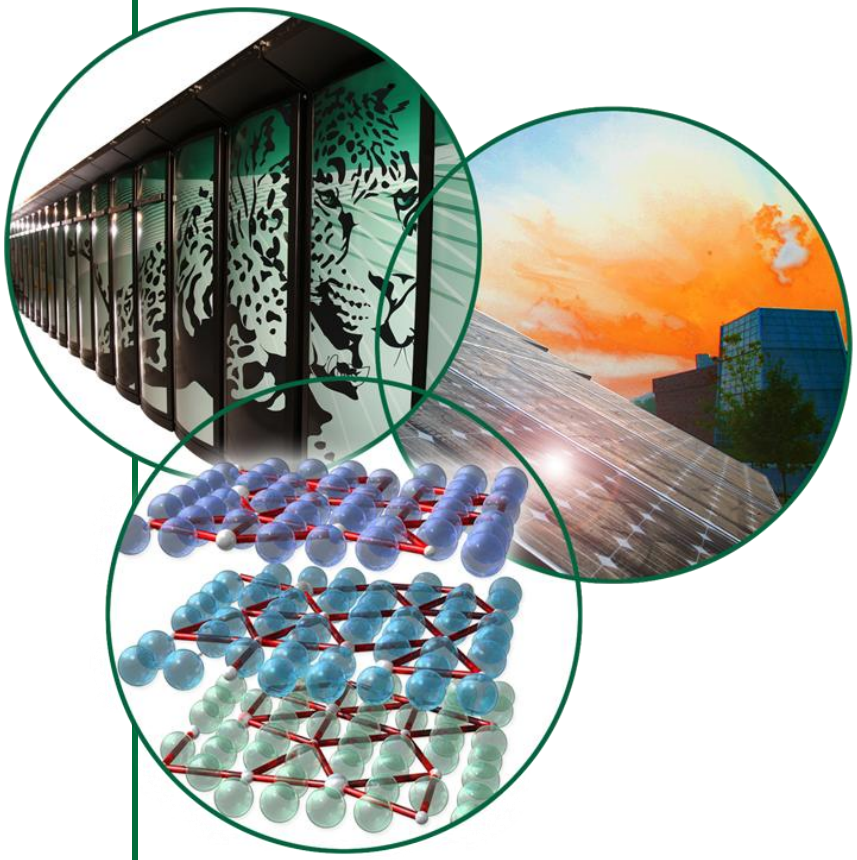
Parallel Simulation of Turbulent Flows using Lattice Boltzmann Models



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Outline

A quick overview of LBM

Multi Relaxation Time LBM (MRT-LBM)

Some results

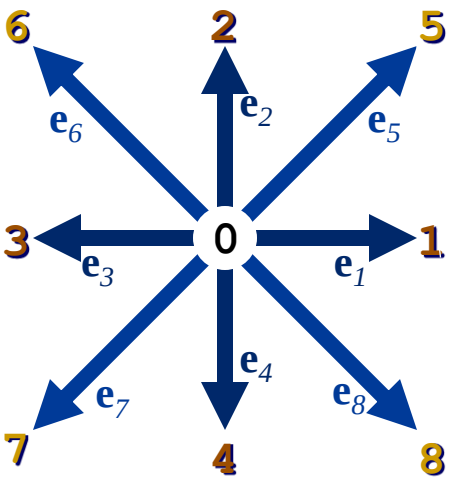
Conclusions

A quick overview of LBM

- An alternative numerical method based on kinetic theory to simulate various hydrodynamic systems
- Developed from Lattice Gas Cellular Automata (LGCA) models (which suffered from intrinsic noise and limited values of transport coefficients)
- Development of LBM continues for compressible, incompressible, visco-elastic, multi-phase and suspensions in fluid
- Two major models:
  - Single Relaxation Time (SRT) LBM
  - Multi Relaxation Time (MRT) LBM or (Generalized LBE method)

