

# Task parallel implementation of a DG solver for implicit kinetic relaxation schemes applied to fluid systems

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# Outline

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  - High order implicit DG scheme
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# Section 1

## Context and overall approach

## Target problem

### Typical problem

Unknowns "macroscopic" fields  $U(t, \mathbf{x}) : \mathbb{R}^{d+1} \rightarrow \mathbb{R}^{n_c}$  macroscopic fields.  
System of (mostly) hyperbolic conservation laws

$$\partial_t U + \partial_\alpha F^\alpha(U) = \left\{ \partial_\alpha \left[ \mathcal{D}^{\alpha\beta}(U) \partial_\beta U \right] + \mathcal{S} \right\}$$

$F^\alpha$  : fluxes (nonlinear) -  $\mathcal{D}$  : parabolic terms (diffusion),  $\mathcal{S}$  source term  
Systems of interest : Euler/Navier Stokes - MHD

### Numerical challenges

- explicit schemes
  - CFL conditions : time scale constrained by space grid
  - forces to resolve possibly unwanted fast times scales
- implicit schemes
  - large nonlinear system
  - costly matrix assembly/storage/inversion.

## Xin-Jin flux relaxation method

### Flux relaxation scheme

- each flux component is replaced by an additional new unknown  $W^\alpha$ .
- $W^\alpha$  linear transport (acoustic like system)
- relaxation of  $V^\alpha$  towards actual flux.

$$\begin{cases} \partial_t U + \partial_\alpha W^\alpha = 0 \\ \partial_t W^\alpha + A^{\alpha\beta} \partial_\beta U = \frac{R}{\varepsilon} (F^\alpha(U) - W^\alpha) \end{cases} \quad (1)$$

- operator splitting : linear transport step + local relaxation step.

### A divide and conquer strategy

- larger system  $n_c \times (d+1)$  but
  - non-locality is solved linearly (wave system)
  - non-linearity is local
- Caveats :
  - the splitting error generates diffusion/dispersion
  - all variables are still coupled in the wave system.

## Diagonalizing transport - the 1D case

Starting from the relaxation system

$$\partial_t \begin{pmatrix} U \\ V \end{pmatrix} + \underbrace{\begin{pmatrix} 0 & 1 \\ a^2 & 0 \end{pmatrix}}_T \partial_x \begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{R}{\varepsilon}(F(U) - V) \end{pmatrix}$$

Transport matrix  $T$  has eigenvalues  $\lambda_{\pm} = \pm|a|$  with eigenvectors  $f_{\pm} \propto [1, \pm a]^t$ .

$$\begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ a & -a \end{pmatrix} \begin{pmatrix} f_+ \\ f_- \end{pmatrix} \quad \begin{pmatrix} f_+ \\ f_- \end{pmatrix} = \frac{1}{2a} \begin{pmatrix} a & 1 \\ a & -1 \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix}$$

so that the system on  $f = [f_+, f_-]$  reads

$$\partial_t \begin{pmatrix} f_+ \\ f_- \end{pmatrix} + \begin{pmatrix} a & 0 \\ 0 & -a \end{pmatrix} \partial_x \begin{pmatrix} f_+ \\ f_- \end{pmatrix} = \begin{pmatrix} \frac{R}{\varepsilon} & 0 \\ 0 & \frac{R}{\varepsilon} \end{pmatrix} \begin{pmatrix} f_+^{eq}(U) - f_+ \\ f_-^{eq}(U) - f_- \end{pmatrix},$$

with the equilibrium functions  $f_{\pm}^{eq}(U) = \frac{U}{2} \pm \frac{F(U)}{2a}$ .

- the transport operator is **diagonal**
- simple advection with **constant** coefficient (no acoustics)
- in a op. splitting scheme  $f_+$  and  $f_-$  might be transported **independently**.

## Generic discrete kinetic relaxation scheme

Kinetic relaxation system [Nat98] [Bou99]

$$\partial_t f + \partial_\alpha V^\alpha f = \frac{\Omega}{\varepsilon} (f^{eq}(Pf) - f)$$

- a vector  $f$  of  $n_v$  kinetic fields  $f_i(t, \mathbf{x}), \mathbf{x} \in \mathbb{R}^d$
  - $n_v$  constant velocities  $\mathbf{v}_i \in \mathbb{R}^d$  and  $d$  diagonal matrices  $V^\alpha, \alpha = x, y, \dots$  with  $V_{ij}^\alpha = \delta_{ij} v_i^\alpha$
  - a  $n_c \times n_v$  ( $n_c < n_v$ ) matrix  $P$  mapping  $f$  to the macroscopic fields vector  $U = Pf$ , with  $U \in \mathbb{R}^{n_c}$ .
  - an equilibrium vector operator  $f^{eq} : \mathbb{R}^{n_c} \rightarrow \mathbb{R}^{n_v}$  such that  $Pf^{eq}(Pf) = Pf, \forall f$ .
  - a  $n_v \times n_v$  relaxation matrix  $\Omega$
  - $U$  conserved during relaxation i.e  $P\Omega g = 0, \forall g \in \text{Ker}P$ .
- 
- Applying  $P$  and  $\varepsilon \rightarrow 0$  :  $\partial_t(Pf^{eq}(Pf)) + \partial_\alpha P V^\alpha f^{eq}(Pf) = 0$
  - consistent with  $\partial_t U + \partial_\alpha F^\alpha(U) = 0$  provided

$$C \begin{cases} Pf^{eq}(U) = U \\ P V^\alpha f^{eq}(U) = F^\alpha(U), \alpha = x, y, \dots \end{cases}$$

## 1D simple example - Euler with standard $D1Q3$ scheme

Model notation :  $DdQq$  from Lattice Boltzmann Method scheme with  $q = n_v$

Macroscopic system : still Euler isothermal

$$\begin{cases} \partial_t \rho + \partial_x q = 0 \\ \partial_t q + \partial_x \left( \frac{q^2}{\rho} + \rho c^2 \right) = 0 \end{cases}$$

- $n_c = 2$  macroscopic fields  $U = (\rho, q = \rho u)$ .
- $n_v = 3$  the velocity set is  $(-\lambda, 0, \lambda)$ .
- $V^x = \text{diag}[\lambda, 0, -\lambda]$

- $P = \begin{pmatrix} 1 & 1 & 1 \\ -\lambda & 0 & \lambda \end{pmatrix} P V^x = \begin{pmatrix} -\lambda & 0 & \lambda \\ \lambda^2 & 0 & \lambda^2 \end{pmatrix}$

- note that  $\text{rank}(C) = 3$ .

