Quasi-explicit, unconditionally stable, Discontinuous Galerkin solvers for conservation laws.

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Conservation laws

System of m conservation laws in dimension d

$$\partial_t W + \sum_{i=1}^{d} \partial_i Q^i(W) = S(W),$$

- Unknown: $W(X,t) \in \mathbb{R}^m$, space variable: $X = (x_1 \dots x_d)$, time variable: t.
- $\partial_i = \frac{\partial}{\partial x_i}$, $\partial_t = \frac{\partial}{\partial t}$. Source term: $S(W) = 0$.
- Hyperbolicity: let $N \in \mathbb{R}^d$ be an arbitrary space direction. The flux

$$Q(W) \cdot N = \sum_{i=1}^{d} N_i Q^i(W)$$

is supposed to be hyperbolic, i.e. the jacobian of the flux $d_W Q(W) \cdot N$ is diagonalizable with real eigenvalues.

Kinetic representation

We consider a set of $d+1$ (or more) kinetic velocities V_k, $k = 0 \dots d$, associated to **vectorial** kinetic functions $F_k(W) \in \mathbb{R}^m$. The macroscopic data are related to the kinetic data by

$$W = \sum_k F_k.$$

We also define "Maxwellian" equilibrium functions $M_k(W) \in \mathbb{R}^m$ such that

$$W = \sum_k M_k(W).$$

The kinetic BGK representation is given by transport equations with relaxation source terms [3, 1]

$$\partial_t F_k + V_k \cdot \nabla_X F_k = \frac{1}{\tau} \left(M_k(W) - F_k \right).$$

Kinetic representation

When the relaxation time $\tau \to 0^+$, the kinetic model is formally equivalent to the initial system of conservation laws if

$$W = \sum_k M_k(W), \quad \sum_k V_k^i M_k(W) = Q^i(W), \quad i = 1, \dots, d.$$

- Linear system of size $m(d+1) \times m(d+1)$ for finding the Maxwellian. One expects a unique solution.
- It is possible to generalize to conservation laws with a source term $\partial_t W + \sum_{i=1}^d \partial_i Q^i(W) = S(W) \neq 0$.
- In practice it is difficult to solve directly the BGK system. A splitting is preferable.

Kinetic algorithm

1. Start with $W(\cdot, 0)$. Construct kinetic vectors $F_k(\cdot, 0)$ such that $W = \sum_k F_k$ (not unique);
2. solve the free transport equations $\partial_t F_k + V_k^i \cdot \partial_i F_k = 0$ for a duration of Δt. This gives

$$F_k(X, \Delta t^-) = F_k(X - \Delta t V_k, 0);$$

3. define

$$W(\cdot, \Delta t) = \sum_k F_k(\cdot, \Delta t^-);$$

4. apply a relaxation

$$F_k(\cdot, \Delta t^+) = \omega M_k(W(\cdot, \Delta t)) + (1 - \omega) F_k(\cdot, \Delta t^-).$$

Interesting cases: $\omega = 1$, $\omega = 2$, ω is a matrix. CFL-less [4, 7].

Flux error representation

During the computations, one expects that $\sum_k V_k^i F_k \simeq Q^i(W)$, we thus introduce the **approximated flux** Z**,** and the **flux error** Y

$$Z^i = \sum_k V_k^i F_k, \quad Y^i = Z^i - Q^i(W).$$

The kinetic algorithm is then a functional operator $\mathcal{M}(\Delta t)$ that maps $(W(\cdot, 0), Y^i(\cdot, 0))$ to $(W(\cdot, \Delta t), Y^i(\cdot, \Delta t^+))$.

1. The operator $\mathcal{M}$ is made of (linear) shift operations and (non-linear) local relaxations.
2. In the (W, Y^i) variables, when $\omega = 2$, the relaxation operation simply reads
$$Y^i(\cdot, \Delta t^+) = -Y^i(\cdot, \Delta t^-).$$
This induces fast oscillations of the flux error. For the analysis it is better to replace $\mathcal{M}$ by $\mathcal{M} \circ \mathcal{M}$.

Equivalent equation

In principle it is now easy, while tedious, to compute the equivalent equation of the kinetic algorithm: simply compute a Taylor expansion of

$$\frac{\mathcal{M}(\Delta t/2) - \mathcal{M}(-\Delta t/2)}{\Delta t}$$

with respect to Δt up to order $O(\Delta t^2)$.

- The term $X - \Delta t V_k$ in the shift operation generates partial derivatives in space.
- Because of symmetries, when $\omega = 2$, the even order terms vanish.
- And finally, the relaxation introduces non linearities. We end up with a system of non-linear conservation laws of first order in (W, Y^i).

One-dimensional case

We consider the case $d = 1$, we have $d + 1 = 2$ kinetic velocities. We take $V_0 = -\lambda$, $V_1 = \lambda$, $W = F_0 + F_1$. The equivalent equation for $\omega = 2$ at order $O(\Delta t^2)$ is

$$\partial_t W + \partial_x Q(W) = 0,$$

(of course) and

$$\partial_t Y - d_W Q(W) \partial_x Y = 0.$$

- We observe that the system is hyperbolic and that the waves for W and Y move in opposite directions.
- No assumption of smallness of Y !
- It is necessary to analyze the third order terms to find the sub-characteristic stability condition

$$\lambda \geq \max_{1 \leq i \leq m} |\lambda_i(W)|,$$

where $\lambda_i(W)$ are the eigenvalues of $d_W Q(W)$.