A quick overview of LBM

D2Q9



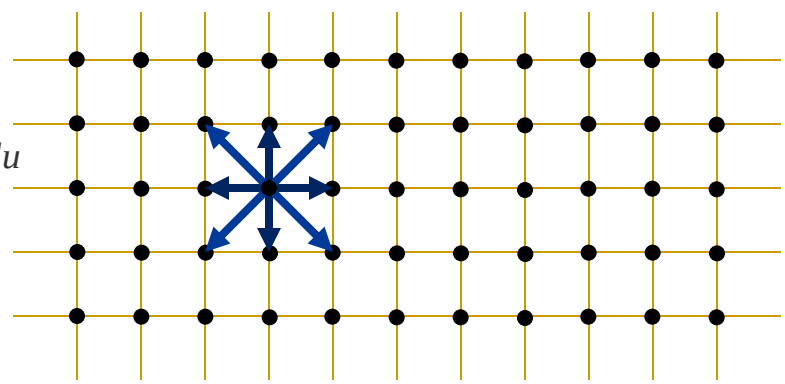
Discrete Velocities $\mathbf{e}_a$

Directional densities f_a

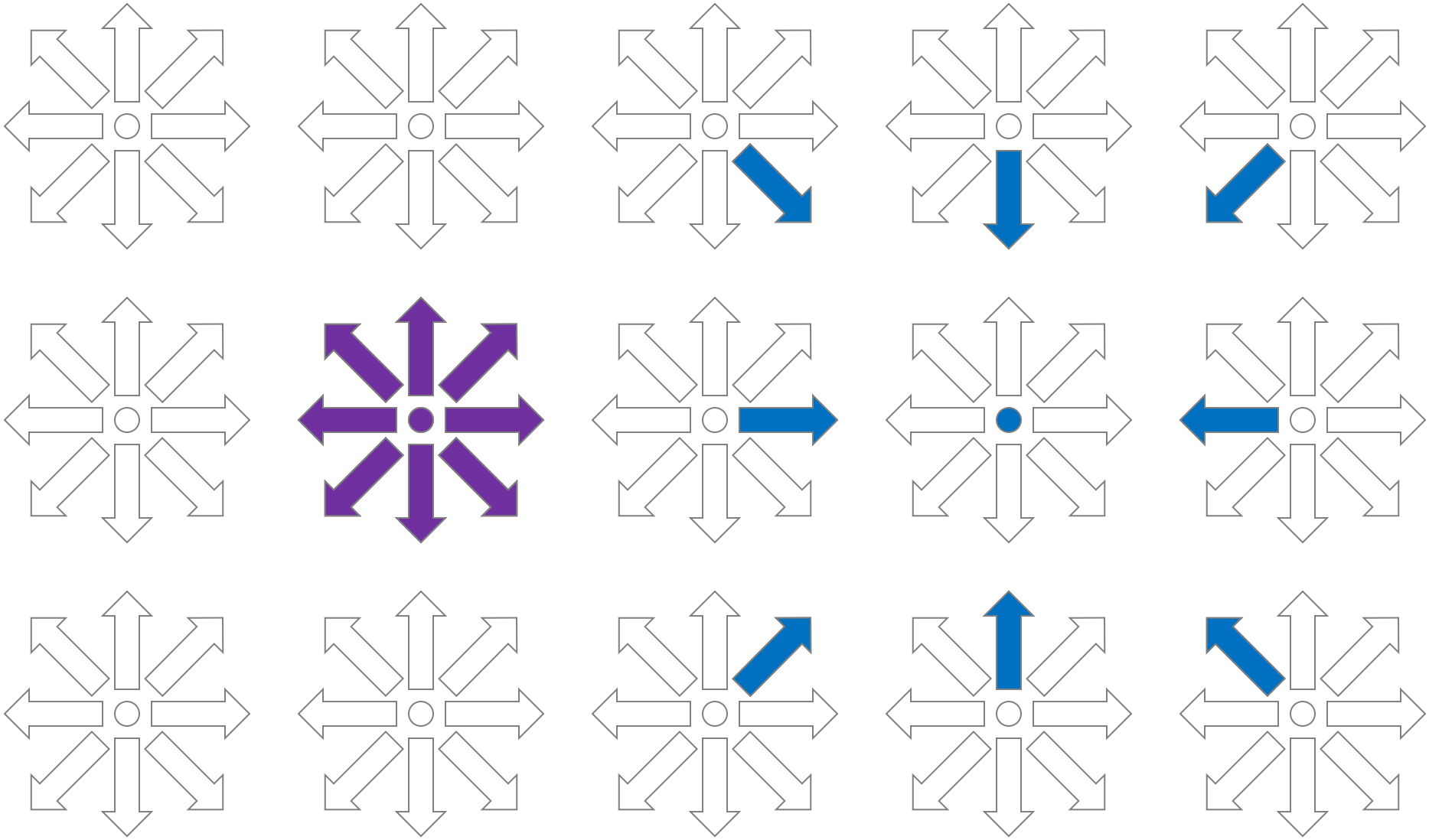
Macroscopic density $\rho = \sum_{a=0}^{8} f_a$

Macroscopic velocity $\mathbf{u} = \frac{1}{\rho} \sum_{a=0}^{8} f_a \mathbf{e}_a$

