A lumped nodal DGTD-PIC method to ensure charge conservation for the 3D Vlasov-Maxwell system on nonconforming grids

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Nuclétudes

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Quick introduction to mesoscopic plasma description

Boltzmann Probability Function

$$f(X, p, t) = f(x, y, z, p_x, p_y, p_z, t)$$

is an observable used to describe particles behavior at the mesoscopic level in phase space : $X = (x, y, z)$ is the position vector, $p = (p_x, p_y, p_z)$ the momentum and t the time.

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{dx}{dt}\frac{\partial f}{\partial x} + \frac{dv}{dt}\frac{\partial f}{\partial v} = \left(\frac{df}{dt}\right)_{coll}$$

Applying Newton's Second Law of Motion, we get Bolzmann equation :

$$\boxed{\frac{\partial f}{\partial t} + v.\nabla f + \frac{F}{m}\frac{\partial f}{\partial v} = \left(\frac{df}{dt}\right)_{coll}}$$

For collionless plasmas F stands for the Lorentz Force (produced by electromagnetic fields E and H) and therefore :

$$\left(\frac{df}{dt}\right)_{coll} = 0$$

Special case of an electron collisionless plasma

Colors used to emphasize nonlinear dependencies between (E, H, f)

Non-consistent DGTD-PIC

- Dynamics of electromagnetic fields : Maxwell equations
  $\mapsto$ *Discontinuous Galerkin in Time Domain* : How to do it in order to numerically conserve charge as a first part

$$\epsilon \partial_t E - \nabla \times H = -J(f)$$

$$\mu \partial_t H + \nabla \times E = 0$$

$$\nabla . E = \frac{\rho}{\epsilon}$$

$$\nabla . H = 0$$

- Vlasov system describing electron behavior : Vlasov equation
  $\mapsto$ *Particle In Cell* How to combine PIC with DGTD as a second part

$$\frac{\partial f}{\partial t} + v . \nabla f + \frac{F(E, H)}{m} \frac{\partial f}{\partial v} = 0$$

What is charge conservation ?

Charge Conservation Equation

$$\partial_t \rho + \nabla . J = 0$$

- A necessary property for both Maxwell and Vlasov equations to make sense
- Involution in Maxwell equations. Given suitable initial conditions thanks to this property, Maxwell's equations reduce to

$$\epsilon \partial_t E - \nabla \times H = -J(f)$$

$$\mu \partial_t H + \nabla \times E = 0$$

- What about a numerical solution not satisfying this property ?
  $\mapsto$ *Accounting for divergence constraints becomes mandatory*

Why DGTD(-PIC) is a most promising method to solve (Vlasov-)Maxwell system

- Purely local Method
- Can be used for lots of other physical applications $\mapsto$ *Multiphysics*
- Natural ability to easily increase resolution order
- High order method compatible with very general meshes (hybrid, with hanging nodes, HP) : possibility of multiscale highly accurate modelling
- Highly parallelizable

Main drawbacks of DGTD(-PIC)

DGTD and DGTD-PIC

High computational cost (worse for complex meshes) depending on the available resources

$\mapsto$ *only cartesian grids with hanging nodes (multiscale)* for this briefing

DGTD

Complete mastery of nonspurious DGTD schemes on general grids not yet achieved

DGTD-PIC

Complete mastery of charge conserving DGTD-PIC schemes on general grids not yet achieved

Nonspurious schemes and charge conserving schemes

$$E(t,.) = \overbrace{E(0,.)}^{\text{initial state}} + \overbrace{\int_0^t [\nabla \times H(s,.) - J(s,.)]\ ds}^{\text{what a convergent scheme computes}} + \overbrace{\nabla\varphi(t,.)}^{\text{divergence error of the scheme}}$$

Charge conserving : nonlinearity but source term prescribed by PIC

$$\epsilon\partial_t E - \nabla \times H = -J(f)$$
$$\mu\partial_t H + \nabla \times E = 0$$

Nonspurious : linear but arbitrary source term J

$$\epsilon\partial_t E - \nabla \times H = -J$$
$$\mu\partial_t H + \nabla \times E = 0$$

Goal : secure charge conservation on 3D cartesian grids with hanging nodes (multiscale)

Can spurious behavior take place in Time Domain ?

yes it can...

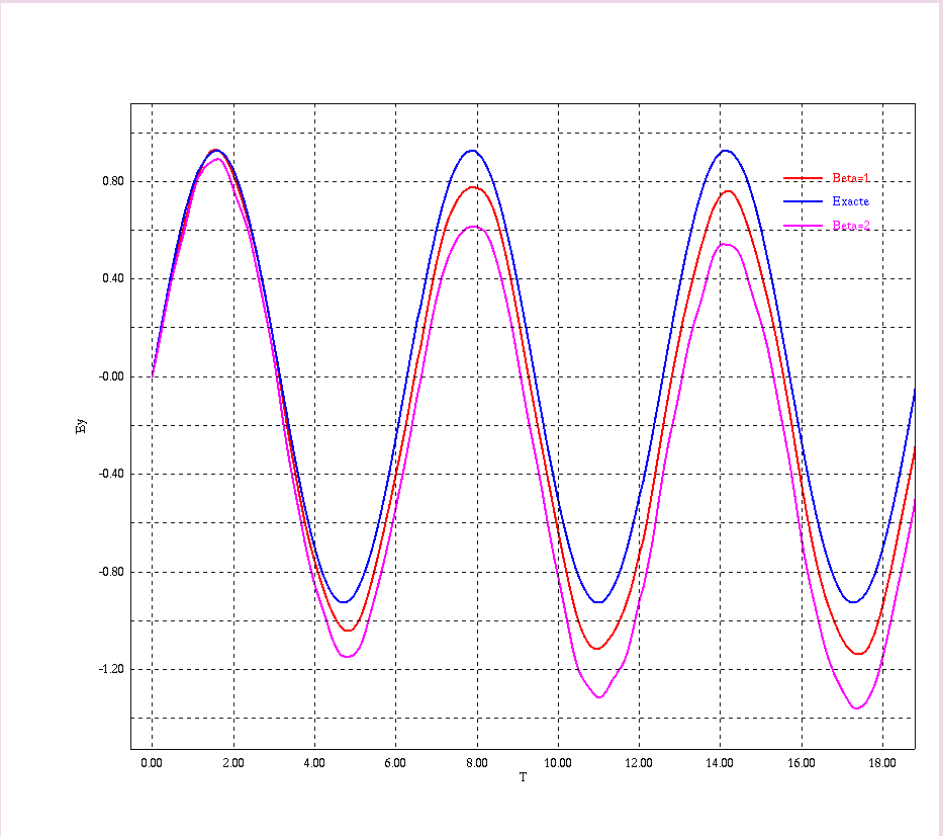

FIG.: E_y field for parameter $\beta = 1$ and $\beta = 2$ Legendre P^1 with centered fluxes on mesh 10x10x10