Two-dimensional case

We consider the case $d = 2$, we have $d + 1 = 3$ kinetic velocities. We take

$$V_k = \lambda \begin{pmatrix} \cos \frac{2k\pi}{3} \\ \sin \frac{2k\pi}{3} \end{pmatrix}$$

The equivalent equation on W for $\omega = 2$ at order $O(\Delta t^2)$ is

$$\partial_t W + \partial_1 Q^1(W) + \partial_2 Q^2(W) = 0,$$

(of course). Setting $A^i(W) = d_W Q^i(W)$, the equation for Y is

$$\partial_t \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix} + \begin{pmatrix} \frac{\lambda}{2} I - A^1(W) & 0 \\ -A^2(W) & -\frac{\lambda}{2} \end{pmatrix} \partial_1 \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix} + \begin{pmatrix} 0 & -\frac{\lambda}{2} I - A^1(W) \\ -\frac{\lambda}{2} & -A^2(W) \end{pmatrix} \partial_2 \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix} = O(\Delta t^2),$$

We can prove that the equivalent system is symmetrizable, and thus hyperbolic, if λ is large enough (sub-characteristic condition). Entropy analysis [3, 5].

Unconditionally stable Discontinous Galerkin

Discontinuous Galerkin (DG) solver

The main task is to solve a single transport equation

$$\partial_t f + V \cdot \nabla f = 0$$

in a domain Ω with a complex geometry. The characteristic method is not necessarily a good idea (problems with stability, conservation, boundaries). Let's do DG [8].

- Unstructured mesh of Ω made of tetrahedral cells.
- The transported function f is approximated in cell L by a linear expansion on basis functions

$$f(x, n\Delta t) \simeq f_L^n(x) = \sum_j f_{L,j}^n \psi_j^L(x), \quad x \in L.$$

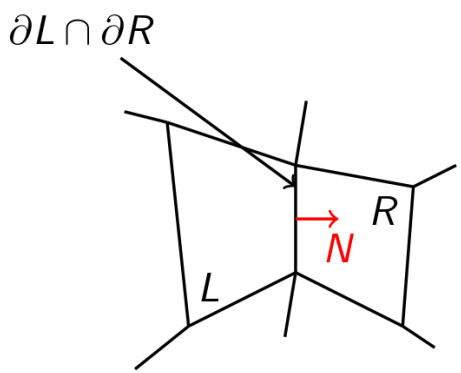
- The unknowns are the coefficients $f_{L,j}^n$ of the linear expansion.

Implicit DG

Implicit DG approximation scheme for going from time step $n-1$ to time step n: for all cell L and $\forall i$,

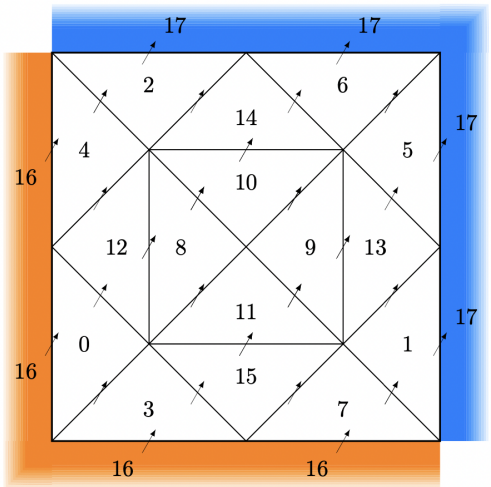
$$\int_L \frac{f_L^n - f_L^{n-1}}{\Delta t}\psi_i^L - \int_L V\cdot\nabla\psi_i^L f_L^n + \int_{\partial L}\left(V\cdot N^+ f_L^n + V\cdot N^- f_R^n\right)\psi_i^L = 0.$$

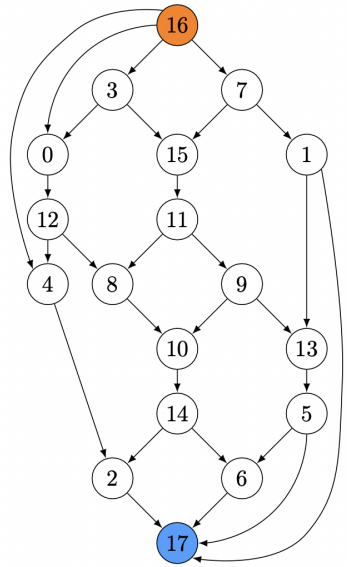
- R denotes the neighbor cells along ∂L.
- $V\cdot N^+ = \max(V\cdot N, 0)$, $V\cdot N^- = \min(V\cdot N, 0)$. We thus use an upwind numerical flux.
- N is the unit normal vector on ∂L oriented from L to R.



Downwind algorithm

The scheme seems to be implicit, but it is actually explicit [2].





- The solution can be explicitly computed by following a topological ordering of a Direct Acyclic Graph (DAG), e.g. 3, 7, 0, 15, 1, etc.
- In addition there is parallelism: (3,7) can be computed in parallel, then (0,15,1) can be computed in parallel, etc.
- Low storage: the solution can be replaced in memory during the computations.

Numerical results

Rust implementation

We have implemented the downwind algorithm in Rust:

- Recent programming language (2010) oriented towards concision, speed and security.
- Most common bugs are avoided at compile time: memory leaks and segfaults, uninitialized data, race conditions.
- Automatic parallelization tools: if the sequential code works, the parallel version is guaranteed to be correct.
- Fast. More details in [6].