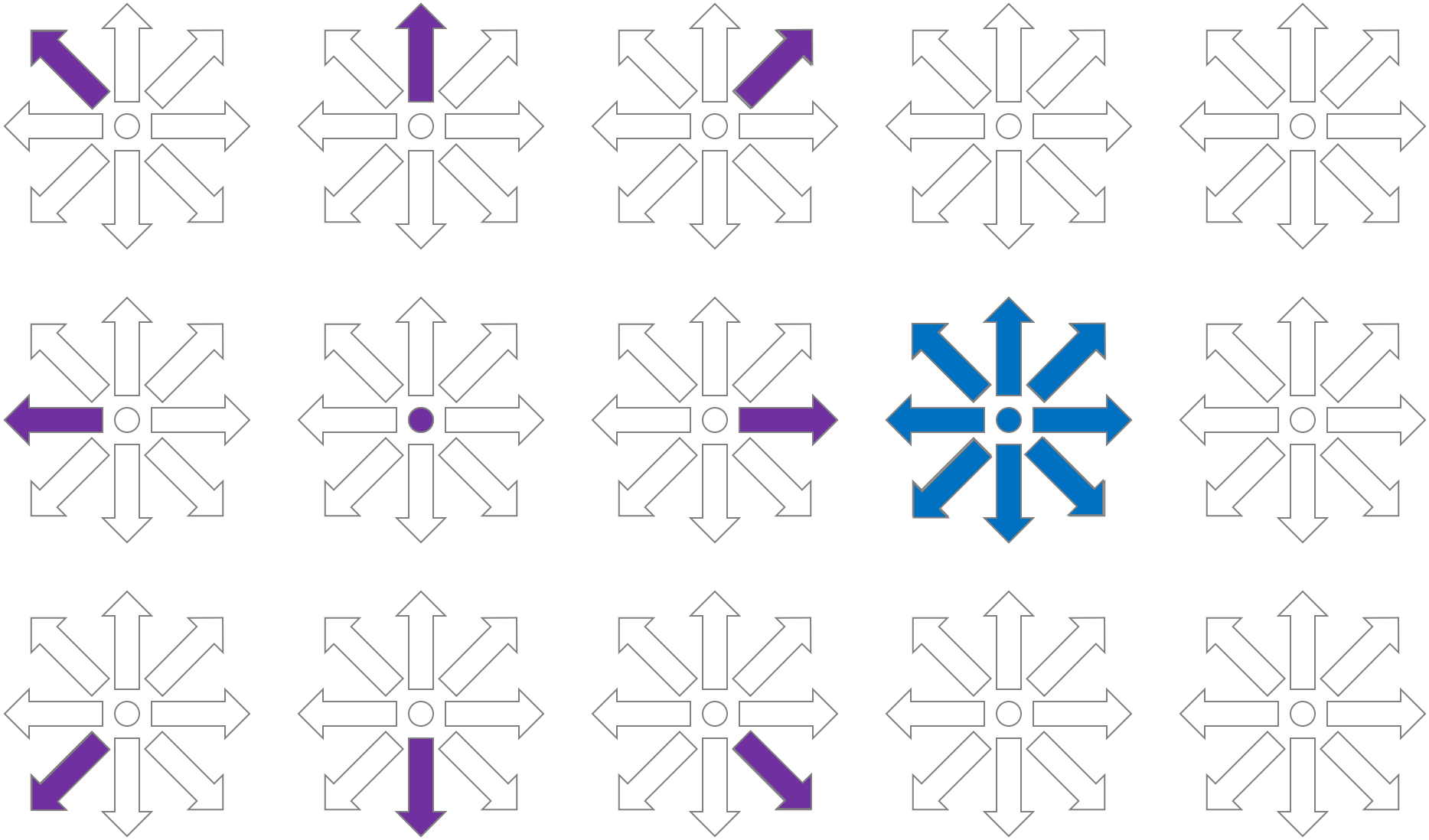
Lattice Unit, *lu*



Streaming step: f → f*



Collision step: $f = f^* + \tau^{-1}(f^{eq} - f^*)$



Typical set up for SRT-LBM

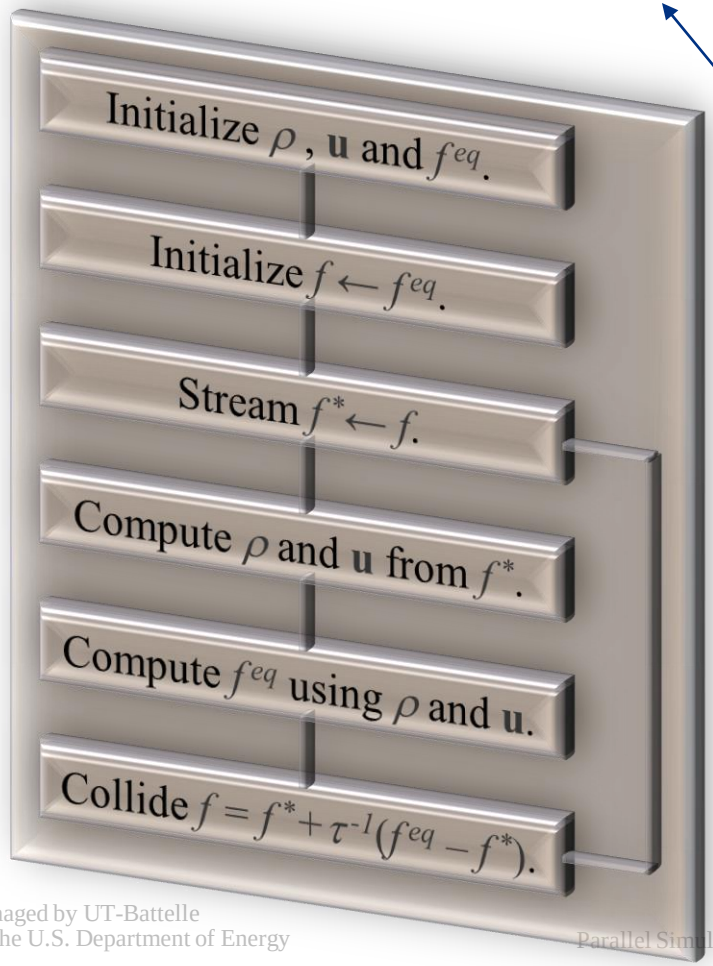
Streaming Step $$f_a^*(\mathbf{x}+\mathbf{e}_a,t) = f_a(\mathbf{x},t), 1 \le a \le 8$$