How is this result obtained ? (Generalization to 3D of 2D Issautier test-case)

$$J = \pi \begin{pmatrix} (\cos(t) - \beta)[\pi \cos(\pi x)(\sin(\pi z) + \sin(\pi y)) + 2\pi^2 x \sin(\pi y) \sin(\pi z)] - \cos(t) x sin(\pi y) \sin(\pi z) \\ (\cos(t) - \beta)[\pi \cos(\pi y)(\sin(\pi x) + \sin(\pi z)) + 2\pi^2 y \sin(\pi z) \sin(\pi x)] - \cos(t) y sin(\pi z) \sin(\pi x) \\ (\cos(t) - \beta)[\pi \cos(\pi z)(\sin(\pi y) + \sin(\pi x)) + 2\pi^2 z \sin(\pi x) \sin(\pi y)] - \cos(t) z sin(\pi x) \sin(\pi y) \end{pmatrix}.$$

$$E = \sin(t) \begin{pmatrix} x \sin(\pi y) \sin(\pi z) \\ y \sin(\pi z) \sin(\pi x) \\ z \sin(\pi x) \sin(\pi y) \end{pmatrix}$$

$$H = \pi(\cos(t) - \beta) \begin{pmatrix} \sin(\pi x)(z \cos(\pi y) - y \cos(\pi z)) \\ \sin(\pi y)(x \cos(\pi z) - z \cos(\pi x)) \\ \sin(\pi z)(y \cos(\pi x) - x \cos(\pi y)) \end{pmatrix}$$

Test-case similar to the one of A. Stock (proceedings of coupled problems 2011 conference) but fields are known explicitly

The same bad results are obtained

- For all $\beta > 0 \mapsto$ a small error can trigger a spurious reaction
- For Bernstein basis functions $\mapsto$ not due to a defect in Legendre basis functions

Upwind fluxes and higher order basis functions delay the appearance of spurious behavior (but do not correct it)

How to get correct results ?

Two kinds of methods

- Reintroduce divergence contraints in the equation via penalization (Issautier et Depeyre, rapport de recherche du CERMICS 1995) or a Lagrange Multiplier (Elliptic correction, Parabolic correction, Hyperbolic correction : PHM)
  $\mapsto$ the data ρ is needed

- Use a proxy space for J, different from the one used to approximate the field H. Based on this principle, many configurations which correct spurious behaviors can be found.

$\mapsto$ Charge conservation in DGTD-PIC is a separate issue

Context

Both Maxwell and Vlasov are hyperbolic, encouraging the use of explicit time integrators.

The correction methods replace Maxwell equations by an augmented formulation that can be :

- Still hyperbolic
- Parabolic or with parabolic/elliptic features

First kind of correction : Depeyre-Issautier's penalization method

Formulation

$$\epsilon \partial_t E - \nabla \times H \overbrace{- \frac{1}{\alpha_E} \nabla \left(\nabla . E - \frac{\rho}{\epsilon} \right)}^{\text{penalization of Gauss' law}} = -J$$

$$\mu \partial_t H + \nabla \times E \underbrace{- \frac{1}{\alpha_H} \nabla \left(\nabla . H \right)}_{\text{penalization of Gauss' law for magnetism}} = 0$$

Analysis of the formulation

No additional unknowns to compute but the equations become parabolic :

- Explicit time stepping loose efficiency
- Discretization of the additional penalization term in DGTD is more technical to perform
- Given suitable assumptions and an initial condition, there is a unique solution $\left(E\left(\alpha_E, \alpha_H \right), H\left(\alpha_E, \alpha_H \right) \right)$

Second kind of correction containing several correction methods

Formulation

Lagrange multiplier enforcing Gauss' law

$$\epsilon\partial_t E - \nabla \times H \overbrace{+\alpha_E \nabla \varphi_E} = -J$$

$$\mu\partial_t H + \nabla \times E \underbrace{+\alpha_H \nabla \varphi_H} = 0$$

Lagrange multiplier enforcing Gauss' law for magnetism

$$\beta_E \partial_t \varphi_E + \gamma_E op(\partial)\left(\nabla . E - \frac{\rho}{\epsilon}\right) = 0$$

$$\beta_H \partial_t \varphi_H + \gamma_H op(\partial)\nabla . H = 0$$

Remarks

- Depending on the choice of parameters $(\alpha_E, \beta_E, \gamma_E)$ and of the differential operator $op(\partial)$, the Cauchy system on the whole space is well-posed.
- The last two equations can be : hyperbolic, parabolic, elliptic
- The PHM (Purely Hyperbolic Maxwell) formulation ensures global hyperbolicity of the system whose unknowns are $(E, H, \varphi_E, \varphi_H)$

Relevant questions

List of questions

- Generalization of classical boundary conditions for Maxwell's equations to the augmented system (existence but no uniqueness)
- Time scheme to use to solve numerically the new augmented system
- Characteristics of waves propagating on (φ_E, φ_H) unknowns. For instance, for PHM, parameters have to be prescribed in a unique way to ensure propagation of these waves at the speed of light.
- Rigourous meaning of charge density ρ

Definition of charge density (I)

Two point of views for the Vlasov-Maxwell system

- ρ obtained from density function f as

$$\rho_{Vlasov} := (t, x) \mapsto \int_{\mathbb{R}^3} f(t, x, v)\, dv$$

- ρ obtained from the electric field through Gauss' law as

$$\rho_{Maxwell} := (t, x) \mapsto \epsilon \nabla . E(t, x)$$

- The two definitions of ρ give different values in DGTD-PIC, for instance on charged metallic surfaces

Definition of charge density (II)