			Error e_r		CPU (s)	
Method	CFL β	Δt	$\nu = 2$	$\nu = 5$	1 thread	24 threads
RK3DG	0.37	0.00009	0.00070	0.01238	4,607.95	785.28
D3Q4P	0.37	0.00009	0.00103	0.01467	1,524.45	234.48
RK3DG	0.93	0.00023	0.00070	0.01238	2,189.76	384.79
D3Q4P	0.93	0.00023	0.00103	0.01467	613.44	90.84
RK3DG	1.85	0.00046	0.00070	0.01238	1,121.96	212.60
D3Q4P	1.85	0.00046	0.00103	0.01467	304.41	45.14
D3Q4P	3.70	0.00091	0.00103	0.01468	153.09	22.40
D3Q4P	9.25	0.00228	0.00104	0.01479	61.60	8.96
D3Q4P	18.50	0.00456	0.00115	0.01619	30.76	4.53
D3Q4P	37.00	0.00912	0.00210	0.02992	15.34	2.46
D3Q4P	92.50	0.02281	0.01107	0.16589	6.17	0.92
D3Q4P	185.00	0.04562	0.04509	0.40344	3.10	0.48

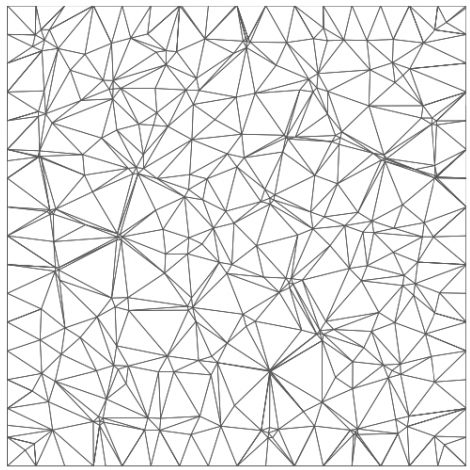
Numerical results

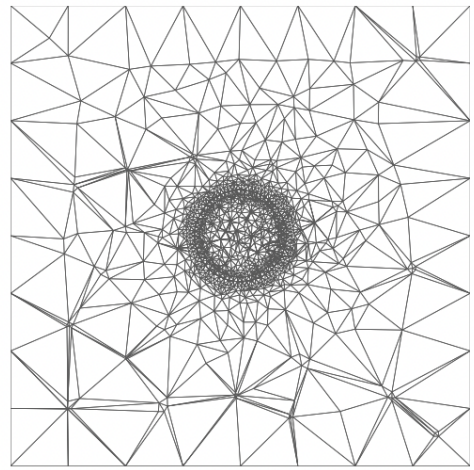
- Maxwell's equation: $W = (E^T, H^T)^T$, with electric field $E \in \mathbb{R}^3$ and magnetic field $H \in \mathbb{R}^3$.
- Maxwell flux:

$$Q(W) \cdot N = \begin{pmatrix} -N \times H \\ N \times E \end{pmatrix}, \quad \partial_t W + \nabla \cdot Q(W) = 0.$$

.

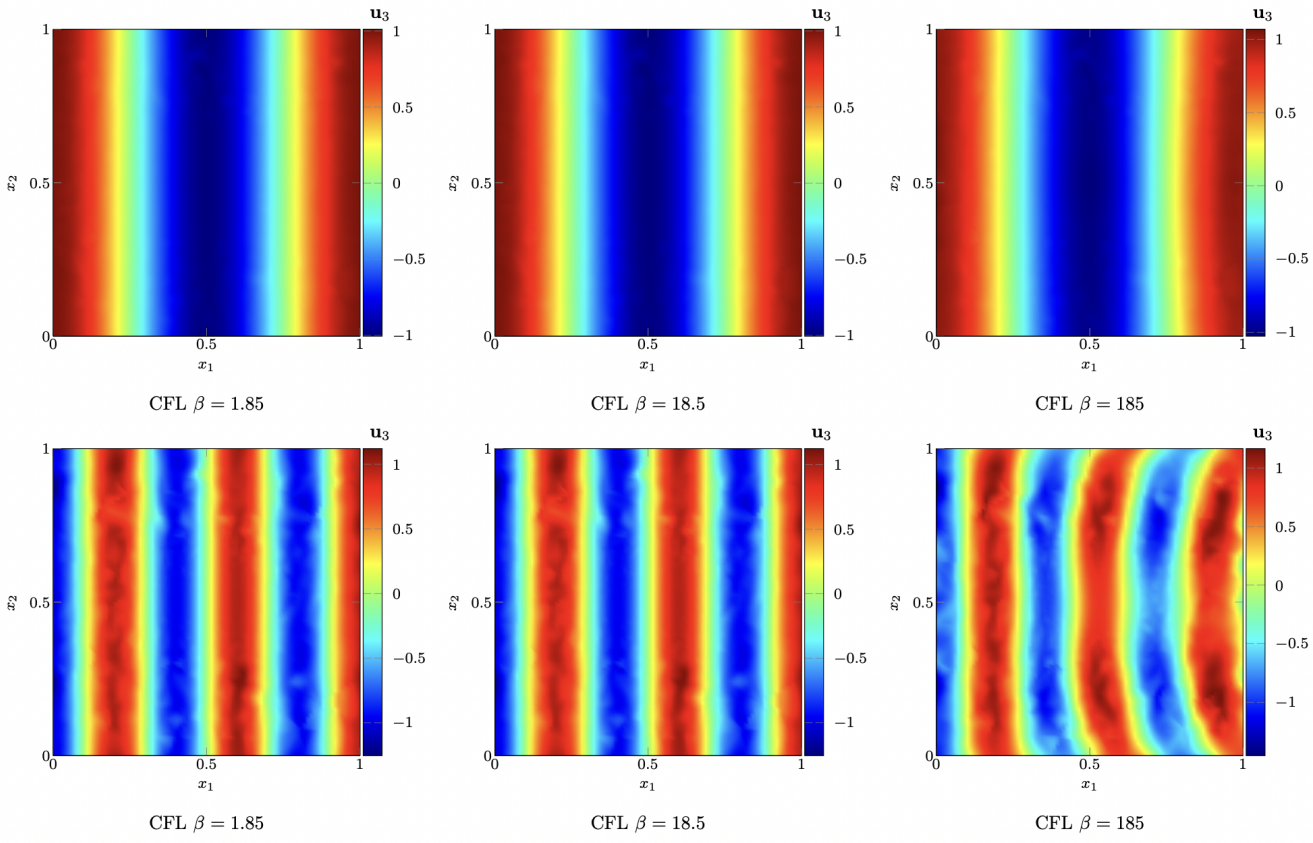
- Unstructured mesh of the unit cube made with large and small cells