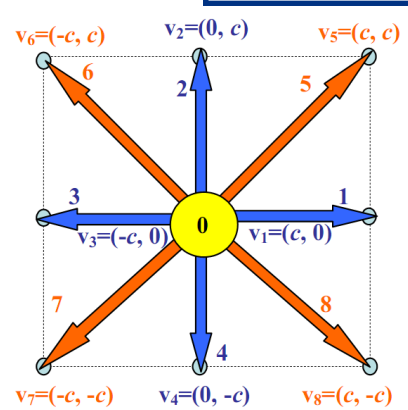
Collision Step $$f_a(\mathbf{x},t+\Delta t) = f_a^*(\mathbf{x},t) + \frac{1}{\tau}\left(f_a^{eq}(\mathbf{x},t) - f_a^*(\mathbf{x},t)\right), 0 \le a \le 8$$

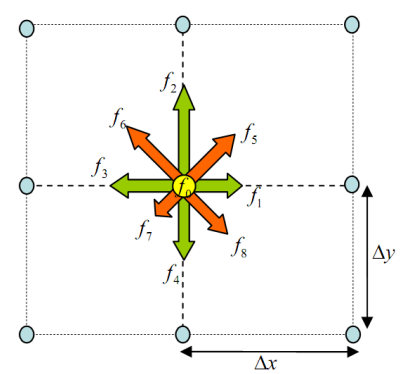
Equilibrium Dist. Func. $$f_a^{eq} = E_a\rho\left[1 + 3\mathbf{e}_a\cdot\mathbf{u} + \frac{9}{2}(\mathbf{e}_a\cdot\mathbf{u})^2 - \frac{3}{2}\mathbf{u}\cdot\mathbf{u}\right], 0 \le a \le 8$$

BGK single relaxation time τ is related to kinematic viscosity $\nu = \frac{1}{3}\left(\tau - \frac{1}{2}\right)$.
Usually $\frac{1}{2} < \tau < 2$.

$$E_a = \begin{cases} \frac{4}{9} & \text{for } a = 0, \\ \frac{1}{9} & \text{for } a \in \{1,2,3,4\}, \\ \frac{1}{36} & \text{for } a \in \{5,6,7,8\}. \end{cases}$$







Multi Relaxation Time (MRT) LBM

- Much more stable than SRT (LBGK-type) models
- Similar steps as in SRT-LBM:
  - Streaming : in discrete velocity space
  - Collision : in kinetic moment space
- From the kinetic theory, hydrodynamic processes can be described by interaction of different 'modes' which are related to the 'kinetic moments'
- Moment representation allows to control each 'mode' independently

Kinetic Moments in D2Q9 MRT Model

#	Moment vectors for the D2Q9 model	Description
1	$\lvert\rho\rangle_\alpha = \lvert\mathbf{e}_\alpha\rvert^0 = 1,$	Density mode
2	$\lvert e\rangle_\alpha = -4\lvert\mathbf{e}_\alpha\rvert^0 + 3(e_{\alpha,x}^2 + e_{\alpha,y}^2)$	Energy mode
3	$\lvert\varepsilon\rangle_\alpha = 4\lvert\mathbf{e}_\alpha\rvert^0 - \frac{21}{2}(e_{\alpha,x}^2 + e_{\alpha,y}^2) + \frac{9}{2}(e_{\alpha,x}^2 + e_{\alpha,y}^2)^2$	Energy-sq mode
4	$\lvert j_x\rangle_\alpha = e_{\alpha,x}$	X-momentum
5	$\lvert q_x\rangle_\alpha = [-5\lvert\mathbf{e}_\alpha\rvert^0 + 3(e_{\alpha,x}^2 + e_{\alpha,y}^2)]e_{\alpha,x}$	X-energy flux
6	$\lvert j_y\rangle_\alpha = e_{\alpha,y}$	Y-momentum
7	$\lvert q_y\rangle_\alpha = [-5\lvert\mathbf{e}_\alpha\rvert^0 + 3(e_{\alpha,x}^2 + e_{\alpha,y}^2)]e_{\alpha,y}$	Y-energy flux
8	$\lvert p_{xx}\rangle_\alpha = e_{\alpha,x}^2 - e_{\alpha,y}^2$	Diag stress tensor
9	$\lvert p_{xy}\rangle_\alpha = e_{\alpha,x}e_{\alpha,y}$	Off-diag stress tensor