Physical description and picture of $\rho_{Maxwell}$

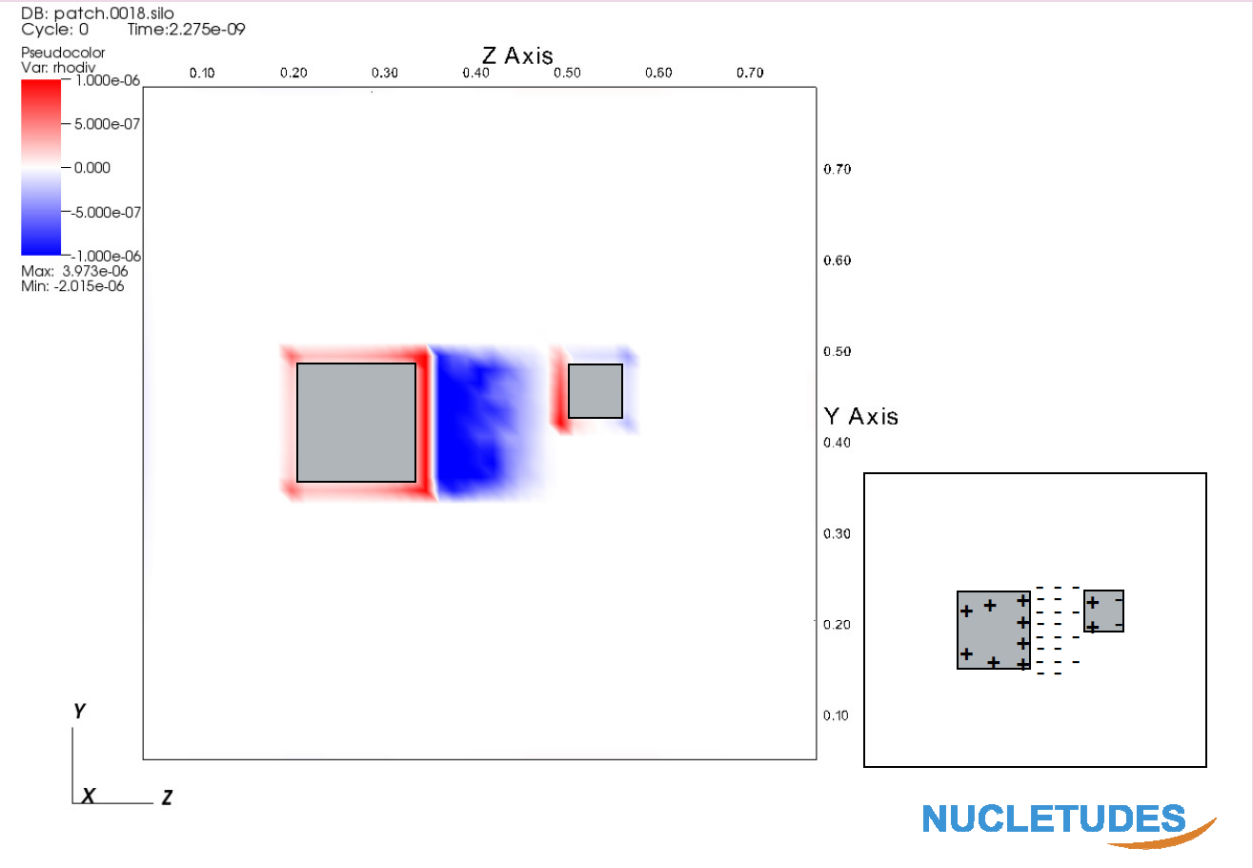

FIG.: Charge influence induced by electrons emitted from the right of the left grey box

Definition of charge density (III)

Physical description and picture of ρ_{Vlasov}

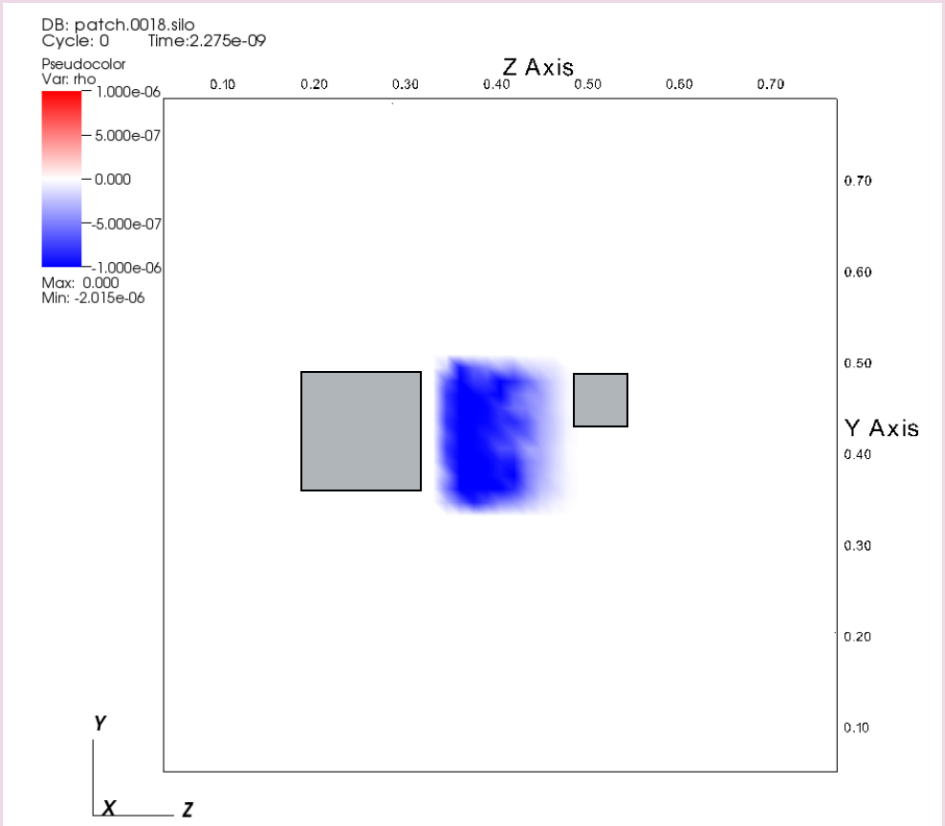

FIG.: Charge influence induced by electrons emitted from the right of the left grey box

Charge density in correction methods

ρ in correction methods for PIC applications

- $\rho = \rho_{vlasov}$ thus correction methods enforce $\nabla.E - \frac{\rho_{vlasov}}{\epsilon} = 0$
- The information contained by ρ_{vlasov} is poorer than the one contained in $\rho_{Maxwell}$ (physical charge density)
- The differences between $\rho_{Maxwell}$ and ρ_{Vlasov} lie on hypersurfaces on which suitable boundary conditions for the augmented system are expected to impose the correct physics

Why correction methods can have tricky effects in a DGTD framework

Correction methods using only DG...