- equilibrium function

$$f^{eq} = \left[ \frac{\rho}{2\lambda^2} (u^2 + c^2 - \lambda u), \frac{\rho}{\lambda^2} (\lambda^2 - u^2 - c^2), \frac{\rho}{2\lambda^2} (u^2 + c^2 + \lambda u) \right]^t$$



1D simple example- Euler with "vectorial" simplicial scheme  $2 \times D1Q2$ 

Macroscopic system

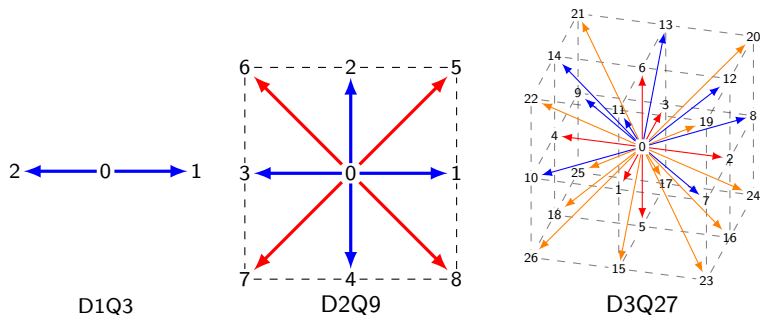
$$\begin{cases} \partial_t \rho + \partial_x q & = 0 \\ \partial_t q + \partial_x \left( \frac{q^2}{\rho} + \rho c^2 \right) & = 0 \end{cases}$$

- $n_c = 2$  macroscopic fields  $U = (\rho, q = \rho u)$ .
- $n_v = 4$ , for each scalar field the velocity set is  $(-\lambda, \lambda)$ .
- $P = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix}$
- $V^x = \text{diag}[\lambda, -\lambda, \lambda, -\lambda]$
- equilibrium function (generic form) :  $f_{k,i}^{eq} = \frac{U_k}{2} + \frac{1}{2\lambda^2} F_k(U) \cdot v_{k,i}$ .
- equilibrium function  $f^{eq} = \left[ \frac{\rho}{2} + \frac{q}{2\lambda}, \frac{\rho}{2} - \frac{q}{2\lambda}, \frac{q}{2} + \frac{q^2/\rho + \rho c^2}{2\lambda}, \frac{q}{2} - \frac{q^2/\rho + \rho c^2}{2\lambda} \right]^t$
- adding a stationary ( $v = 0$ ) nodes for each scalar quantity is straightforward. With arbitrary  $f_{\rho,0}^{eq}(U), f_{q,0}^{eq}(U)$  we have

$$f^{eq} = \left[ \frac{\rho - f_{\rho,0}^{eq}}{2} + \frac{q}{2\lambda}, \frac{\rho - f_{\rho,0}^{eq}}{2} - \frac{q}{2\lambda}, \frac{q - f_{q,0}^{eq}}{2} + \frac{q^2/\rho + \rho c^2}{2\lambda}, \frac{q - f_{q,0}^{eq}}{2} - \frac{q^2/\rho + \rho c^2}{2\lambda} \right]^t$$

## Standard Lattice Boltzmann models

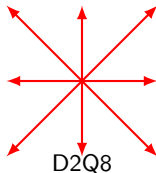
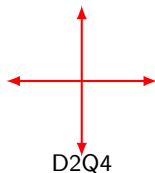
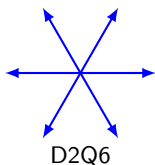
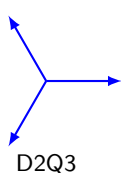
Notation :  $DdQq$  with  $d = 1, 2, 3$  space dimension  $q$  number of velocities.



- $P$  built from low-order polynomials : macro quantities are moments.
- splitting error generates diffusive terms : can mimic physical diffusion
- Can be applied to any hyperbolic system of conservations laws (fluid mechanics [CD98], Maxwell [Gra14], MHD [Del02], etc.)
- transport is exact : regular mesh generated from the velocity set (translation group)
- transport is easy but  $\Delta t/\Delta x$  linked : integer CFL-like condition

## "Vectorial" kinetic model

- Rationale : for some hyperbolic system of interest (eg MHD ), macroscopic variables cannot be considered as moments of various order of the same discrete kinetic set (ie.  $\mathcal{C}$  is structurally unsolvable).
- Basic idea : one (small) set of  $q$  velocities  $\mathbf{v}_{k,i}$  per scalar macroscopic field  $U_k$ .
- the velocity sets need not be the same for each  $U_k$ .
- $P$  has a block diagonal structure :  $1 \leq k \leq n_c : U_k = \sum_{i=1}^{q_k} f_{k,i}$ . (all scalar fields are  $0^{th}$  order moments.
- examples:
  - minimal set for solvability : a  $d$  simplex,  $q = d + 1$  velocities. (D1Q2,D2Q3,D3Q4)
  - velocity pairs along cartesian axes :  $q = 2d$  (D1Q2; D2Q4,D3Q6)
- more complex sets can be obtained by adding velocities : "arbitrary" , zero velocity node, scaled, rotated sets...
- strike a balance between number of velocities and artifacts (anisotropy...)



## Chapman-Enskog expansion

Micro/Macro splitting : we write  $f = f^{eq}(U) + g$ , with  $U = Pf \in \mathbb{R}^{n_c}$  and  $g \in \text{Ker}P$ .

$$\begin{cases} \partial_t U + \partial_\alpha P V^\alpha f^{eq}(U) = -\partial_\alpha P V^\alpha g \\ \partial_t g + \partial_\alpha V^\alpha g = -\Omega g - [\partial_U f^{eq} \partial_t U + V^\alpha \partial_U f^{eq} \partial_\alpha U] \end{cases}$$

Expansion up to first order of  $U = U_0 + \varepsilon U_1 + \mathcal{O}(\varepsilon^2)$  and  $g = \varepsilon g_1 + \mathcal{O}(\varepsilon^2)$  yields

$$\partial_t U + \partial_\alpha F^\alpha(U) = \varepsilon \partial_\alpha \left\{ \underbrace{P V^\alpha \Omega^{-1} [V^\beta \partial_U f^{eq} - \partial_U f^{eq} \partial_U F^\beta]}_{D^{\alpha\beta}} \partial_\beta U \right\} + \mathcal{O}(\varepsilon^2)$$

In the BGK case ( $\Omega = I$ ) the diffusion tensor reads

$$D^{\alpha\beta} = P V^\alpha V^\beta \partial_U f^{eq} - \partial_U F^\alpha \partial_U F^\beta$$

- dissipation criterion  $X^t D^{\alpha\beta} X \geq 0, X \in \mathbb{R}^{n_c}$  constrains the velocity scale  $\lambda$  of  $V^\alpha$ .
- the diffusion term of a discrete first order time implicit scheme has the same structure.
- at finite but small  $\varepsilon$ ,  $D^{\alpha\beta}$  can be used to mimic (small) physical diffusion.

## Comparison with Xin-Jin scheme

For  $d > 1$  is the kinetic system still equivalent to the Xin-Jin relaxation scheme ?

- Compare Xin-Jin system on the variables/flux pairs  $U, W^\alpha$  to the kinetic system on  $(Pf, PV^\alpha f)$  assuming only  $Pf^{eq}(U) = U$  and  $PV^\alpha f^{eq}(U) = F^U$ .
- equation on the conserved variables

$$\partial_t U + \partial_\alpha W^\alpha = 0 \quad \text{vs} \quad \partial_t Pf + \partial_\alpha PV^\alpha f$$

- equation on the discrete flux variables

$$\partial_t W^\alpha + B^{\alpha\beta} \partial_\beta U = \frac{R}{\varepsilon} (F^\alpha(U) - W^\alpha) \quad \text{vs} \quad \partial_t (PV^\alpha f) + \partial_\beta PV^\alpha V^\beta f = \frac{PV^\alpha \Omega}{\varepsilon} (f^{eq} - f)$$

- diffusion term from Chapman-Enskog expansion  $\varepsilon \partial_\alpha [D^{\alpha\beta} \partial_\beta U]$

$$D^{\alpha\beta}(U) = \Omega^{-1} [a^2 B^{\alpha\beta} - \partial_U F^\alpha \partial_U F^\beta] \quad \text{vs} \quad D^{\alpha\beta}(U) = PV^\alpha \Omega^{-1} [V^\beta \partial_U f^{eq} - \partial_U f^{eq} \partial_U F^\beta]$$

### Remarks

- overall structure is similar
- all the transport structure is fixed by the choice of velocity basis.
- dissipation criterion on velocity scale  $\lambda$ .

