The Abdus Salam
International Centre
for Theoretical Physics

Lattice-Boltzmann parallelization

Introductory School on Parallel Programming and Parallel Architecture for High-Performance Computing

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ICTP

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What do I do and why do I need HPC?

- I work in magnetohydrodynamics (MHD)

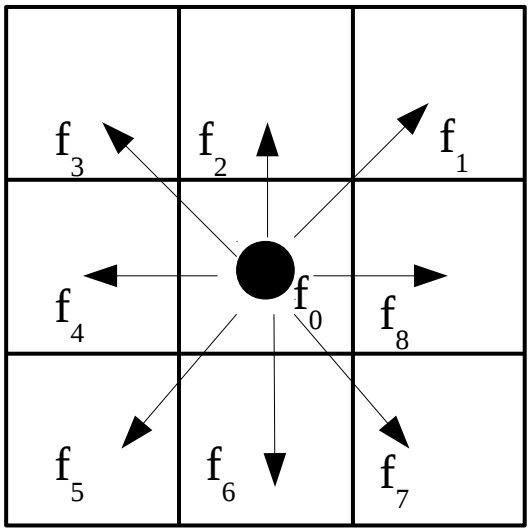
$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{1}{\rho}\nabla p + \mathbf{j} \times \mathbf{B} + \frac{1}{R}\nabla^2 \mathbf{v}$$

$$\frac{\partial \mathbf{b}}{\partial t} = \nabla \times (\mathbf{v} \times \mathbf{B}) + \frac{1}{R_m}\nabla^2 \mathbf{b}$$

- Non-linear equations with no analytic solutions. So, numerical methods.
- Grids of 512^3 points, pseudospectral method (Fourier transformations), etc.

Lattice-Boltzmann Method

- Class of computational fluid dynamics (CFD) methods.
- The discrete Boltzmann equation is solved to simulate the flow of a Newtonian fluid with collision models such as Bhatnagar–Gross–Krook (BGK).
- D2Q9