Transformation b/w moment and phase space

$$\rho = \langle \rho | f \rangle = \langle f | \rho \rangle,$$
$$e = \langle e | f \rangle = \langle f | e \rangle,$$
$$\varepsilon = \langle \varepsilon | f \rangle = \langle f | \varepsilon \rangle,$$
$$j_x = \langle j_x | f \rangle = \langle f | j_x \rangle,$$
$$q_x = \langle q_x | f \rangle = \langle f | q_x \rangle,$$
$$j_y = \langle j_y | f \rangle = \langle f | j_y \rangle,$$
$$q_y = \langle q_y | f \rangle = \langle f | q_y \rangle,$$
$$p_{xx} = \langle p_{xx} | f \rangle = \langle f | p_{xx} \rangle,$$
$$p_{xy} = \langle p_{xy} | f \rangle = \langle f | p_{xy} \rangle.$$

Transformation Matrix for D2Q9 lattice

$$\mathsf{M} \equiv \begin{pmatrix} \langle \rho | \\ \langle e | \\ \langle \varepsilon | \\ \langle j_x | \\ \langle q_x | \\ \langle j_y | \\ \langle q_y | \\ \langle p_{xx} | \\ \langle p_{xy} | \end{pmatrix} \equiv \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -4 & -1 & -1 & -1 & -1 & 2 & 2 & 2 & 2 \\ 4 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \\ 0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 & -1 \\ 0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \end{pmatrix}$$

$$|m\rangle \equiv (\rho, e, \varepsilon, j_x, q_x, j_y, q_y, p_{xx}, p_{xy})^{\mathsf{T}}$$

$$|m\rangle = \mathsf{M}|f\rangle,$$
$$|f\rangle = \mathsf{M}^{-1}|m\rangle.$$

Transformation between moment and phase space

Governing equation for MRT-LBM

- Evolution equation

$$|f(\boldsymbol{r}_i + \boldsymbol{e}_\alpha \delta t, t + \delta t)\rangle - |f(\boldsymbol{r}_i, t)\rangle = \quad M^{-1} S[|m(\boldsymbol{r}_i, t)\rangle - |m^{(\mathrm{eq})}(\boldsymbol{r}_i, t)\rangle]$$

  - S: Diagonal Relaxation Matrix (or Collision Matrix)

$$\mathsf{S} \equiv \mathrm{diag}(0, -s_2, -s_3, 0, -s_5, 0, -s_7, -s_8, -s_9)$$

  - M: Transformation Matrix

- Collisions do not change conserved quantities, only non-conserved moments are updated

$$e^* = e - s_2[e - e^{(\mathrm{eq})}],$$

$$\varepsilon^* = \varepsilon - s_3[\varepsilon - \varepsilon^{(\mathrm{eq})}],$$