## Back to our example

*D1Q3* model

$$D = \begin{bmatrix} 0 & 0 \\ 2u(u^2 - c^2) & \lambda^2 - c^2 - u^2 \end{bmatrix}$$

Dissipation condition

$$\lambda^2 \geq c^2 + u^2$$

*2D1Q2* vectorial model

$$D = \begin{bmatrix} -c^2 + 2\lambda^2 + u^2 & -2u \\ 2u(-c^2 + u^2) & -c^2 + 2\lambda^2 - 3u^2 \end{bmatrix}$$

Dissipation condition

$$\lambda^2 \geq (c \pm u)^2$$

Trade-off on the choice of  $\lambda$

- sufficiently large to ensure dissipation (avoid anti-diffusion)
- sufficiently small to avoid over-diffusion (and dispersion...)

## Section 2

### Space discretization - transport scheme

# Transport schemes

## Whishlist

- complex geometry, curved meshes
- flexibility  $h - p$  refinement
- cfl-free
- efficiency

## Candidates

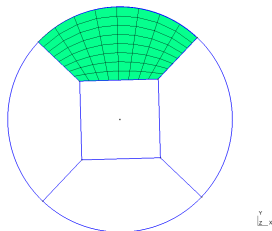
- finite volumes
- discontinuous galerkin
- semi-lagrangian
- stochastic schemes (Glimm)



# DG - Implicit upwind transport scheme 1

We consider a coarse mesh made of hexahedral curved macrocells

- Each macrocell is itself split into smaller subcells of size  $h$ .
- In each subcell  $L$  we consider polynomial basis functions  $\psi_k^L$  of degree  $p$ .
- Expansion on the polynomial basis: discontinuous approximation of  $f$ .



$$f(x, v, p\Delta t) \simeq f_L^p(x, v) = \sum_k f_{L,k}^p(v) \psi_k^L(x), \quad x \in L.$$

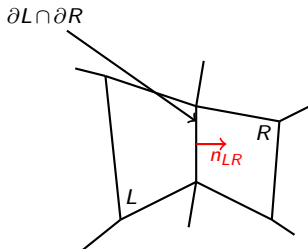
## DG - Implicit upwind transport scheme 2

### Implicit DG approximation scheme

$\forall L, \forall k$

$$\int_L \frac{f_L^p - f_L^{p-1}}{\Delta t} \psi_k^L - \int_L v \cdot \nabla \psi_k^L f_L^p + \int_{\partial L} (v \cdot n^+ f_L^p + v \cdot n^- f_R^p) \psi_k^L = 0.$$

- time step index:  $p$
- $R$  denotes the neighbor cells along  $\partial L$ .
- $v \cdot n^+ = \max(v \cdot n, 0)$ ,  
 $v \cdot n^- = \min(v \cdot n, 0)$ .
- $n_{LR}$  is the unit normal vector on  $\partial L$  oriented from  $L$  to  $R$ .



### Features

- implicit scheme , unconditionally stable ,  $(h, p)$  refinement
- requires a priori the resolution of a large linear system for each  $v$ .

## Getting high order in time : symmetric splitting

Bibliography: [MQ02]

### Splitting schemes made of **symmetric** building blocks

All steps implemented as  $\theta$  weighted schemes: setting  $\theta = 1/2$  (Crank-Nicolson)  $\rightarrow$  symmetric

- Transport (T)
- Macroscopic source (S)
- BGK Relaxation (R).

$1^{st}$ order	$T(\Delta t)$	$S(\Delta t)$	$R(\Delta t)$			
$2^{nd}$ order	$T(\Delta t/2)$	$R(\Delta t/2)$	$S(\Delta t)$	$R(\Delta t/2)$	$T(\Delta t/2)$	
$2^{nd}$ order collapsed	$R(\Delta t/2)$		$S(\Delta t)$	$R(\Delta t/2)$	$T(\Delta t)$	

### Beyond second order : composition methods

Using the  $2^{nd}$  order scheme as a basic building block, we can build higher-order time schemes using composition methods [KL97] [Suz90]

Example : Suzuki  $4^{th}$  order fractal scheme with 5 fractional substeps  $\gamma_i \Delta t$  with  $\gamma_0 = \gamma_1 = \gamma_3 = \gamma_4 = (4 - 4^{1/3})^{-1}$  and  $\gamma_2 = -4^{1/3}(4 - 4^{1/3})^{-1}$ .

## Section 3

### Task-Based parallel solver

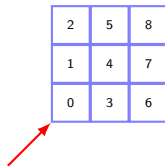
## The benefits of upwinding

upwind flux  $\rightarrow$  data dependencies follow the (constant) velocity

- transport operator can be cast into Block Triangular Form (BTF) by appropriate data renumbering.
- inversion : BTF + inversion of diagonal blocks.
- data blocks at the subcell scale : too small for efficient parallelism.

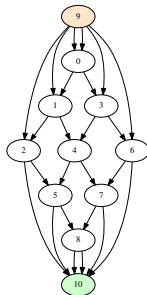
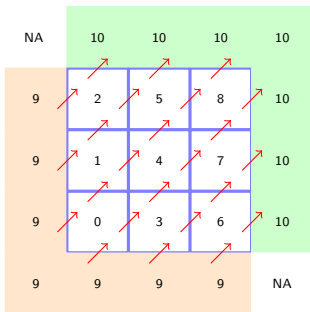
Coarse grain block structure at macrocell level

- $L$  is *upwind* with respect to  $R$  if  $v \cdot n_{LR} > 0$  on  $\partial L \cap \partial R$ .
- In a cell  $L$ , the solution depends only on the values of  $f$  in the upwind macrocells.



## Dependency graph

For a given velocity  $v$  we can build a dependency graph. Vertices are associated to macrocells and edges to macrocells interfaces or boundaries. We consider two fictitious additional vertices: the “upwind” vertex and the “downwind” vertex.

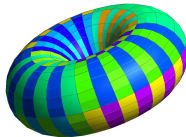


- The dependency graph yields a coarse block triangular ordering
- the local system in each macrocell is solved "on the fly" using the KLU library.
- no need to assemble, store, and factorize the global system.

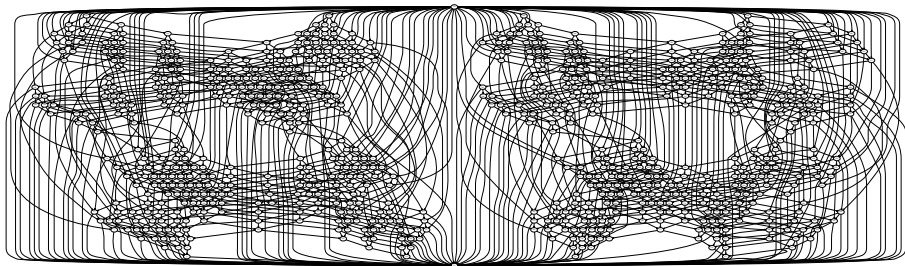
# Transport solver parallelism

- ideal across velocities (uncoupled)
- across macrocells : can be high but load imbalance
- realistic mesh : complex to manage...