We do not want to loose the advantages of DG by mixing it with finite elements

Physical case for which DGM correction Methods give nonphysical results

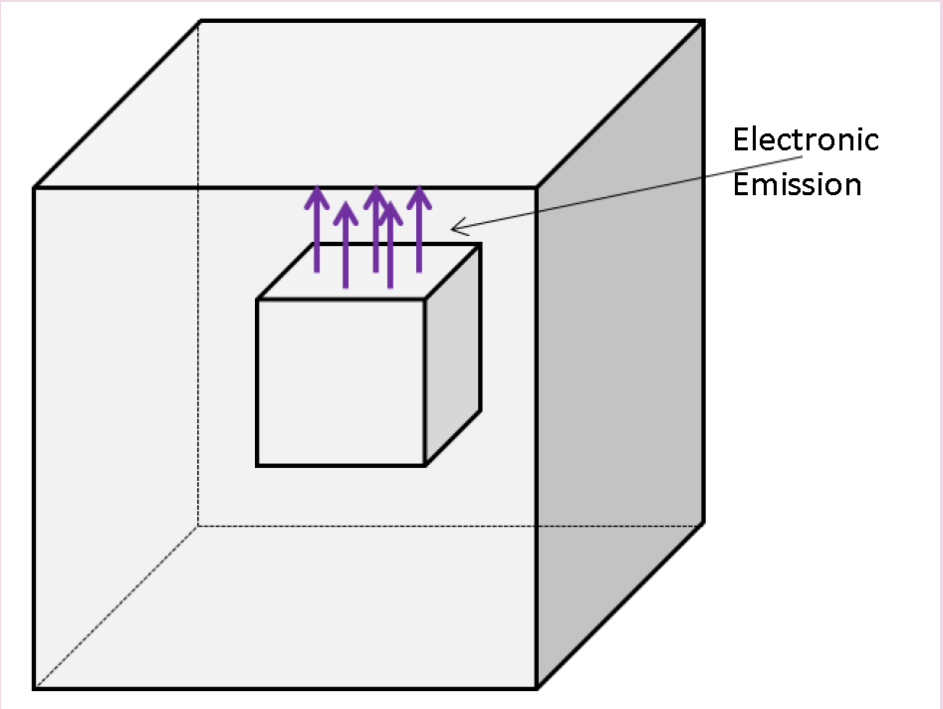

FIG.: A metallic box inside another one

Comment on the nonphysical results

Tests performed

- In 3D with PHM (preferred correction method)
- In 2D with Boris correction (reference method in terms of quality for most people)

Unphysical results how ?

Charge density near the emissive zone goes to zero instead of maintaining a constant positive value at late times.

Expected results and results obtained when charge is not conserved

Bad charge conservation

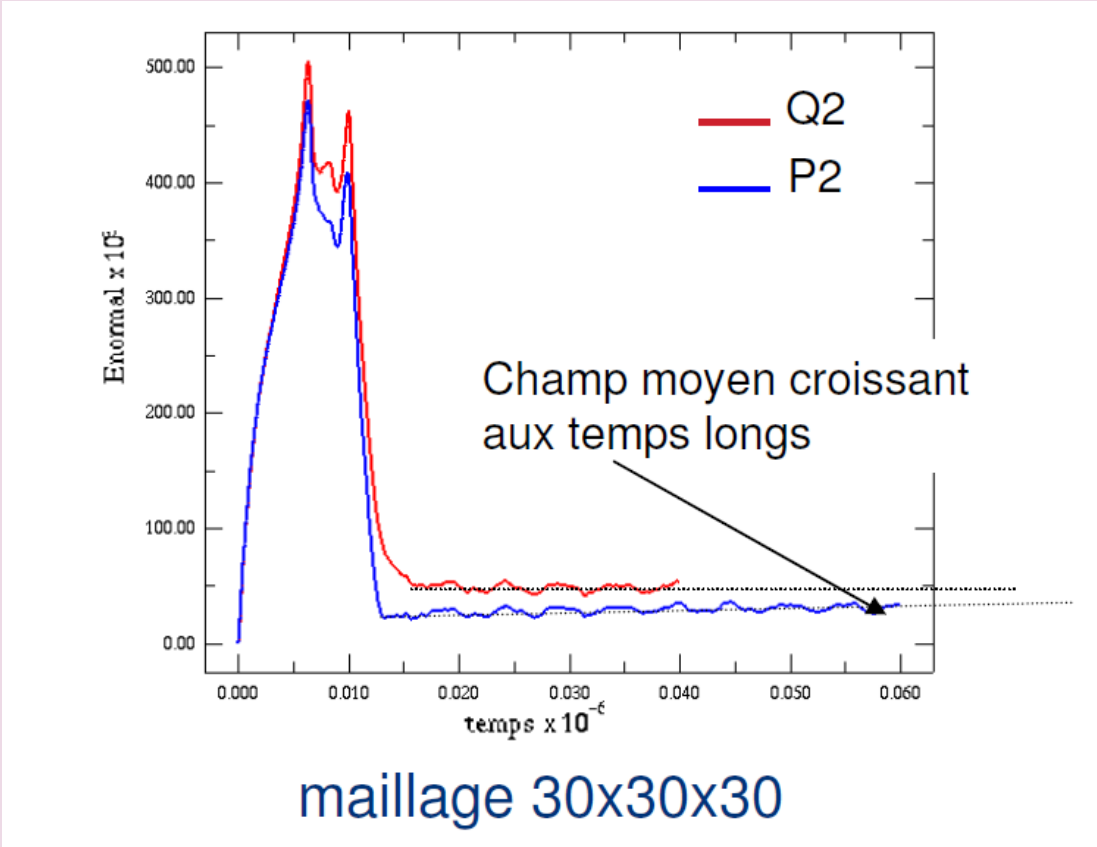

FIG.: Normal electric field near emissive plate

Results obtained after correction can be even worse than those without correction !