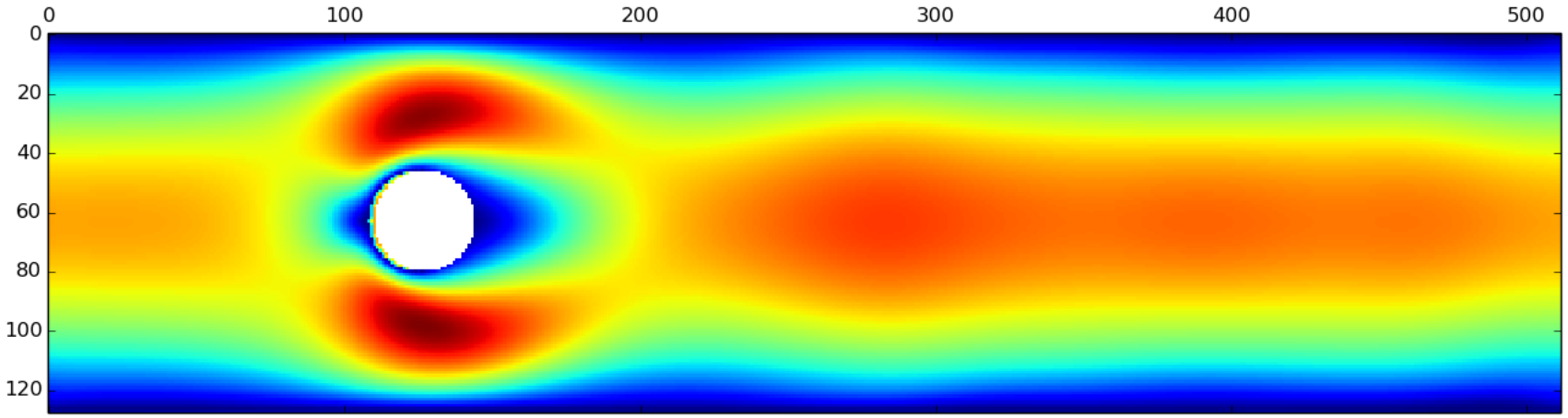


Streaming

+ Collision

ICTP Project

2D Cylinder in a periodic flow



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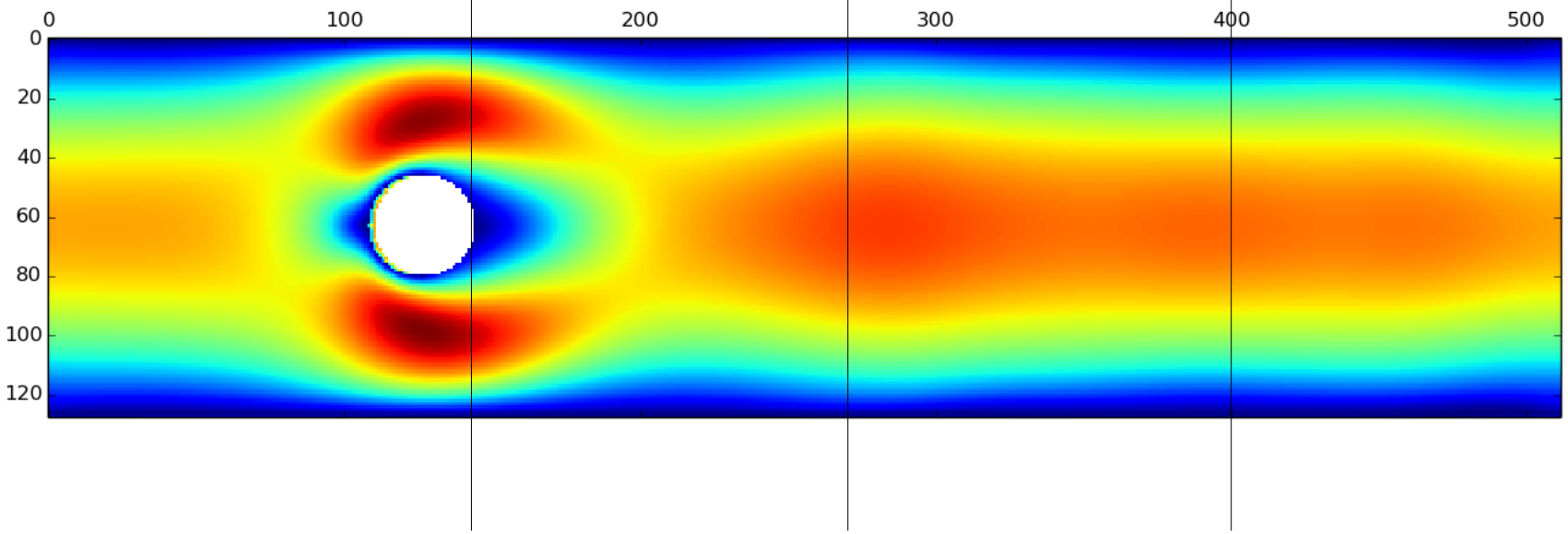

ICTP Project

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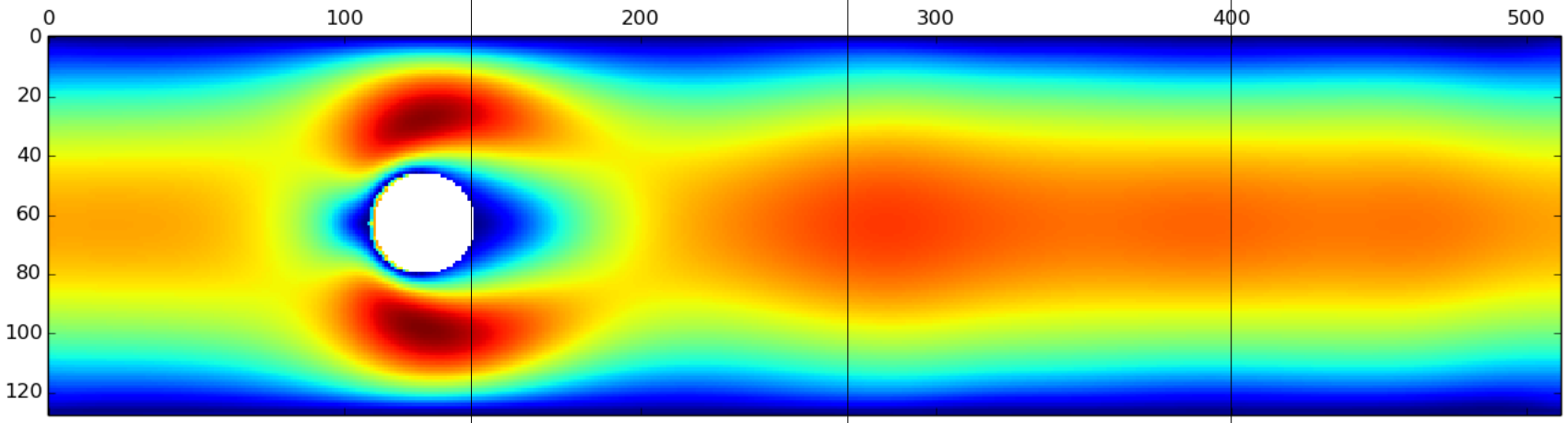
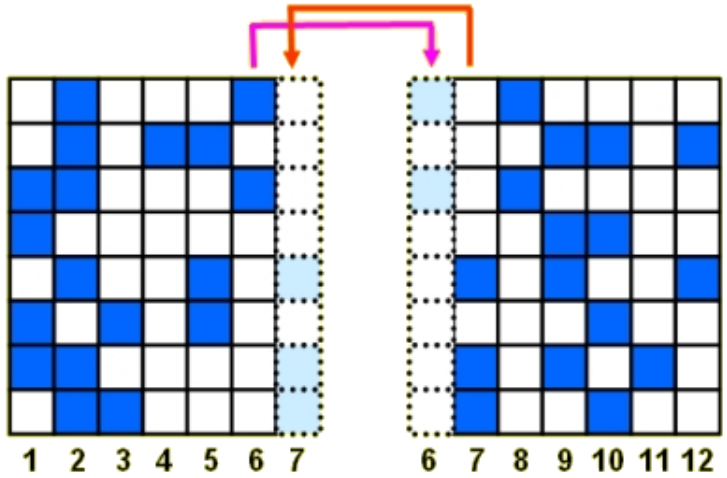