Toroidal mesh - 720 macrocells



Toroidal mesh - transport graph for  $(1, 0, 0)$  velocity.



We need smart task scheduling

## Kirsch : Task-Based parallel DG-LBM solver

Here comes StarPU(<http://starpu.gforge.inria.fr>)

- StarPU is a task-based scheduling library developed at Inria Bordeaux
- Task description : codelets, inputs (R), outputs (W or RW).
- The user submits tasks in a correct sequential order.
- StarPU schedules the tasks in parallel if possible.
- MPI extension easy : dispatch data and declare owner process : communications handled transparently.

SCHNAPS + StaRPU + Kinetic Schemes = KIRSCH

- starting point SCHNAPS : general DG explicit solver.
- StarPU + Optimization for Kinetic Relaxation schemes
- KIRSCH : Kinetic Representation for SCHnaps

KIRSCH design

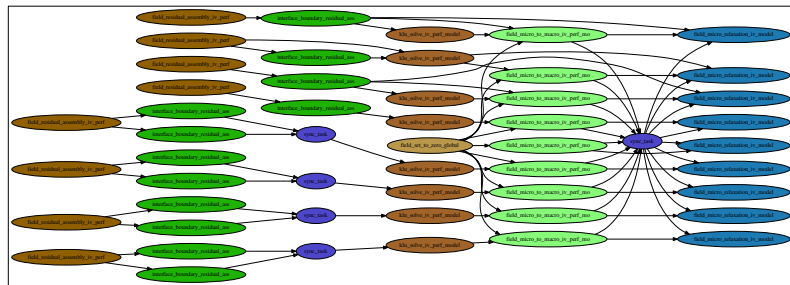
- base ops : transport(T), relaxation(R), sources (S) weighted implicit integrators.
- each op encapsulated in a StarPU codelet.
- physics in the equilibrium functions : flexibility.
- high order time schemes are built from second order blocks.



# What StarPU does for us

## Task graph for D2Q9 model

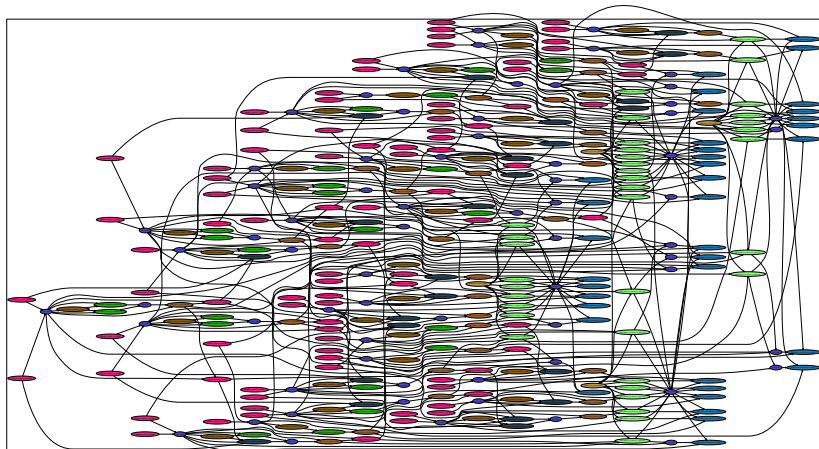
- a single 2D macrocell
- a single time step of the first order scheme ( T + R )



Pretty simple...

## What StarPU does for us

- 4 macrocells in a 2D square
- a single time step of the first order scheme ( T + R)



Slightly more complicated....

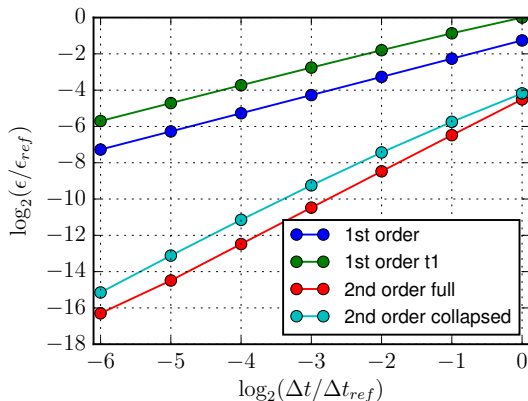
## Section 4

### Some numerical results

## Euler gravity stationary

- D2Q9 model ,Euler stationary state in a constant gravity field  $\mathbf{g} = g\mathbf{e}_y$ .
- Analytical solution  $\rho = \rho_0 e^{-gy/T}$

$\Delta t$  Convergence of  $L_2$  error on macroscopic data wrt analytical solution.

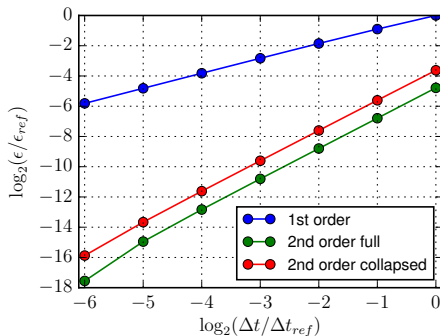


First order t1 : first order splitting with fully implicit  $\theta = 1$  blocks.

First order : first order splitting with  $\theta = 1/2$  second order symmetric blocks.

## Euler Gaussian pulse

- D2Q9 model on a square :  $8 \times 8$  elements,  $10 \times 10$  subcells,  $3^{\text{rd}}$  order
- Initial condition : narrow gaussian density bump  $\rho = 1 + 0.1 \exp(-40 * (x^2 + y^2))$ .
- Convergence evaluated from highly time-resolved solution.



## Drifting MHD stationary vortex : $7 \times D2Q4$

$$\text{Basic MHD} \quad \left\{ \begin{array}{l} \partial_t \rho + \nabla \cdot \rho \mathbf{u} = 0 \\ \partial_t \rho \mathbf{u} + \nabla \cdot \left[ \rho \mathbf{u} \mathbf{u} + \left( \rho + \frac{B^2}{2} \right) \mathbf{I} - \mathbf{B} \mathbf{B} \right] = 0 \\ \partial_t Q + \nabla \cdot \left[ \left( Q + \rho + \frac{B^2}{2} \right) \mathbf{u} - (\mathbf{B} \cdot \mathbf{u} \mathbf{B}) \right] = 0 \\ \partial_t \mathbf{B} + \nabla \cdot (\mathbf{B} \mathbf{u} - \mathbf{u} \mathbf{B} + \psi \mathbf{I}) = 0 \\ \partial_t \psi + \nabla \cdot (c_h^2 \mathbf{B}) = 0 \end{array} \right.$$

(+divergence cleaning)

Closure

$$p = (\gamma - 1) \rho e = (\gamma - 1) \left[ Q - \rho \frac{u^2}{2} + \frac{B^2}{2} \right]$$

Simple 2D stationary solution (azimuthal symmetry) + constant drift velocity

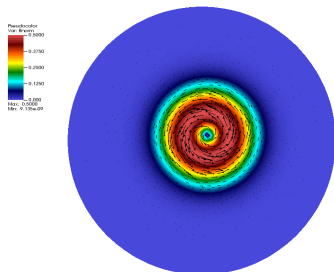
$$\left\{ \begin{array}{l} \rho = \rho_0 \\ \mathbf{u} = u_0 [\mathbf{u}_{drift} + h(r) \mathbf{e}_\vartheta] \\ \mathbf{B} = b_0 h(r) \mathbf{e}_\vartheta \\ p(r) = p_0 + \frac{b_0^2}{2} (1 - h^2(r)) \\ b_0^2 = \rho u_0^2 \end{array} \right.$$

expressed in cylindrical coordinates in the drifting frame ( $\mathbf{r}_0 = \mathbf{u}_{drift} t$ ).