Numerical artefacts induced by PHM

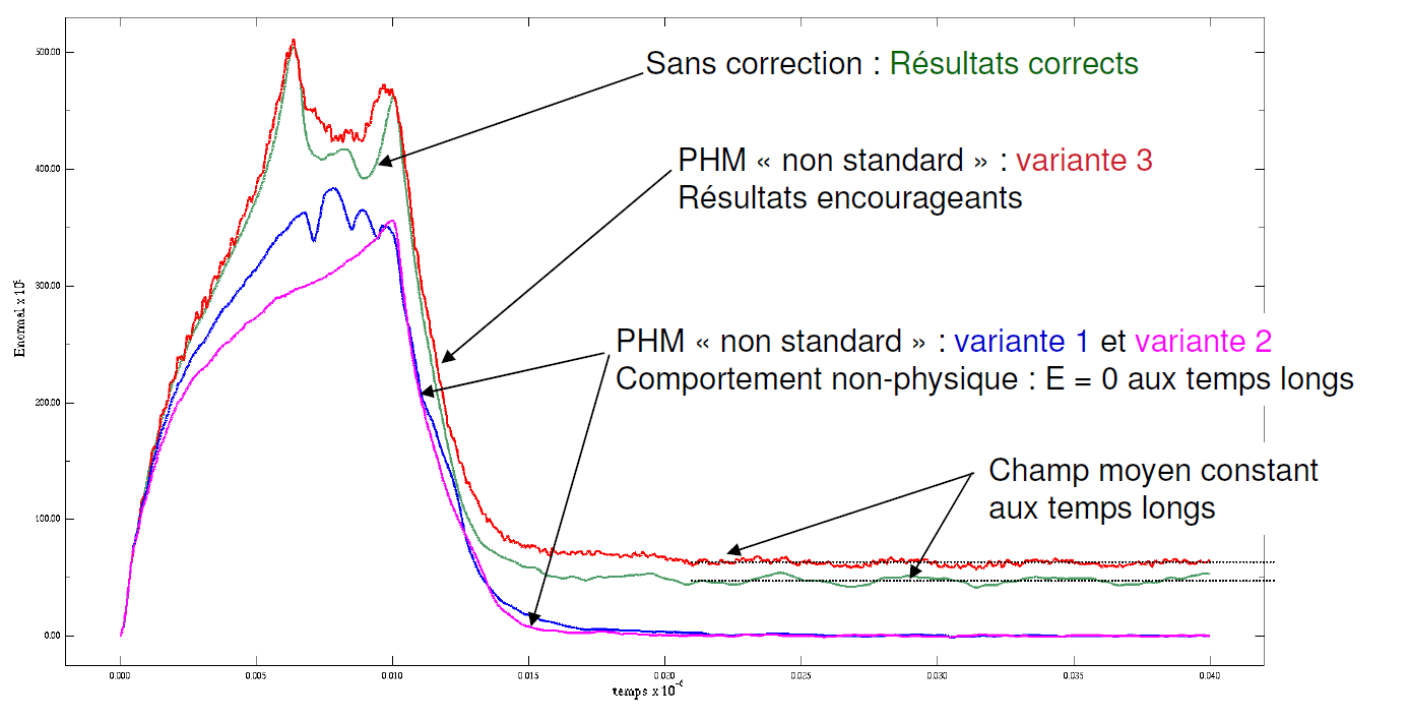

FIG.: Normal electric field near emissive plate

Results obtained with centered fluxes

DGTD

- Bad with general meshes (lower convergence order, unphysical solutions for discontinuous meshes)
- For spurious schemes, encourage spurious errors
- For nonspurious schemes (Mounier, Campos-Pinto, Sonnendrücker (to appear in Applied Math and Computation 2015)) cannot cope with meshes with hanging nodes

DGTD-PIC

- Bad with general meshes (Example of Crestetto : 2D PHM on triangular meshes)
- Encourage false statistical-like noise
- Bad for charge conservation on general meshes including grids with hanging nodes

DGTD scheme (part one)

From equation :

$$A_0 \partial_t U + A(\partial) U = S(t, x, y, z),$$

A way to write the DGTD scheme is :

$$\frac{d}{dt}\mathbf{U}_K + (M_K^{-1} R_K)\mathbf{U}_K + \sum_{L \in \nu(K)} M_K^{-1} F_{KL}^{in} \mathbf{U}_K + \sum_{L \in \nu(K)} (M_K^{-1} F_{KL}^{out})\mathbf{U}_L + \sum_{L \in \nu_{bound}(K)} M_K^{-1} F_{KL}^{bound} \mathbf{U}_K = M_K^{-1} \mathbf{S}_K.$$

With Mass Matrix :

$$M_K = \begin{pmatrix} \left\langle \left\langle A_0 \psi_1^K, \psi_1^{test,K} \right\rangle \right\rangle_{L^2(\Omega_K)} & \cdots & \left\langle \left\langle A_0 \psi_{dof_{tot}^K}^K, \psi_1^{test,K} \right\rangle \right\rangle_{L^2(\Omega_K)} \\ \vdots & \ddots & \vdots \\ \left\langle \left\langle A_0 \psi_1^K, \psi_{dof_{tot}^{test,K}}^{test,K} \right\rangle \right\rangle_{L^2(\Omega_K)} & \cdots & \left\langle \left\langle A_0 \psi_{dof_{tot}^K}^K, \psi_{dof_{tot}^{test,K}}^{test,K} \right\rangle \right\rangle_{L^2(\Omega_K)} \end{pmatrix}$$

DGTD scheme (part two)

Stiffness Matrix :

$$R_K = -\begin{pmatrix} \left\langle\left\langle \psi_1^K, A(\partial)\psi_1^{test,K} \right\rangle\right\rangle_{L^2(\Omega_K)} & \cdots & \left\langle\left\langle \psi_{dof_{tot}^K}^K, A(\partial)\psi_1^{test,K} \right\rangle\right\rangle_{L^2(\Omega_K)} \\ \vdots & \ddots & \vdots \\ \left\langle\left\langle \psi_1^K, A(\partial)\psi_{dof_{tot}^{test,K}}^{test,K} \right\rangle\right\rangle_{L^2(\Omega_K)} & \cdots & \left\langle\left\langle \psi_{dof_{tot}^K}^K, A(\partial)\psi_{dof_{tot}^{test,K}}^{test,K} \right\rangle\right\rangle_{L^2(\Omega_K)} \end{pmatrix}$$