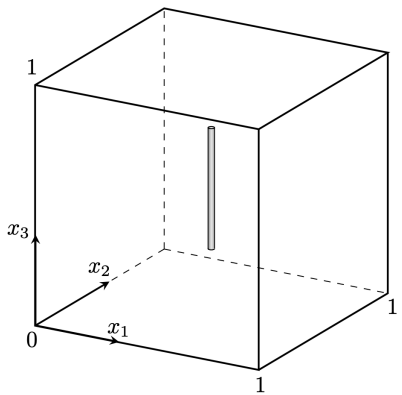
Numerical results

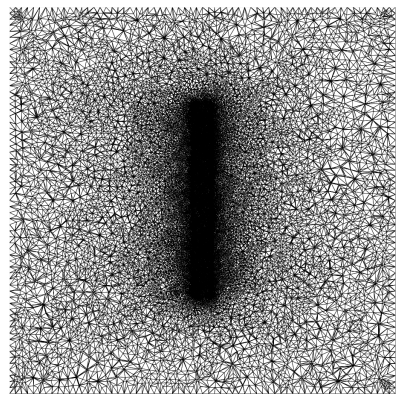
- We compute a plane wave on the above mesh.
- We check second order accuracy and the CFL-less feature

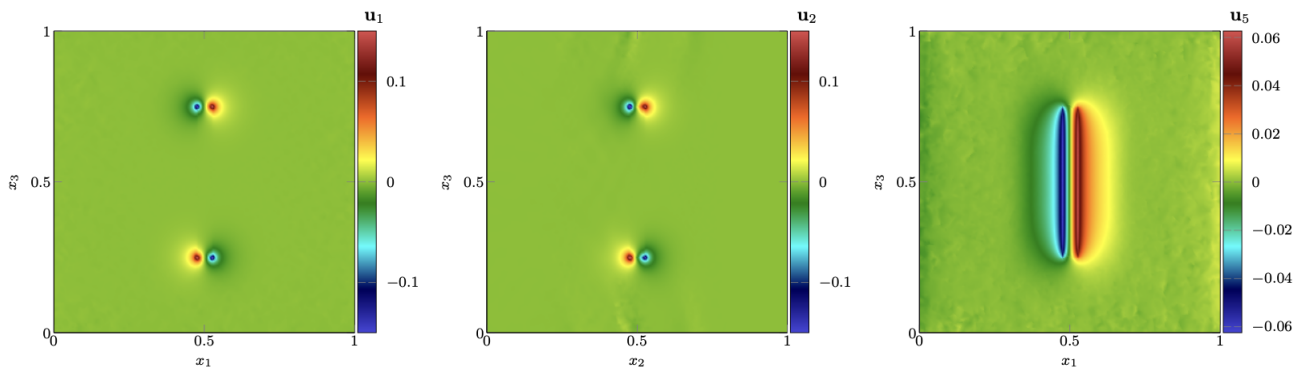


Antenna simulation

- Unstructured mesh of the unit cube made of large and small cells. A small electric wire at the middle of the mesh.
- Resolution of the Maxwell equations with a conductivity source term $S(W) = (\sigma E, 0)$. Plane wave pulse.