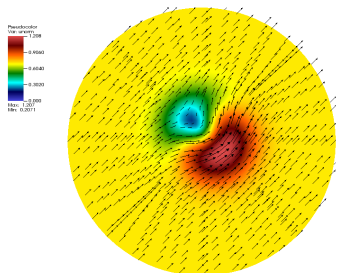
## 2D MHD drifting vortex

Parameters :  $\rho = 1.0, p_0 = 1, u_0 = b_0 = 0.5, \mathbf{u}_{drift} = [1, 1]^t, h(r) = \exp[(1 - r^2)/2]$

Magnetic field



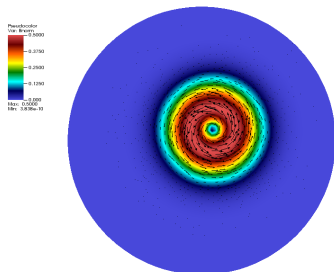
Velocity



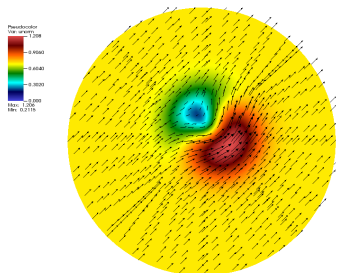
## 2D MHD drifting vortex

Parameters :  $\rho = 1.0, p_0 = 1, u_0 = b_0 = 0.5, \mathbf{u}_{drift} = [1, 1]^t, h(r) = \exp[(1 - r^2)/2]$

Magnetic field



Velocity

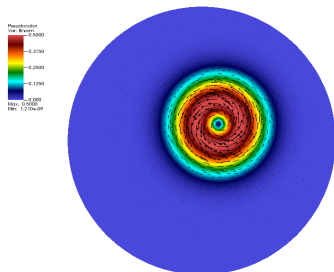




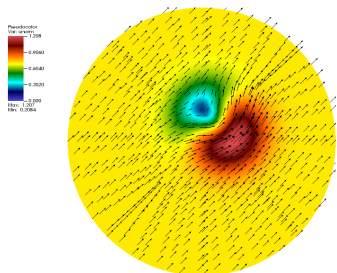
## 2D MHD drifting vortex

Parameters :  $\rho = 1.0, p_0 = 1, u_0 = b_0 = 0.5, \mathbf{u}_{drift} = [1, 1]^t, h(r) = \exp[(1 - r^2)/2]$

Magnetic field



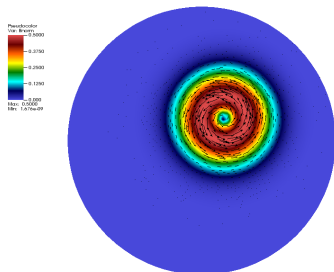
Velocity



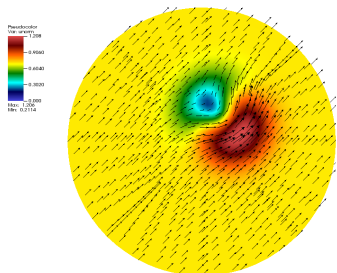
## 2D MHD drifting vortex

Parameters :  $\rho = 1.0, p_0 = 1, u_0 = b_0 = 0.5, \mathbf{u}_{drift} = [1, 1]^t, h(r) = \exp[(1 - r^2)/2]$

Magnetic field



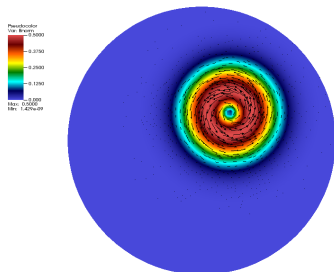
Velocity



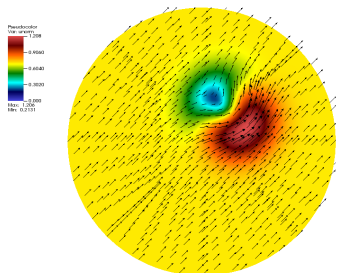
## 2D MHD drifting vortex

Parameters :  $\rho = 1.0, p_0 = 1, u_0 = b_0 = 0.5, \mathbf{u}_{drift} = [1, 1]^t, h(r) = \exp[(1 - r^2)/2]$

Magnetic field



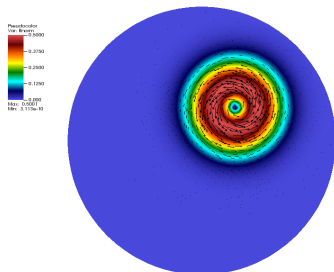
Velocity



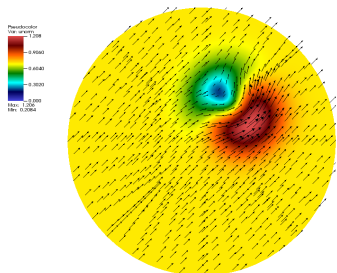
## 2D MHD drifting vortex

Parameters :  $\rho = 1.0, p_0 = 1, u_0 = b_0 = 0.5, \mathbf{u}_{drift} = [1, 1]^t, h(r) = \exp[(1 - r^2)/2]$

Magnetic field



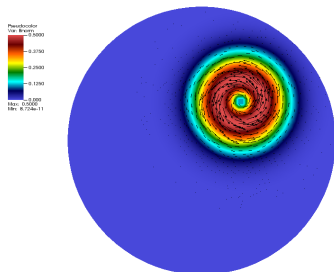
Velocity



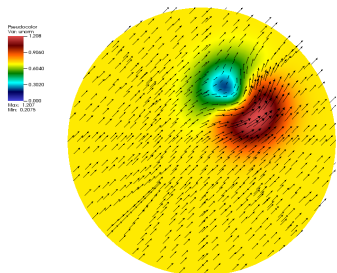
## 2D MHD drifting vortex

Parameters :  $\rho = 1.0, p_0 = 1, u_0 = b_0 = 0.5, \mathbf{u}_{drift} = [1, 1]^t, h(r) = \exp[(1 - r^2)/2]$

Magnetic field



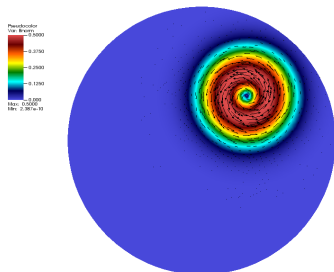
Velocity



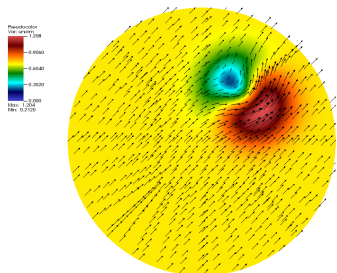
## 2D MHD drifting vortex

Parameters :  $\rho = 1.0, p_0 = 1, u_0 = b_0 = 0.5, \mathbf{u}_{drift} = [1, 1]^t, h(r) = \exp[(1 - r^2)/2]$