$$q_x^* = q_x - s_5[q_x - q_x^{(\mathrm{eq})}],$$

$$q_y^* = q_y - s_7[q_y - q_y^{(\mathrm{eq})}],$$

$$p_{xx}^* = p_{xx} - s_8[p_{xx} - p_{xx}^{(\mathrm{eq})}],$$

$$p_{xy}^* = p_{xy} - s_9[p_{xy} - p_{xy}^{(\mathrm{eq})}],$$

* post-collision quantities

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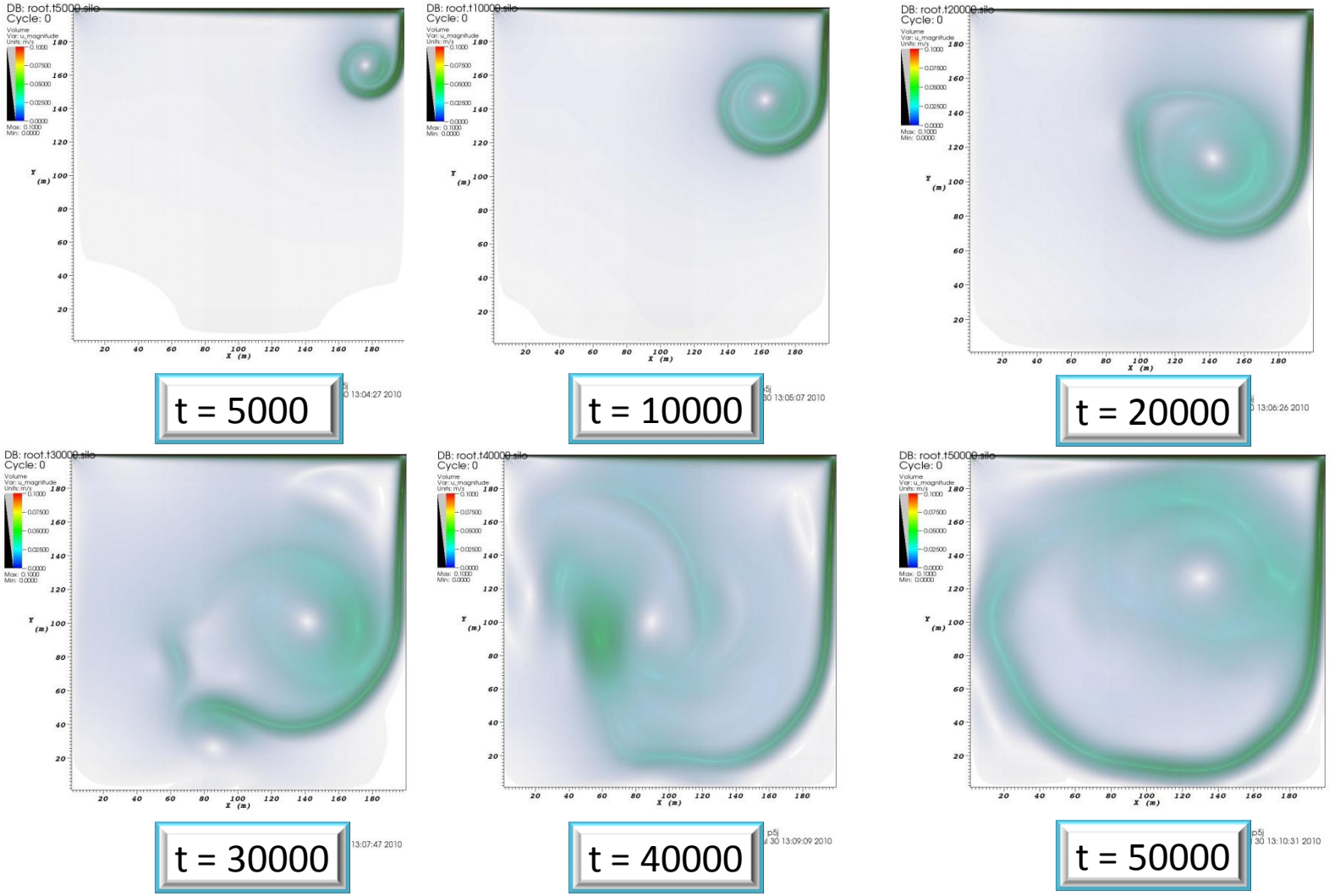
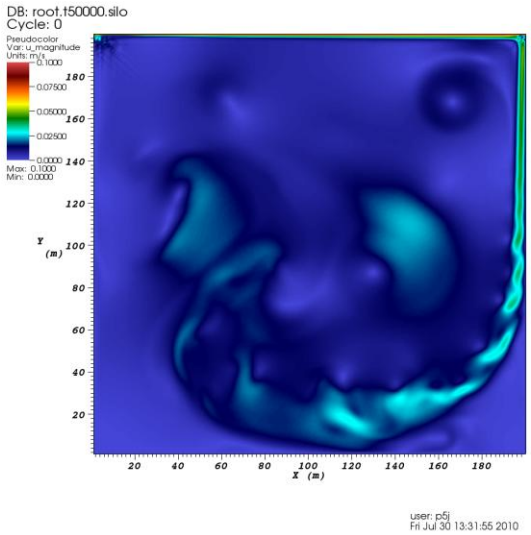
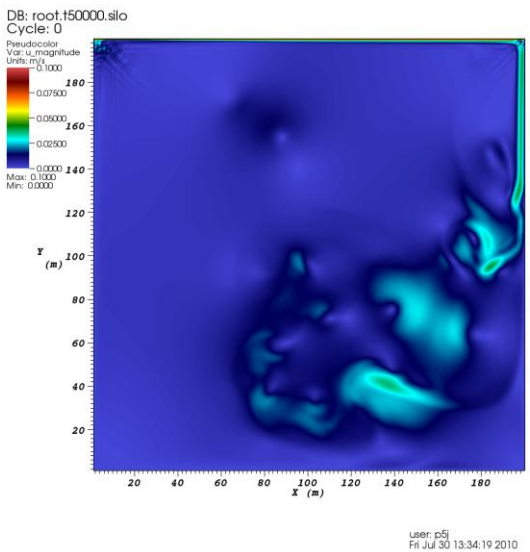
2D Lid Driven Cavity at Re = 12,000