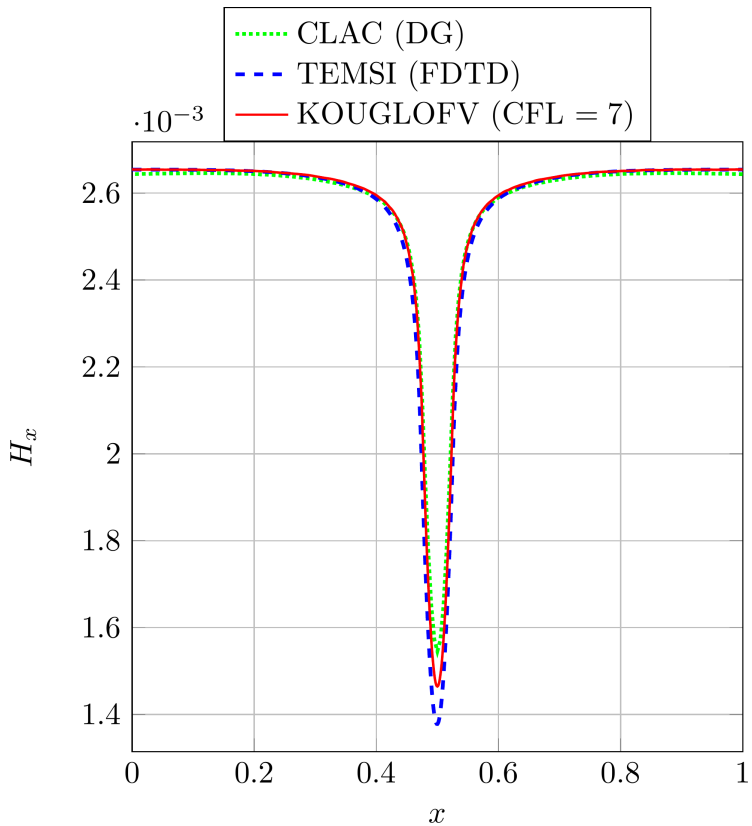


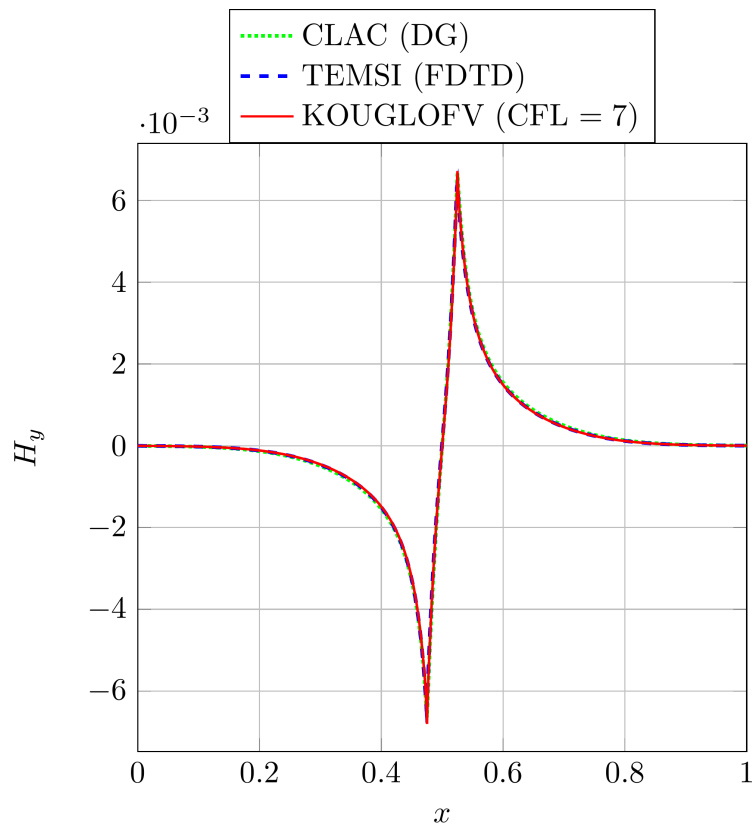


(a) Solution at time $t = 0.75$; left panel: $E_1|_{x_2=0.5}$; middle panel: $E_2|_{x_1=0.5}$; right panel: $H_2|_{x_2=0.5}$.

FDTD comparison, $\sigma = 3$

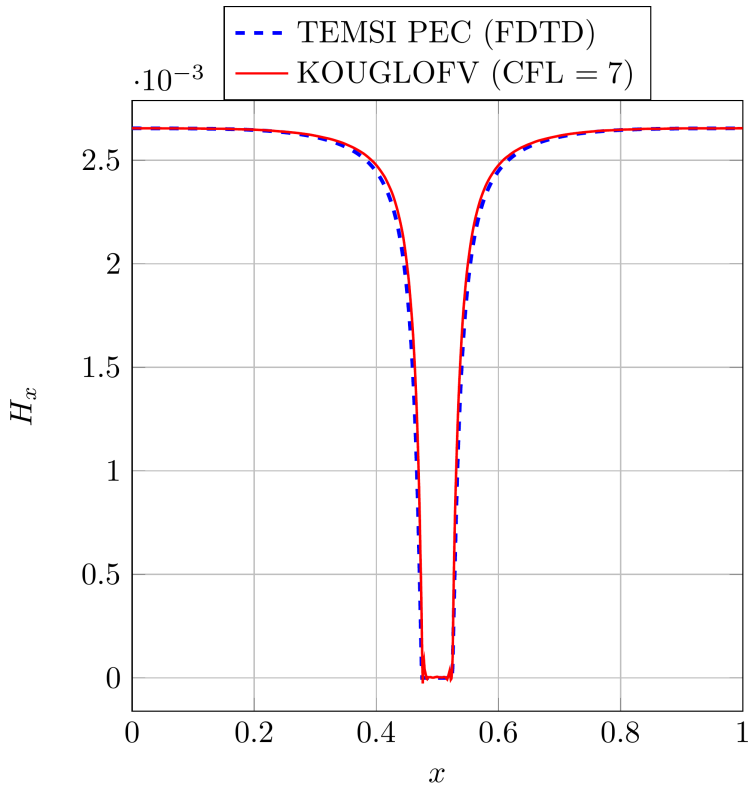
- Comparison with an FDTD solver. H_x and H_y on the line $y = z = 1/2$ when the pulse reaches the wire.
- Computation time: FDTD 20 hours: (uniform fine mesh), Kinetic DG: 70 s.