Interior Fluxes

$$F_{KL}^{in} = \begin{pmatrix} \left\langle \frac{A_{in}^{\gamma}(n_{KL})}{2}\psi_1^K, \psi_1^{test,K} \right\rangle_{L^2(\partial\Omega_K)} & \cdots & \left\langle \frac{A_{in}^{\gamma}(n_{KL})}{2}\psi_{dof_{tot}^K}^K, \psi_1^{test,K} \right\rangle_{L^2(\partial\Omega_K)} \\ \vdots & \ddots & \vdots \\ \left\langle \frac{A_{in}^{\gamma}(n_{KL})}{2}\psi_1^K, \psi_{dof_{tot}^{test,K}}^{test,K} \right\rangle_{L^2(\partial\Omega_K)} & \cdots & \left\langle \frac{A_{in}^{\gamma}(n_{KL})}{2}\psi_{dof_{tot}^K}^K, \psi_{dof_{tot}^{test,K}}^{test,K} \right\rangle_{L^2(\partial\Omega_K)} \end{pmatrix}$$

DGTD scheme (part three)

Exterior flux linked with neighboring unknown U_L is :

$$F_{KL}^{out} = \begin{pmatrix} \left\langle \frac{A_{out}^{\gamma}(n_{KL})}{2}\psi_1^L, \psi_1^{test,K} \right\rangle_{L^2(\partial\Omega_K)} & \cdots & \left\langle \frac{A_{out}^{\gamma}(n_{KL})}{2}\psi_{dof_{tot}^L}^L, \psi_1^{test,K} \right\rangle_{L^2(\partial\Omega_K)} \\ \vdots & \ddots & \vdots \\ \left\langle \frac{A_{out}^{\gamma}(n_{KL})}{2}\psi_1^L, \psi_{dof_{tot}^{test,K}}^{test,K} \right\rangle_{L^2(\partial\Omega_K)} & \cdots & \left\langle \frac{A_{out}^{\gamma}(n_{KL})}{2}\psi_{dof_{tot}^L}^L, \psi_{dof_{tot}^{test,K}}^{test,K} \right\rangle_{L^2(\partial\Omega_K)} \end{pmatrix}$$

Boundary fluxes are added to inforce chosen boundary conditions whenever needed

Fluxes are parametrized through the choice of $0 \leq \gamma \leq 1$

$$A_{in}^{\gamma}(n_{KL}) = (1+\gamma)A^+(n_{KL}) + (1-\gamma)A^-(n_{KL})$$

$$A_{out}^{\gamma}(n_{KL}) = (1-\gamma)A^+(n_{KL}) + (1+\gamma)A^-(n_{KL})$$

New DGTD(-PIC) scheme

Choices

- Explicit time scheme : RK4 or LF2
- Full Upwind Fluxes : $\gamma = 1$
  ($\gamma = 0$ would be Centered Fluxes)

Nodal basis functions used for new DGTD(-PIC)

Approximation space

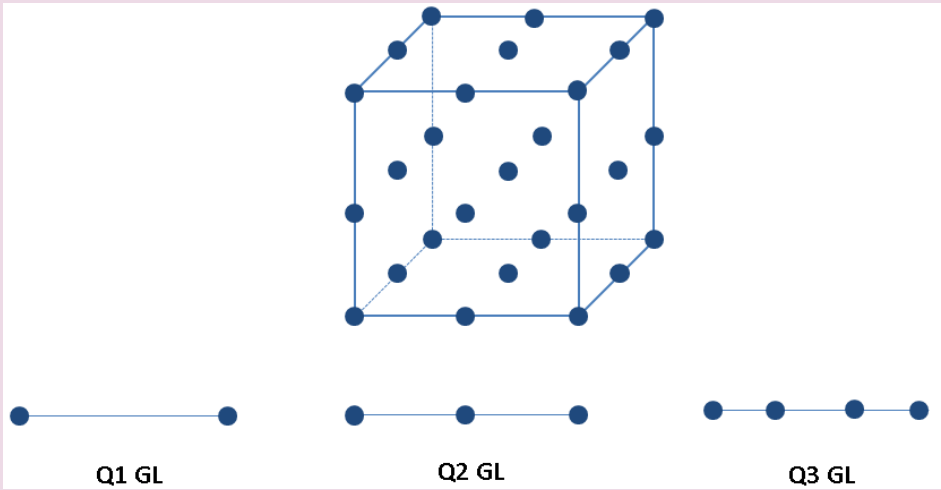

FIG.: Gauss Lobatto tensor product basis functions

Lumping

- Lagrange basis functions defined from Gauss-Lobatto quadrature points
- Gauss-Lobatto quadrature rule $\mapsto$ Approximation of Integrals in DG matrices

PIC to solve Vlasov equation

Macro-particle α is a clustering of particles with same position and momentum :

$$f(X,p,t) = \sum_{\alpha=1}^{N} w_\alpha \ \delta(X - X_\alpha(t)) \ \delta(p - p_\alpha(t))$$

δ denotes the Dirac measure.

Current density $J(f)$ is given by :

$$J(X,t) = q_e \int f \ v \ dp = \sum_{\alpha=1}^{N} q_\alpha v_\alpha(t) \delta(X - X_\alpha(t)) \qquad (1)$$

Each macro-particle evolution is described by the fundamental laws of dynamics (ODE) :

$$\begin{cases} \frac{dX_\alpha}{dt} = v_\alpha \\ \frac{dp_\alpha}{dt} = q_\alpha(E_\alpha + v_\alpha \times B_\alpha) \end{cases}$$

Details of charge conserving PIC algorithm

1. Classical relativistic Boris pusher based on DG fields at macroparticle location
2. Each macroparticle α of charge qw_α remaining in cell Ω_K for $t \in [\tau_\alpha, \tau_\alpha + \Delta\tau_\alpha) \subset [t_n, t_{n+1})$ contributes to create in Ω_K the DGTD current source term given as follows (no Dirac smoothing, like Crestetto and Helluy)

$$\int_{\Omega_K} J\varphi_i^K = \sum_{\alpha=1}^{N_{inside}^K} \frac{1}{\Delta t} \int_{\tau_\alpha}^{\tau_\alpha+\Delta\tau_\alpha} qw_\alpha v(t)\ \varphi_i^K(x_\alpha(t))\ dt$$

Since $\int_{\Omega_K} \delta(X - X_\alpha(t))\varphi_i^K(x)\ dX = \varphi_i^K(x_\alpha(t))$.

