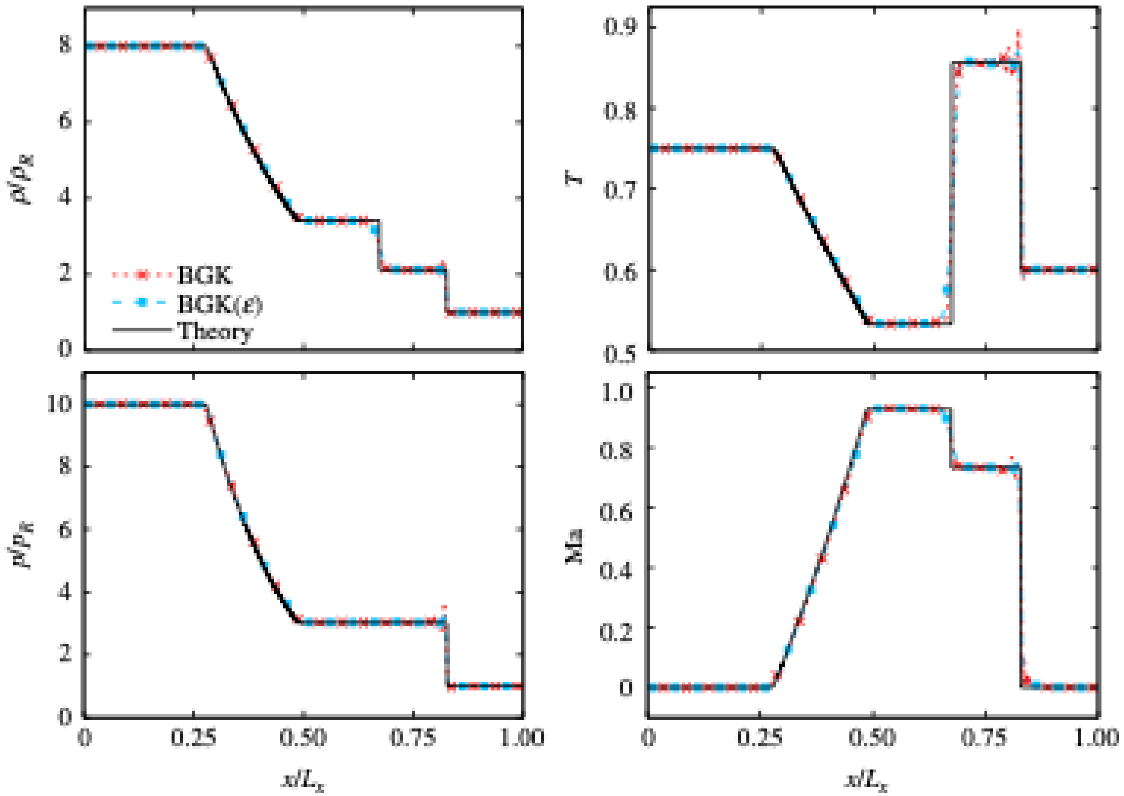


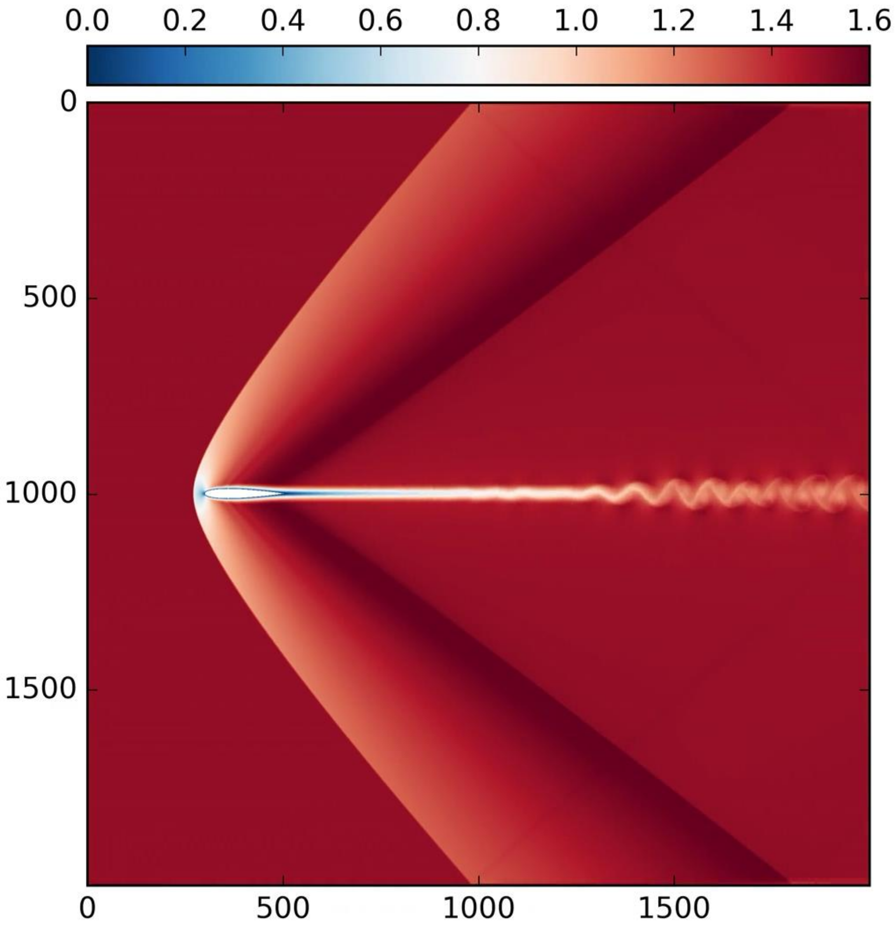
- Good robustness even using the BGK operator
- Kinetic sensor allows for **inviscid** simulations

$$\epsilon = \frac{1}{V} \sum_{i=0}^{V-1} \frac{|f_i - f_i^{eq}|}{f_i^{eq}}$$

Latt et al., Efficient supersonic flow simulations using lattice Boltzmann methods based on numerical equilibria
Phil. Trans. R. Soc. A, **2020**, 378, 20190559

Results – 2D NACA0012

Mach number field



- **Surprisingly**, all BCs have a **good** behavior
- **Only the BB** leads to **spurious** oscillations

Latt et al., Efficient supersonic flow simulations using lattice Boltzmann methods based on numerical equilibria
Phil. Trans. R. Soc. A, **2020**, 378, 20190559

D3Q27 Lattice – CPU (Xeon Gold x48)