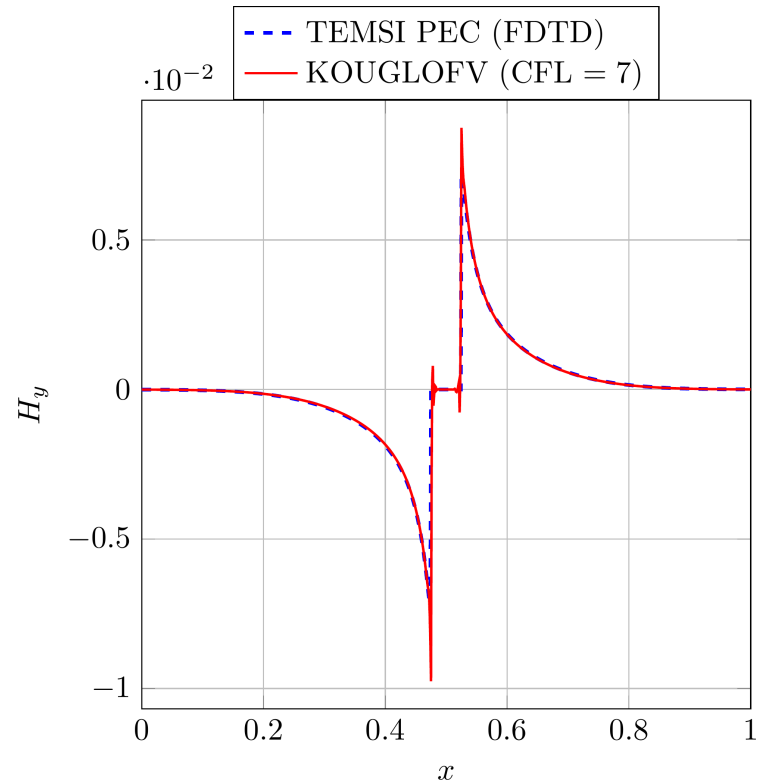




FDTD comparison, $\sigma = +\infty$

The source term is solved in the relaxation step. It amounts to perform $E \leftarrow -E$, before relaxing to the Maxwellian state. It seems to work, even for perfect conductor.





3D multiphase flow

Fluid of density ρ, velocity U, pressure p. Color function ϕ: $\phi = 0$ in the liquid and $\phi = 1$ in the gas.

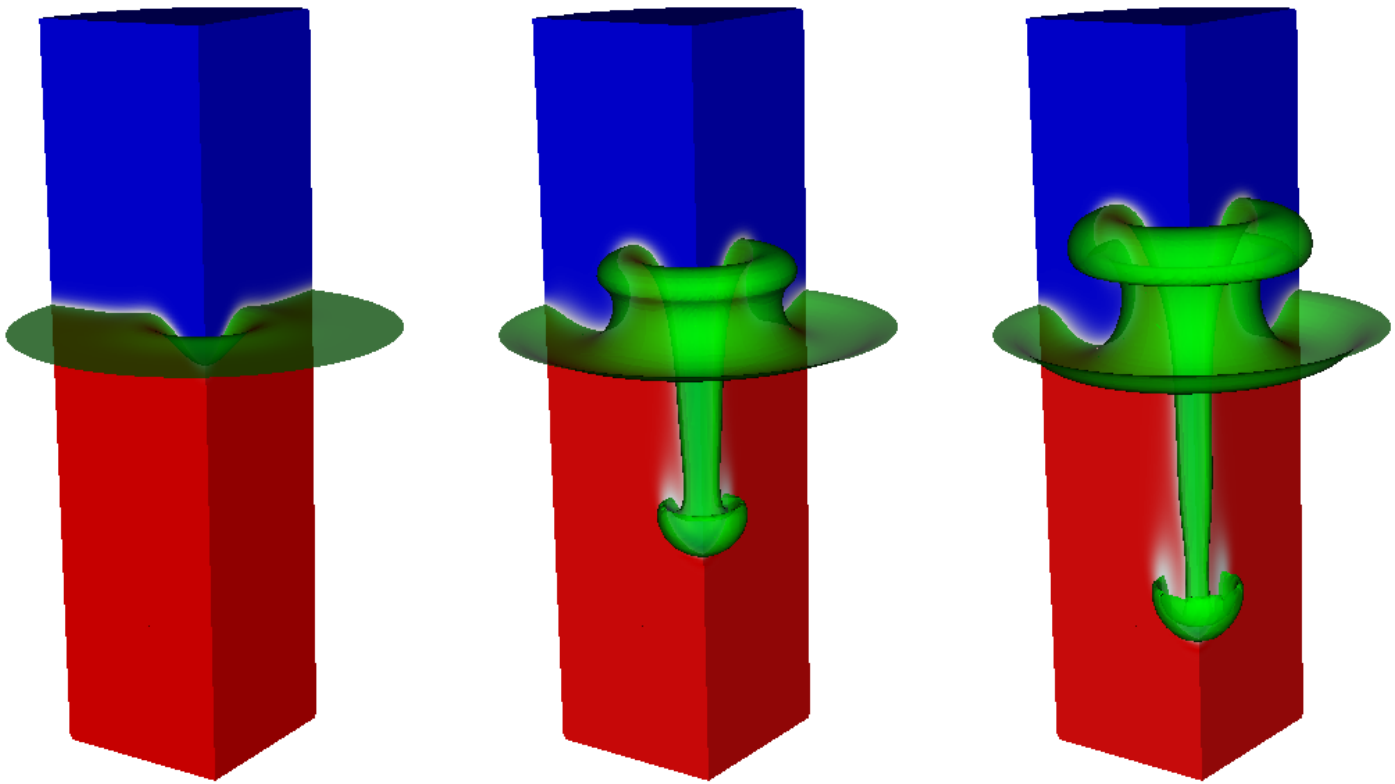
$$W = \begin{pmatrix} \rho \\ \rho U \\ \rho\varphi \end{pmatrix}, \quad Q(W)\cdot N = \begin{pmatrix} \rho U \cdot N \\ \rho(U \cdot N)U + pN \\ \rho\phi U \cdot N \end{pmatrix}, \quad S(W) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -\rho g \\ 0 \end{pmatrix}$$

The pressure is a function of ρ and ϕ, $p = \pi(\rho, \phi)$.

$$\partial_t W + \nabla \cdot Q(W) = S(W).$$

3D multiphase flow

Rayleigh-Taylor instability. Two immiscible fluids with gravity. CFL=10 on the symmetry axis.



Better parallelism ?