Magnetic field



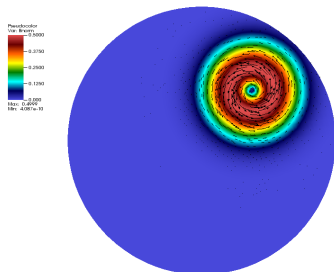
Velocity



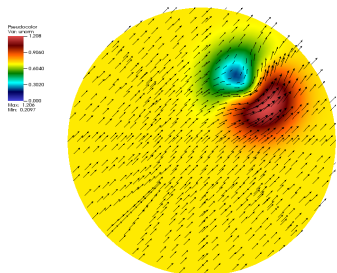
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Parameters :  $\rho = 1.0, p_0 = 1, u_0 = b_0 = 0.5, \mathbf{u}_{drift} = [1, 1]^t, h(r) = \exp[(1 - r^2)/2]$

Magnetic field



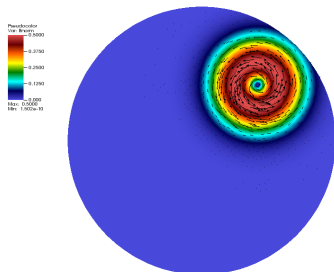
Velocity



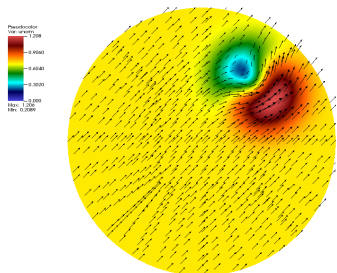
## 2D MHD drifting vortex

Parameters :  $\rho = 1.0, p_0 = 1, u_0 = b_0 = 0.5, \mathbf{u}_{drift} = [1, 1]^t, h(r) = \exp[(1 - r^2)/2]$

Magnetic field



Velocity

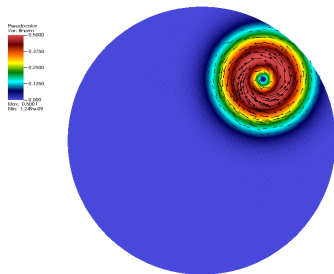




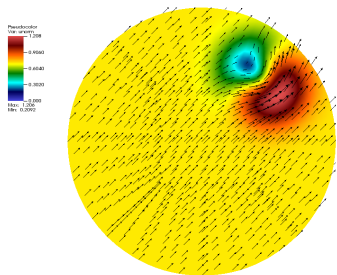
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Parameters :  $\rho = 1.0, p_0 = 1, u_0 = b_0 = 0.5, \mathbf{u}_{drift} = [1, 1]^t, h(r) = \exp[(1 - r^2)/2]$

Magnetic field



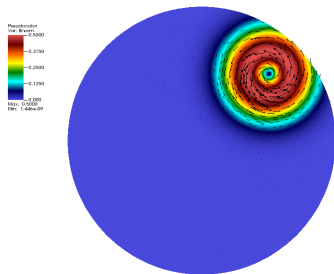
Velocity



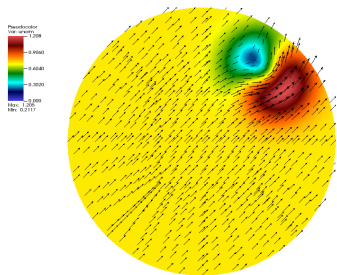
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Magnetic field



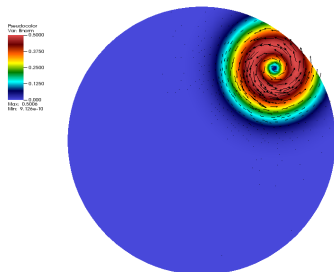
Velocity



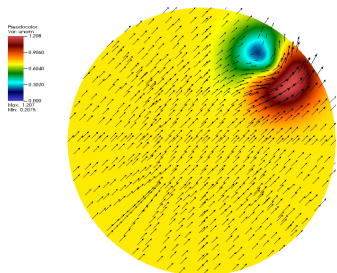
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Magnetic field



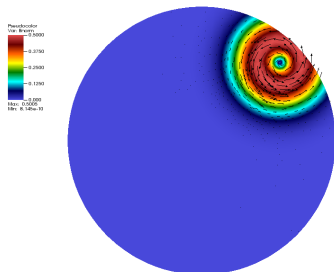
Velocity



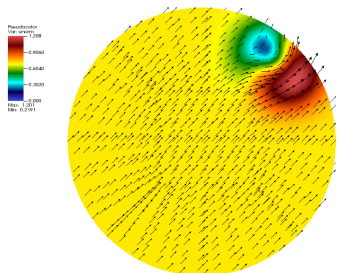
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Magnetic field



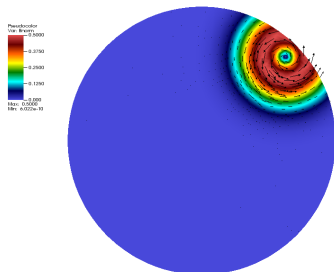
Velocity



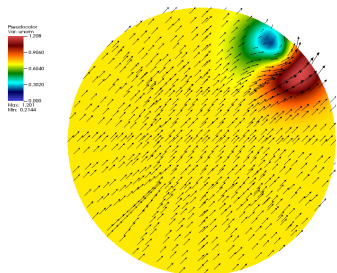
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Magnetic field



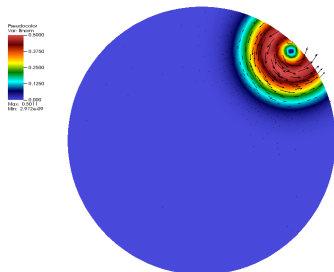
Velocity



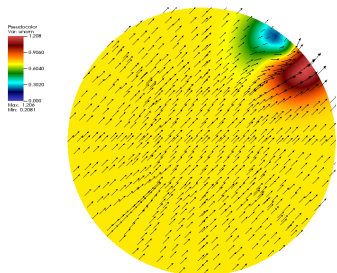
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Parameters :  $\rho = 1.0, p_0 = 1, u_0 = b_0 = 0.5, \mathbf{u}_{drift} = [1, 1]^t, h(r) = \exp[(1 - r^2)/2]$

Magnetic field



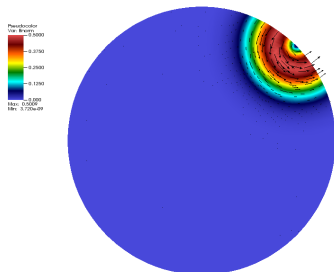
Velocity



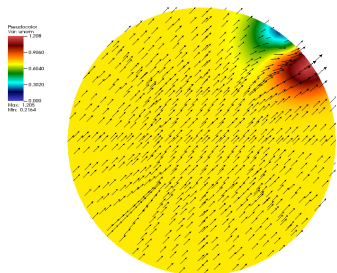
## 2D MHD drifting vortex

Parameters :  $\rho = 1.0, p_0 = 1, u_0 = b_0 = 0.5, \mathbf{u}_{drift} = [1, 1]^t, h(r) = \exp[(1 - r^2)/2]$