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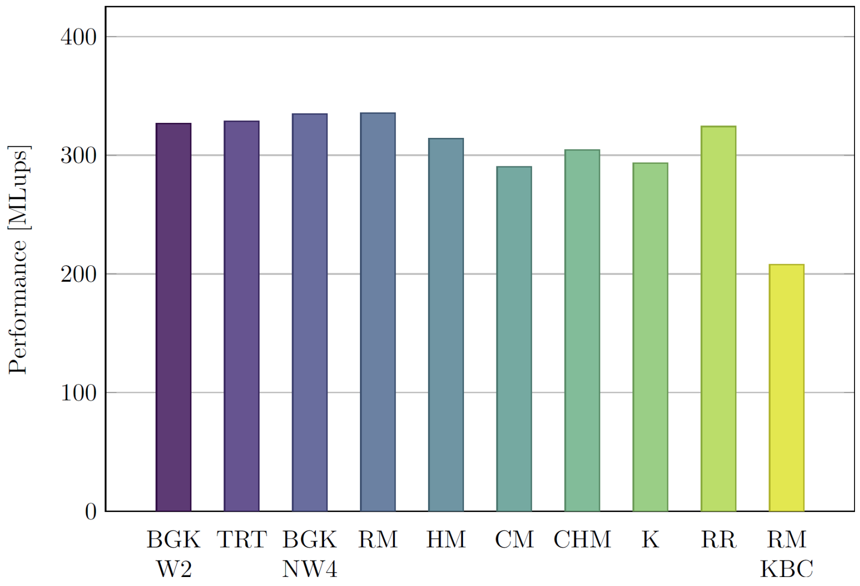
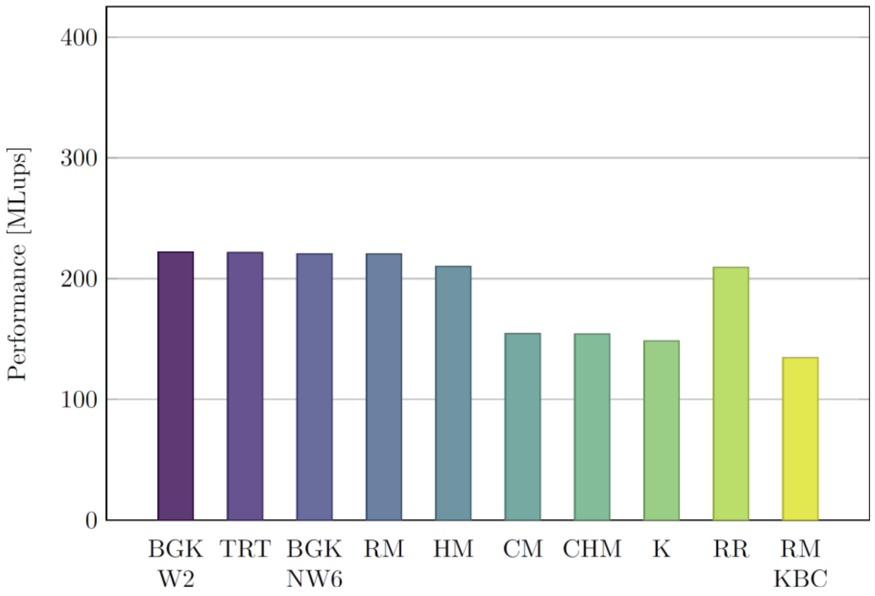
D3Q19



D3Q27



D3Q27 Lattice – GPU (V100)

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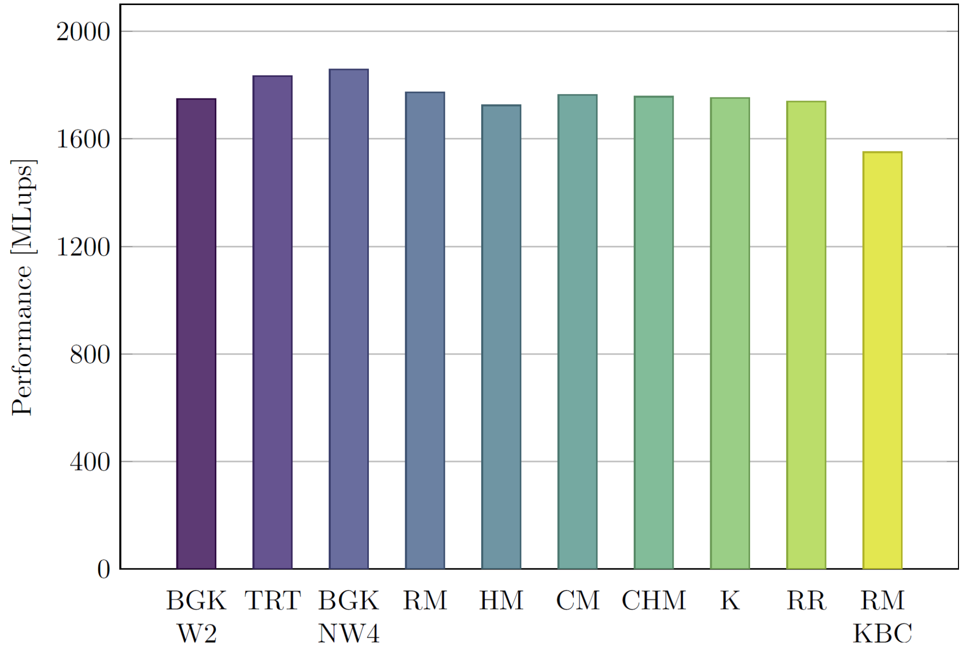
D3Q19



D3Q27