- The downwind algorithm is parallelized with a work stealing thread based algorithm.The parallel scaling is good for a few threads.
- In order to increase it we also applied a subdomain strategy with a coupling between the subdomains.

Subdomain decomposition

Resolution of the transport equation with initial data in $\Omega \times [0, \Delta t]$:

$$\partial_t f + V \cdot \nabla f = 0, \quad f(X, 0) = f^0(X).$$

Decomposition of Ω into subdomains Ω_i (for simplicity, we assume that Ω is a periodic domain or the whole space).

- We denote by f_i the restriction of f to subdomain Ω_i,
- by $N_i(X)$ the outward normal vector on $\partial\Omega_i$,
- and by $\partial\Omega_i^-$ the upwind part of the boundary of Ω_i: $\partial\Omega_i^- = \{X \in \partial\Omega_i, N_i(X) \cdot V < 0\}$.

Iterative algorithm

We set $f_i^0(X,t) = f_i^0(X)$ and consider the iterative algorithm

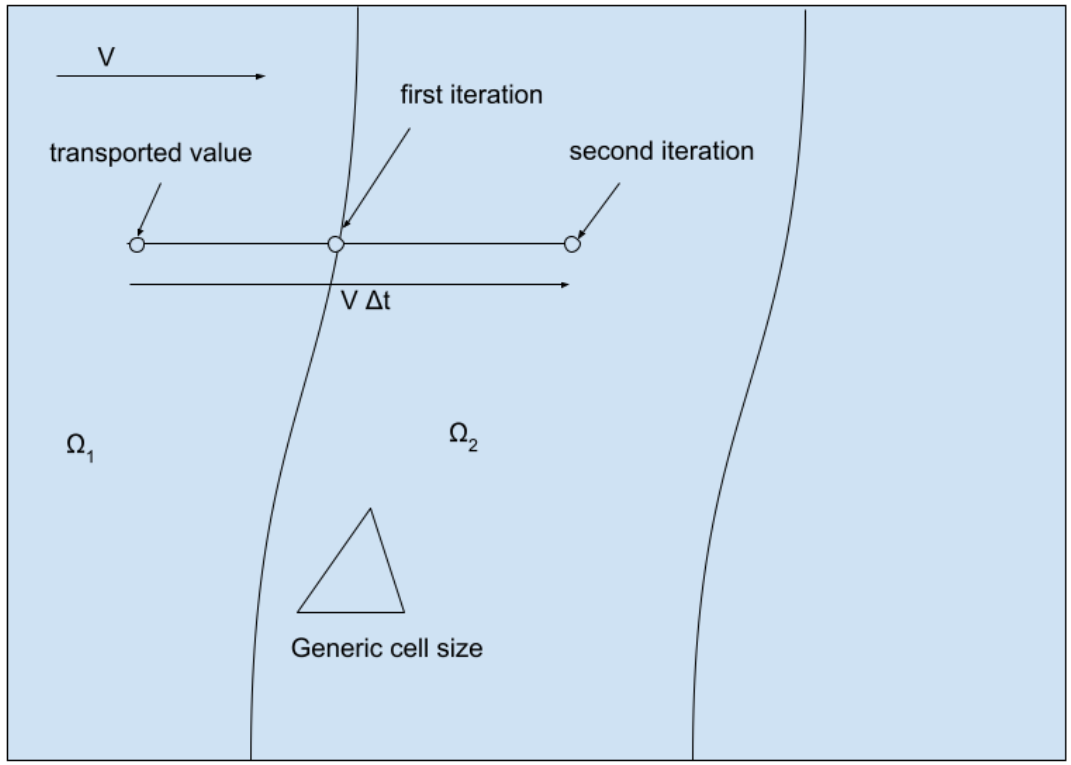
$$\begin{aligned} \partial_t f_i^p + V \cdot \nabla f_i^p &= 0, \quad \text{in } \Omega_i, \\ f_i^p(X,0) &= f_i^0(X), \quad X \in \Omega_i, \\ f_i^p(X,t) &= f_j^{p-1}(X,t), \quad X \in \partial\Omega_i^- \cap \partial\Omega_j. \end{aligned}$$

Proposition: let L be the maximum diameter of the subdomains. Under the condition

$$\Delta t \leq \frac{L}{|V|},$$

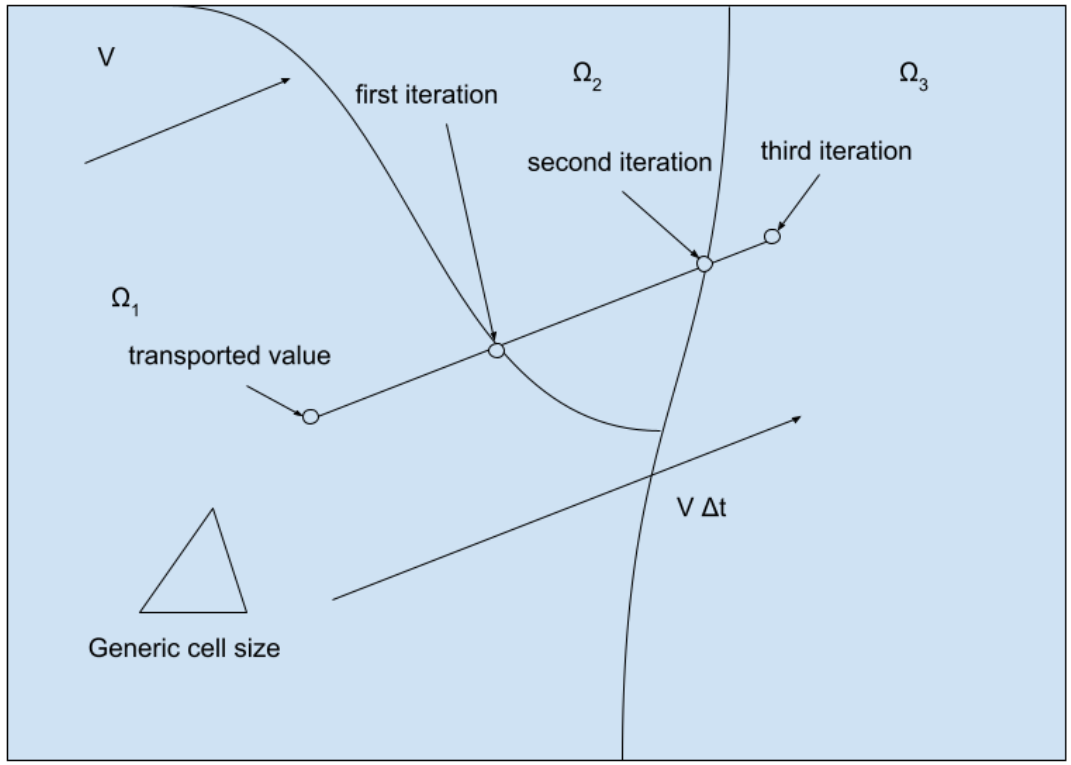
in the generic case, the above algorithm converges to the exact solution in at most three iterations: $f_i^3 = f_i$.
Proof: by the characteristic method.