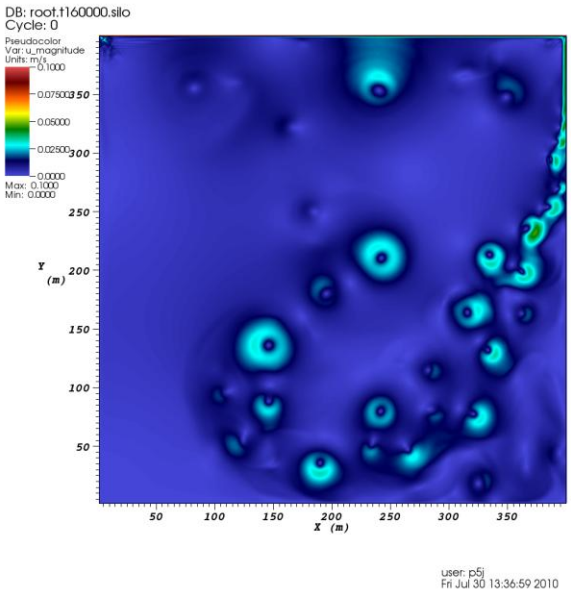
2D Lid Driven Cavity at High Re



Re = 60,000

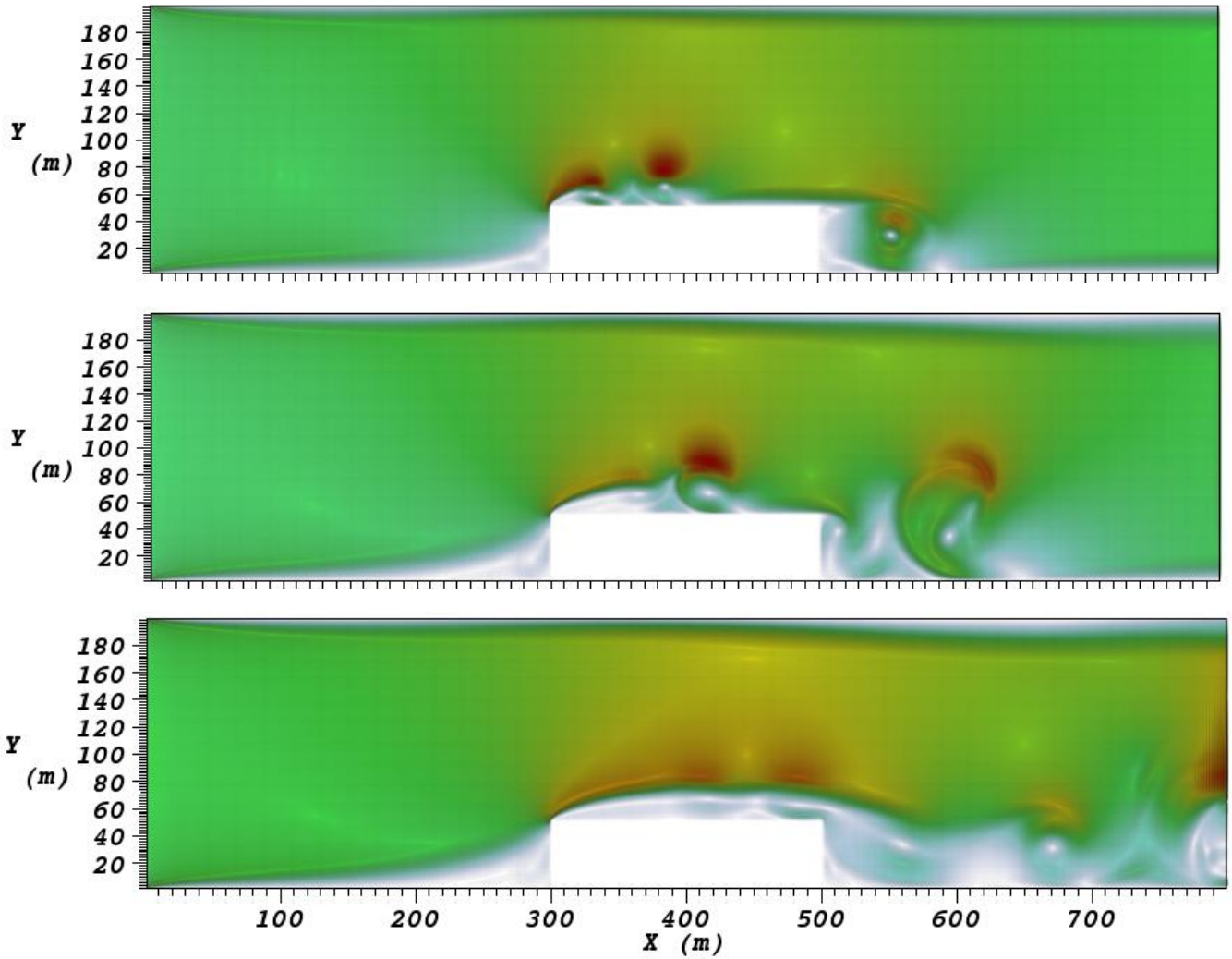


Re = 120,000



Re = 400,000

2D Flow past a boundary obstacle



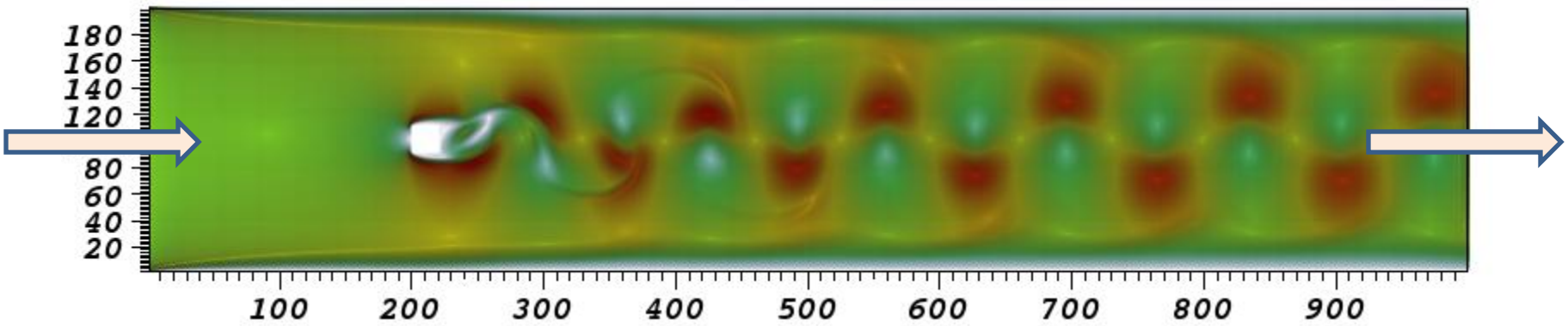
$t = t_1$

$t = t_2$

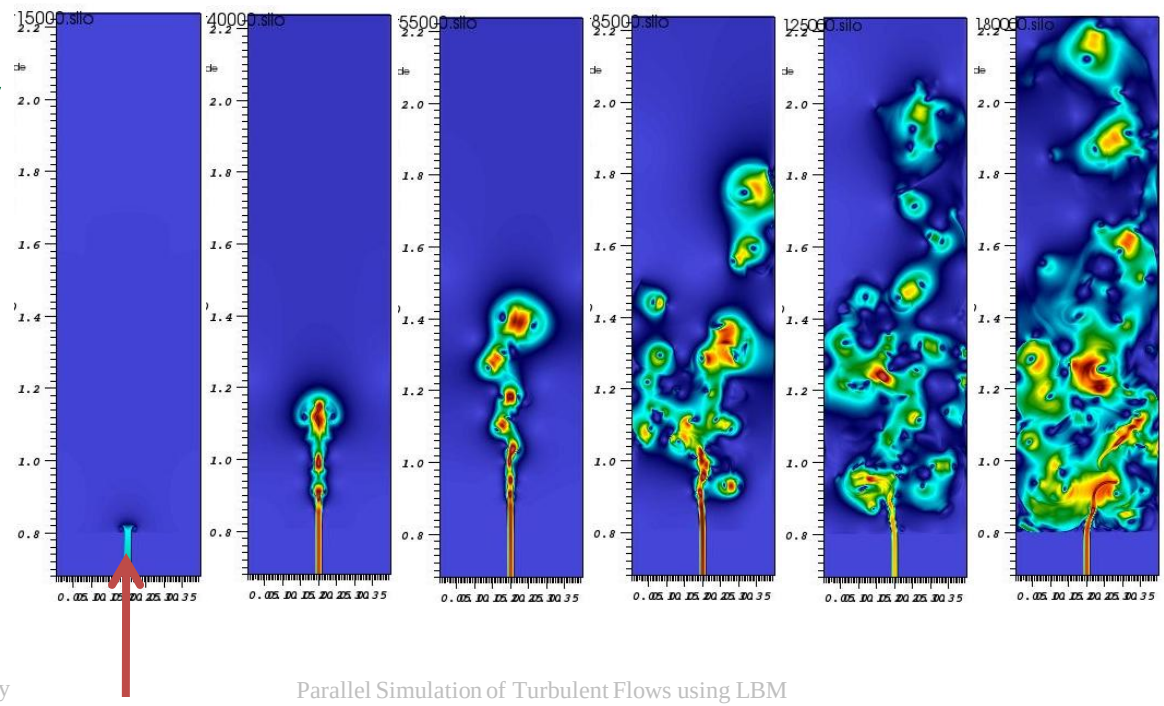
$t = t_3$

Temporal snapshots

Flow past a square obstacle



Jet Flow



Conclusions

- LBM can be a powerful alternative for turbulent flow simulations.
- Large-scale computing is necessary for such solvers. LBM-based turbulent flow solvers will not be available for desktop computing in near future.
- LBM is bringing out the qualitative physics correctly, however, more quantitative numerical verification and experimental validation is needed.
- Accuracy of LBM for general flow situations (in 3D, for realistic geometries) should be quantified (error margins etc.) and reported as compared to the available LES/DNS results.
- Robust thermal models should be developed to enable solution of conjugate heat transfer problems and thus, opening it up for realistic nuclear engineering applications.

Thank you for your attention.

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