Timing the code (not profiling...)

- For a grid of 512 x 128 point (really small), 2000 steps (really small) and not saving files:

  NP = 1 ⟶ T = 30.0s

  NP = 2 ⟶ T = 16.6s

  NP = 4 ⟶ T = 18.9s (?)

  NP = 8 ⟶ T = 12.4s

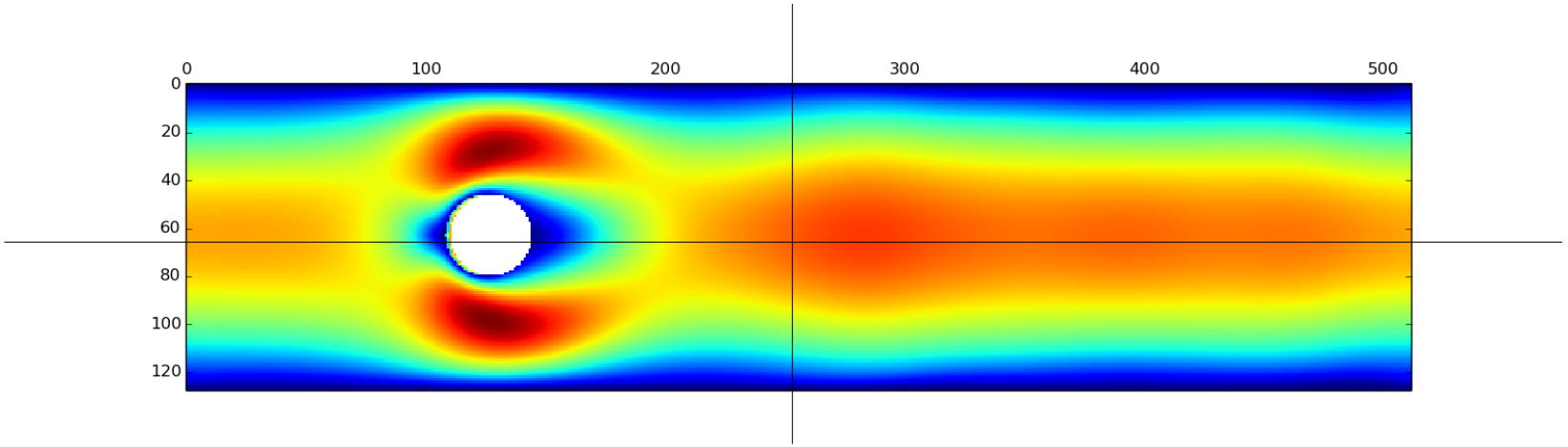
- If I save data every 100 steps, it takes 30% more time.

MPI implementations

- Introduce variables in the code to do it parallelizable.
- MPI_ISEND + MPI_RECV + MPI_WAIT (I need to transfer the data to the ghost cells)
- MPI_SENDRECV (not in the last version)
- Personalized MPI Datatypes to transfer the data in one buffer.

Future MPI implementations

- Implementation of NetCFD to save the data.
- Different division of work for each processor (maybe a grid)



- (not MPI, but) Use of more libraries (don't reinvent the wheel, steal it from someone better).

Movie time

Thanks!