Magnetic field



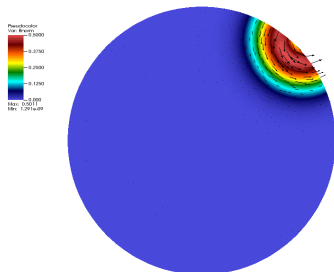
Velocity



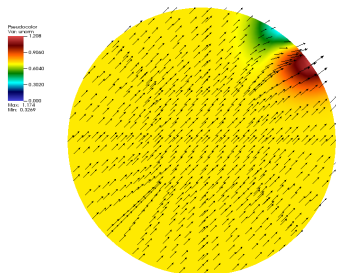
## 2D MHD drifting vortex

Parameters :  $\rho = 1.0, p_0 = 1, u_0 = b_0 = 0.5, \mathbf{u}_{drift} = [1, 1]^t, h(r) = \exp[(1 - r^2)/2]$

Magnetic field



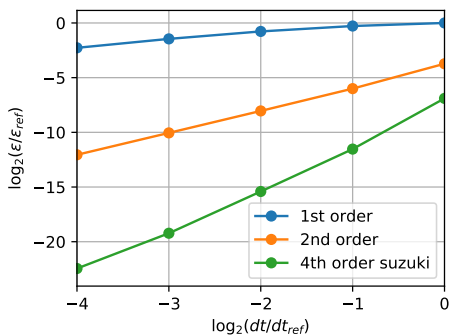
Velocity





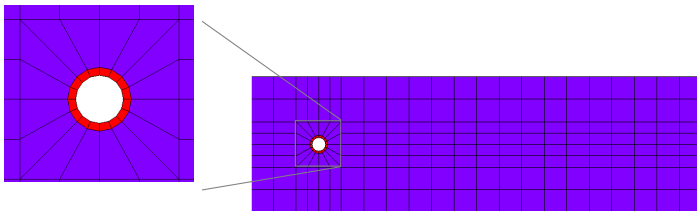
## MHD drifting vortex : time order check

- 2D disk mesh : 20 macro-elements
- refinement 8 , degree 5 : 2304 quadrature points per element
- six scalar fields (no div B cleaning)
- $dt$  ranges from  $dt_{ref} = 0.2$  to  $dt = 0.006250$
- $hmin \approx 0.02$  , discrete velocities norm  $\|v_i\| = 4$ ;



## 2D flow around a cylinder

- D2Q9 model for Isothermal Euler
- mesh is adapted to the geometry of the obstacle
- no-slip ( $u = 0$ ) condition on the obstacle imposed using a penalization method in a small volume (red ring)
  - relaxation of each  $f_i$  towards  $0.5(f_i + f_{\bar{i}})$  where  $v_{\bar{i}} = -v_i$ .
  - with CN scheme and ( $\tau = 0$ )  $\rightarrow$  "bounce-back" operator : simply swap  $f_i$  values between opposite velocities.
- imposed state at boundaries with constant low Mach flow.



- imposed velocity field at inlet  $u \approx 0.07c$ .
- finite  $\tau = 0.0001$ .

Velocity field norm



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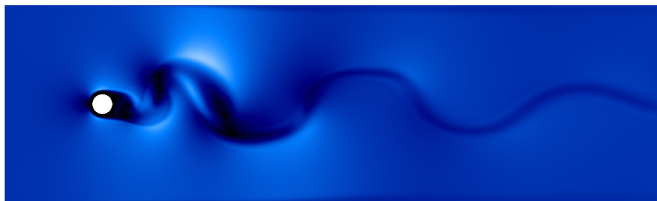
- imposed velocity field at inlet  $u \approx 0.07c$ .
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Velocity field norm



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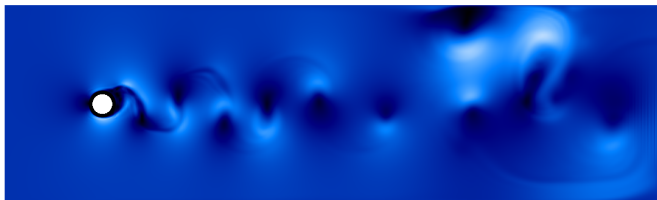
Velocity field norm





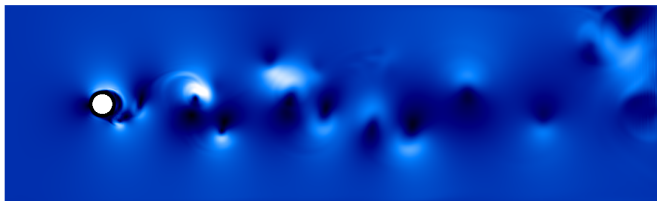
- imposed velocity field at inlet  $u \approx 0.07c$ .
- finite  $\tau = 0.0001$ .

Velocity field norm



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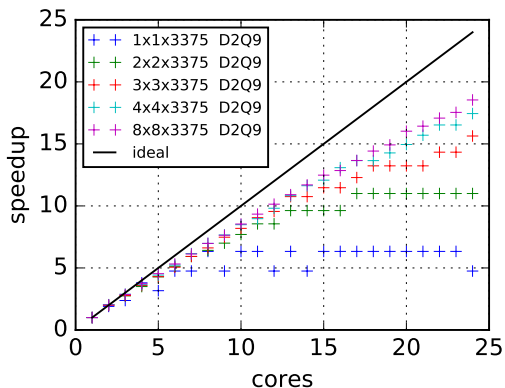
Velocity field norm



## D2Q9 multithread performance

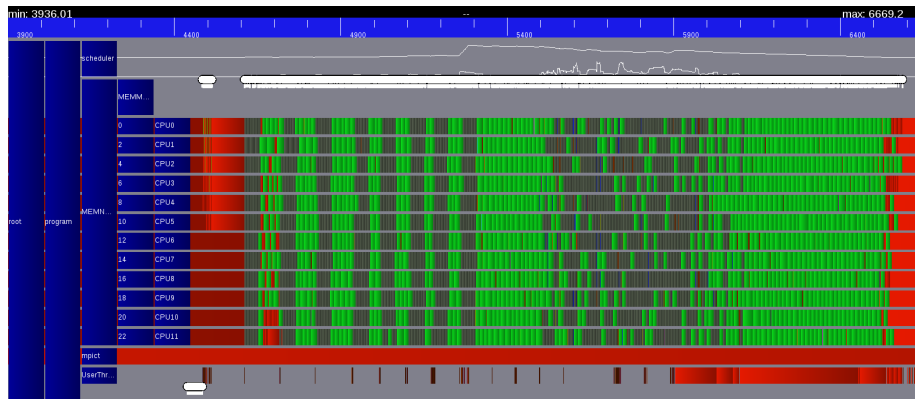
Full D2Q9 scheme on square grids. Constant dof number per macrocell. Number  $N$  of macrocells  $N$  from 1 to  $64 = 8 \times 8$ .

- for 1 macrocell : saturation at  $n_{core} = n_v$ . This is expected.
- efficiency grows with  $N$  due to topological parallelism.