Stringent case to validate charge conservation $\mapsto$ OK

3D diode (validated over 1 μs)

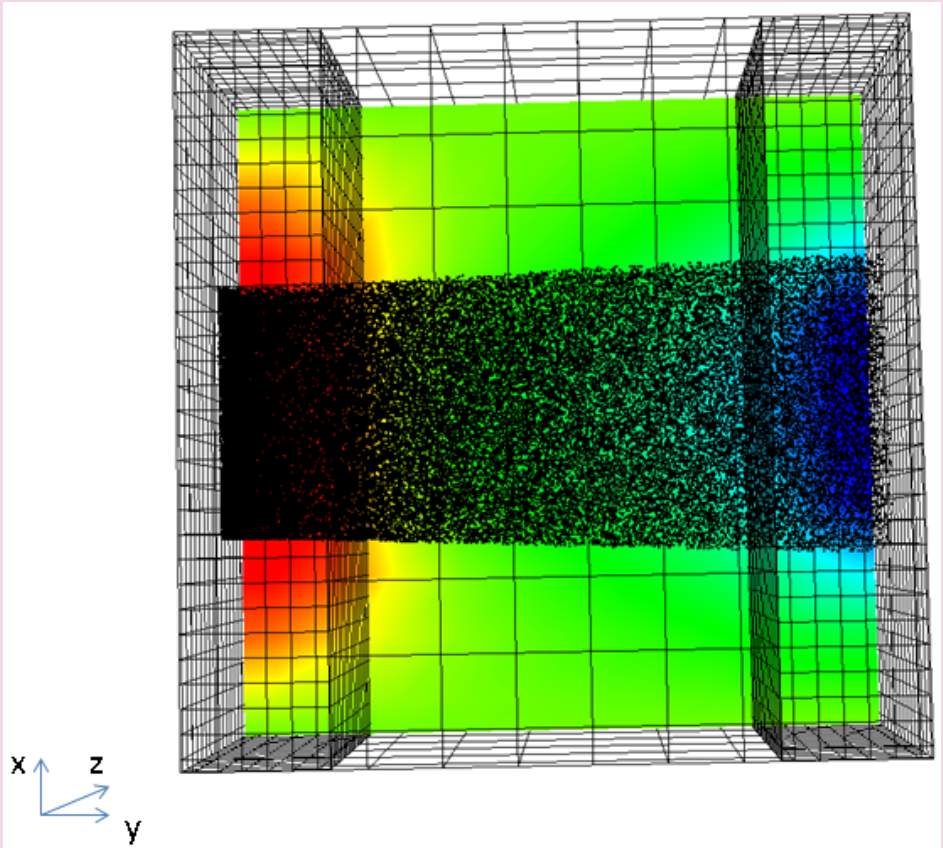

FIG.: Electronic emission is caused by an external electrical field. After a transient phase, the induced field should remain static (equilibrium state). A coarser mesh is successfullly used in the middle.

What happens without a charge conserving scheme

3D diode

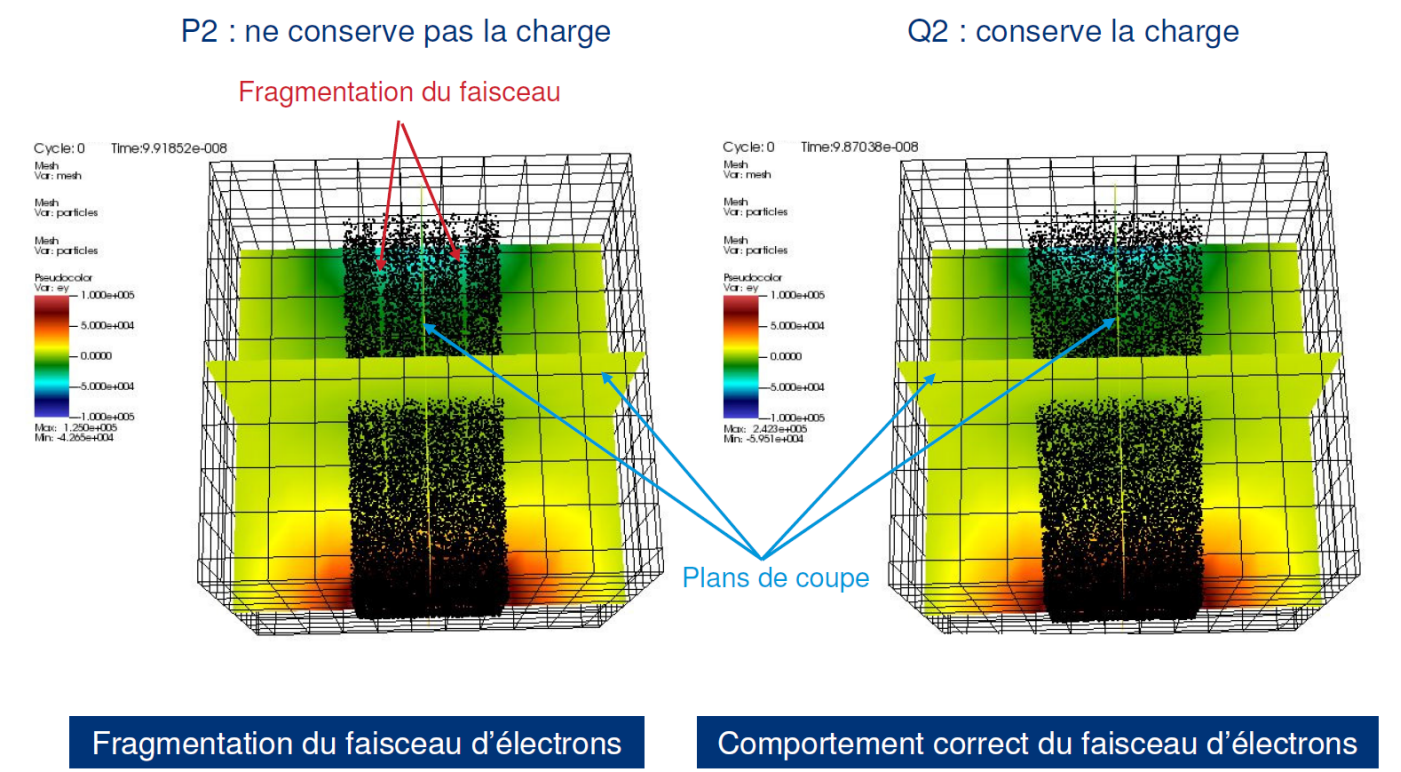

FIG.: Simulation time : 10 ns, results obtained with and without charge conservation

Interest of high order

Question

PIC algorithm is pretty inaccurate (assumption that the Lorentz Force remains constant during a time step).