Aligned subdomains case



- First iteration: the boundary value is updated.
- Second iteration: the correct value is transported.

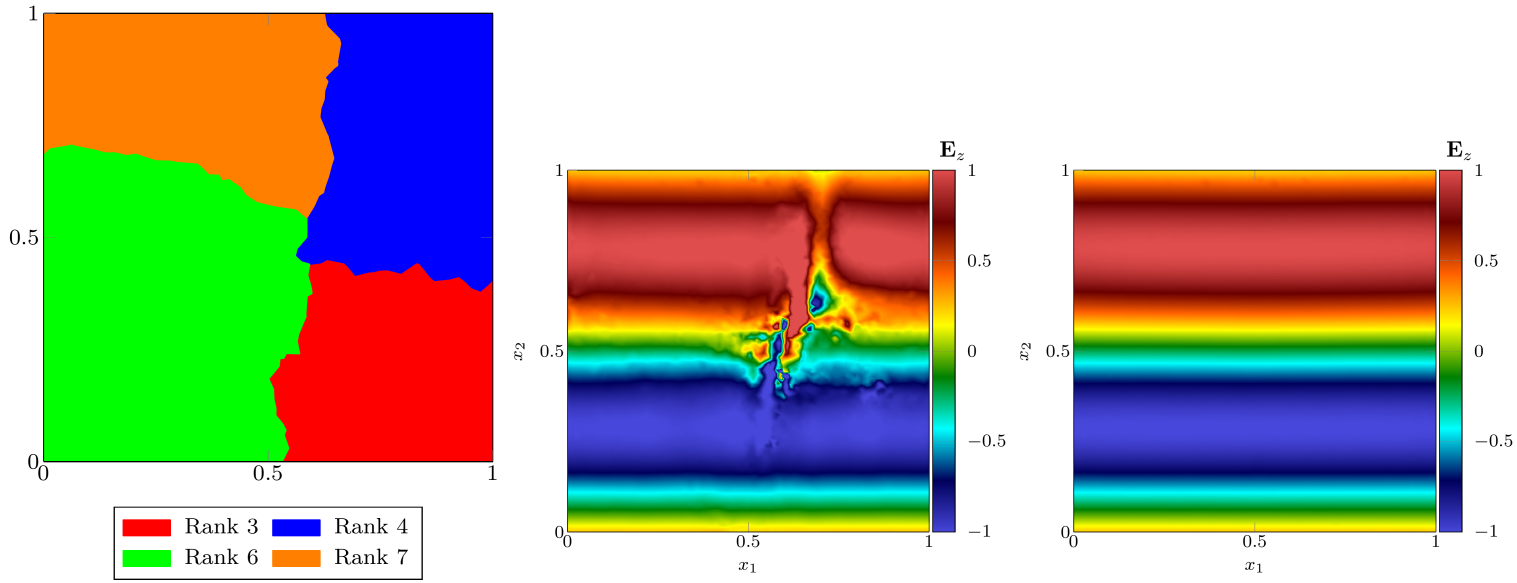
Generic case



- First iteration: the boundary value on $\partial\Omega_2^-$ is updated.
- Second iteration: the boundary value on $\partial\Omega_3^-$ is updated.
- Third iteration: the correct value is transported.

Subdomain stability condition

Numerical experiments indicate that the number of iterations is also related to stability.



Left: subdomains, Middle: 2 iterations scheme, Right: 3 iterations scheme

MPI scaling

The subdomain algorithm relaxes the computational tasks dependency and allows to get a better parallel (strong) scaling of the method:

MPI nodes	Threads	#CPU	Time (s)	Accel.
1	2	2	1314	1
1	8	8	346	0.95
1	16	16	209	0.79
1	32	32	132	0.62
1	**64**	**64**	**106**	**0.39**
2	32	64	75	0.55
4	16	64	59	0.70
8	**8**	**64**	**57**	**0.72**
128	2	256	24	0.43

Conclusion

The kinetic approach:

- Can handle arbitrary conservation laws.
- Construction of CFL-free explicit DG scheme on unstructured meshes.
- Equivalent equation: useful theoretical tool (stability analysis, boundary conditions, behavior of hidden variables).
- Good parallelization features, for both shared memory and distributed memory computers.

Ongoing works: boundary conditions, other applications (cavitation).

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