# Gantt diagram

## D2Q9 model - 12 threads



Low overhead - low sleep/idle time (in red)

## Gantt diagram

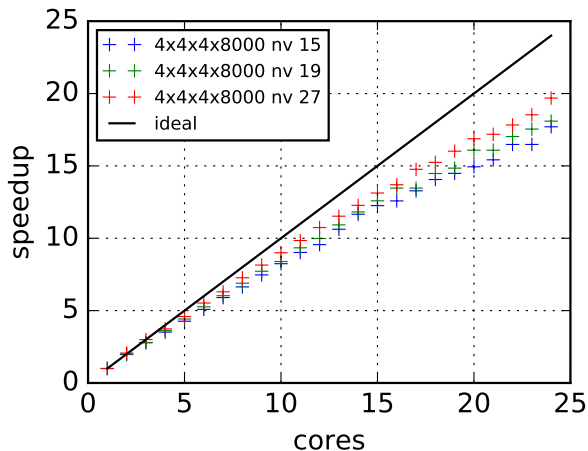
8x8 square - D2Q9 model - 24 threads



No enough work to do !

## D3Q\* multithread performance

D3Q15, D3Q19, D3Q27 models on a cube with  $4 \times 4 \times 4$  elements and 8000 dof per elements with eager scheduler.



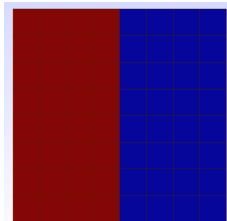
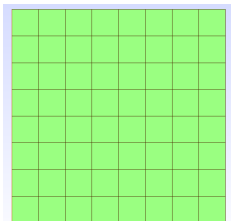
## Preliminary MPI scalings : D2Q9

Irma Atlas : 4 nodes - 24 CPU per node

D2Q9 model square  $8 \times 8$  elts  $\times 3200$  dof

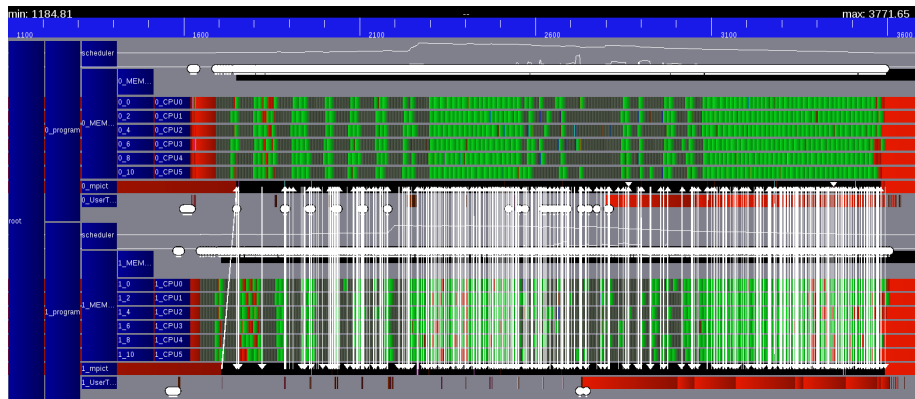
Wall time (s) for 100 iterations

Nmpi/Nthreads	8	12	24
1	153	105	92
2	75	52	95



## Gantt diagram

D2Q9 model - 2x6 threads



Low overhead/sleep time



## Gantt diagram

8x8 square - D2Q9 model - 2x12 threads



Again : not enough work to do !

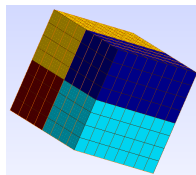
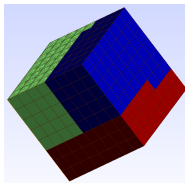
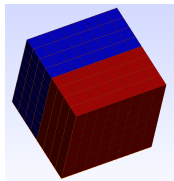
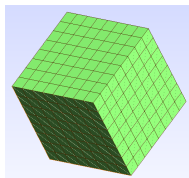
## MPI scalings : D3Q15

D3Q15 - 4x4x4x8000 cubic macromesh - 50 iterations -Wall time (s)

Nthreads/Nmpi	1	2	3
10	303	151	103
15	207	105	71

D3Q15 8x8x8x4096 cubic macromesh 50 iterations - Wall time (s)

Nthreads/Nmpi	1	2	3	4
14	1290	752	409	312

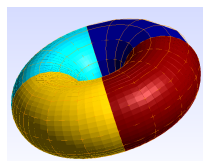
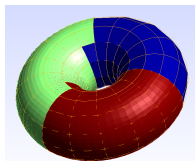
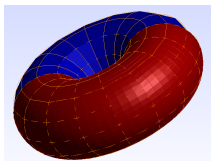
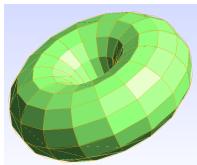


## MPI Scaling : D3Q15 in a torus

Toroidal mesh : 720 macroelements  $\times$  3335 dof  
 2064 interfaces - 192 boundary faces

Wall time in sec for 100 iterations.

Nthreads/Nmpi	1	2	3	4
14	6862	2772	1491	1014



## Section 5

## Conclusions

## Advantages

- resolution of a set of simple independent problems (divide and conquer)
- major cost stems from transport solver DG OK, other solvers must be tried (SL, particle, ....)
- (very) low storage implicit solvers.
- high order in time.

## Challenging points on the theory side / Ongoing Work on model generation

- stability/consistency/error control conditions are complex, particularly at high order
- adapt entropy based methods to vectorial models [Bou99] [Dub13].
- use 0 velocity nodes to perform better for stationary states.

## Drawbacks (no free lunch)

- similar to relaxation model (diffusion, dispersion)
- BC implementation not trivial.

## Design remark

- task based parallelization : flexibility in parallelization scheme
- the transport solver can be changed.

# Bibliography I

- [Bou99] F. Bouchut.  
Construction of bgk models with a family of kinetic entropies for a given system of conservation laws.  
*Journal of Statistical Physics*, 95(1):113–170, 1999.
- [CD98] Shiyi Chen and Gary D Doolen.  
Lattice boltzmann method for fluid flows.  
*Annual review of fluid mechanics*, 30(1):329–364, 1998.
- [Del02] Paul J Dellar.  
Lattice kinetic schemes for magnetohydrodynamics.  
*Journal of Computational Physics*, 179(1):95–126, 2002.
- [Dub13] François Dubois.  
Stable lattice boltzmann schemes with a dual entropy approach for monodimensional nonlinear waves.  
*Computers & Mathematics with Applications*, 65(2):142–159, 2013.
- [Gra14] Benjamin Graille.  
Approximation of mono-dimensional hyperbolic systems: A lattice boltzmann scheme as a relaxation method.  
*Journal of Computational Physics*, 266:74–88, 2014.
- [KL97] William Kahan and Ren-Cang Li.  
Composition constants for raising the orders of unconventional schemes for ordinary differential equations.  
*Mathematics of Computation of the American Mathematical Society*, 66(219):1089–1099, 1997.
- [MQ02] Robert I McLachlan and G Reinout W Quispel.  
Splitting methods.  
*Acta Numerica*, 11:341–434, 2002.
- [Nat98] Roberto Natalini.  
A discrete kinetic approximation of entropy solutions to multidimensional scalar conservation laws.  
*journal of differential equations*, 148:292–317, 1998.
- [Suz90] Masuo Suzuki.  
Fractal decomposition of exponential operators with applications to many-body theories and monte carlo simulations.  
*Physics Letters A*, 146(6):319–323, 1990.