$\mapsto$ Is there any use in coupling PIC with a high order DGTD scheme ?

Answer

It is not only useful but sometimes necessary given performance requirements

Next numerical results

Illustrated by results given on cubic mesh (allows comparison with FDTD-PIC)

Interest of high order : first example

Coarsest mesh allowing convergence : increased computational efficiency

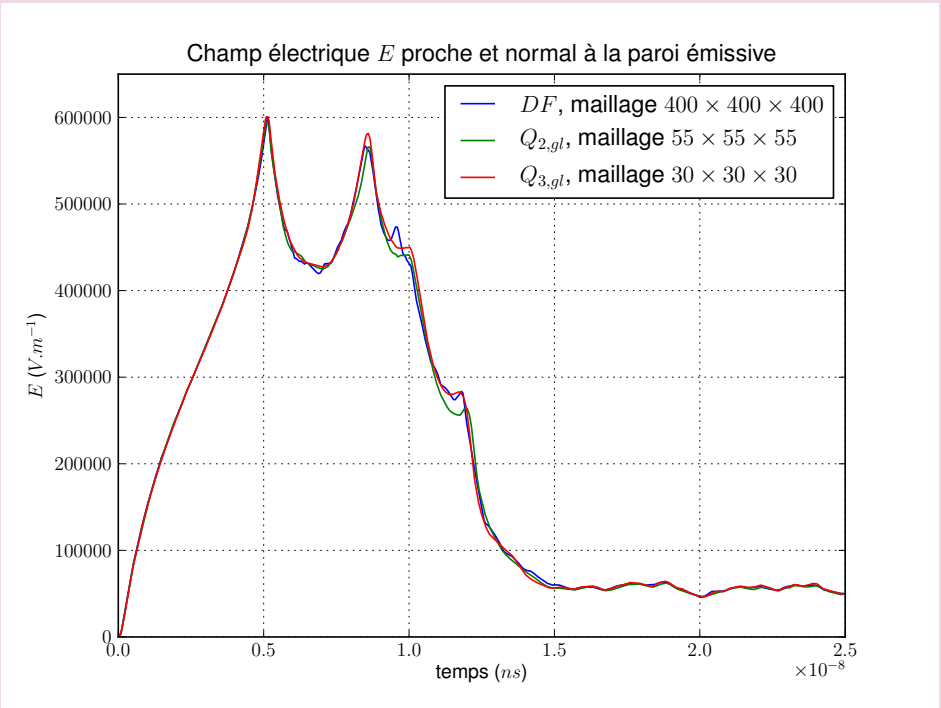

FIG.: Normal field in the case mentioned as a counterexample for correction methods

Necessity of high order

What is high order ?

The scheme must converge at speed 3, which is true for polynomial basis functions of order greater than 1

Fluctuation in convergence for low orders $\mapsto$ not happening for high order !

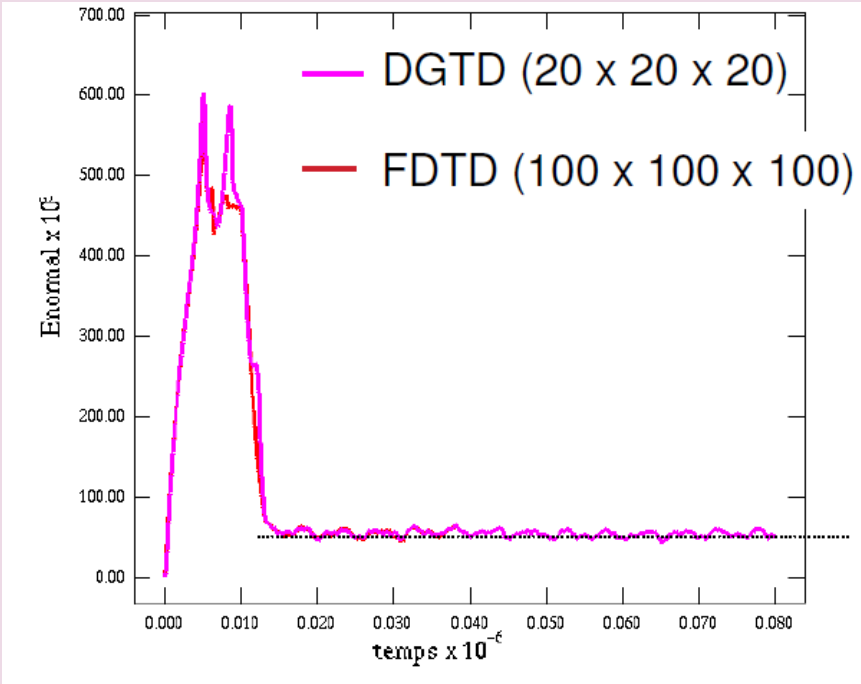

FIG.: Abnormal damping of the plasma oscillation for mesh $100 \times 100 \times 100$

Conclusion

Presentation of a new DGTD-PIC method

- Charge is conserved even with hanging nodes (cartesian mesh with subgrids)
- Coupling high order DGTD with PIC has been shown to be a very rewarding choice since High order convergence (obvious in DGTD) has been achieved in DGTD-PIC (ability to reach converged state using much coarser meshes)

Outlook

More general meshes

1. This new method is genuinely discontinuous (no continuous reconstruction assumed)

2. No feature of the method is mesh-dependent (most DGTD-PIC relying on Dirac regularization scaled on local cell size)

   $\mapsto$ The proposed method is a good candidate to conserve charge on general meshes

Computational efficiency

Increase efficiency by using tensor product structure of proposed basis functions

Thank you for your attention !