On structure-preserving DG-PIC schemes for the Vlasov-Maxwell system

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— jointwork with —

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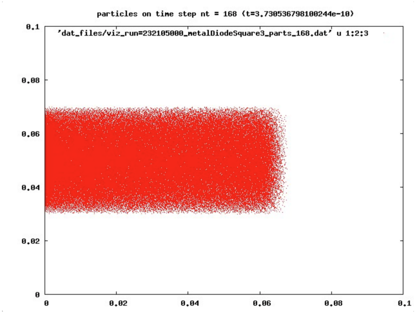
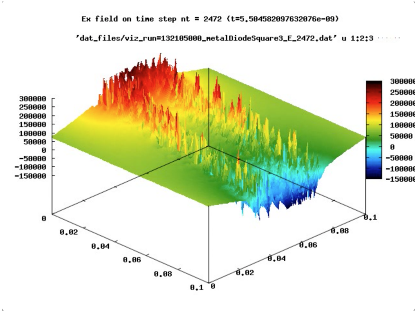
London Kinetic conference, Imperial College

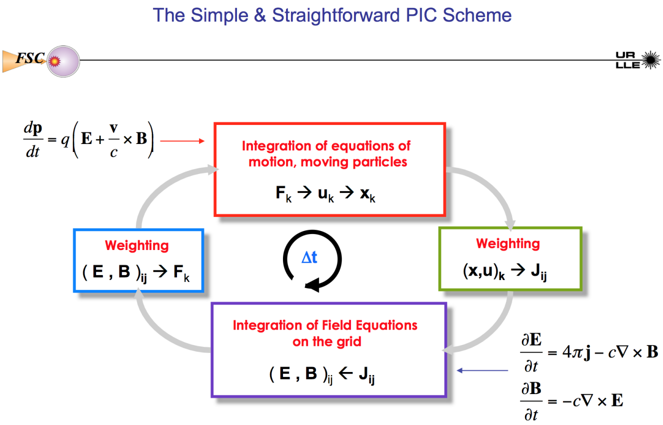
Motivation : an academic diode with DG-PIC





- beam of electrons emitted on the left boundary, accelerated by $\boldsymbol{E}_{\text{ext}}$
- Vlasov-Maxwell solved with DG-PIC scheme (here without dissipation)
- plots : point particles (left) and self-consistent E_x (right)

A well-respected approach : Particle-in-Cell + Maxwell



(Slide borrowed from Chuang Ren (Rochester), 2011 HEDP Summer School)

▷ Bob Glassey and Jack Schaeffer (SINUM '91), convergence analysis in 1.5D

DG for the 2D Maxwell system

- time-dependent 2D Maxwell

$$\begin{cases} \partial_t \boldsymbol{E} - \mathbf{curl}\, B = -\boldsymbol{J} & \text{(Ampère)} \\ \partial_t B + \mathrm{curl}\, \boldsymbol{E} = 0 & \text{(Faraday)} \end{cases}$$

- DG solutions sought in discontinuous spaces :

$$\tilde{\boldsymbol{E}}_h \in \tilde{V}_h^1 := \mathbb{P}_p(\mathcal{T}_h)^2, \qquad B_h \in V_h^2 := \mathbb{P}_p(\mathcal{T}_h)$$

- (semi-discrete) centered DG formulation

$$\begin{cases} \langle \partial_t \tilde{\boldsymbol{E}}_h, \tilde{\varphi}^1 \rangle - \langle B_h, \mathrm{curl}_h\, \tilde{\varphi}^1 \rangle - \langle \{B_h\}, [\tilde{\varphi}^1] \rangle_{\mathcal{F}_h} = -\langle \boldsymbol{J}, \tilde{\varphi}^1 \rangle, & \tilde{\varphi}^1 \in \tilde{V}_h^1 \\ \langle \partial_t B_h, \varphi^2 \rangle + \langle \tilde{\boldsymbol{E}}_h, \mathbf{curl}_h\, \varphi^2 \rangle + \langle \{\tilde{\boldsymbol{E}}_h\}, [\varphi^2] \rangle_{\mathcal{F}_h} = 0, & \varphi^2 \in V_h^2 \end{cases}$$

- convergence estimates (Fezoui, Lanteri, Lohrengel, Piperno '05)

$$\|(\boldsymbol{E} - \tilde{\boldsymbol{E}}_h)(T)\| + \|(B - B_h)(T)\| \leq C(T) h^p \|(\boldsymbol{E}, B)\|_{\mathcal{C}^0(0,T:H^{p+1})}$$

with $C(T) \sim T$, see also (Hesthaven, Warburton '02)

▷ Can we remove the dependence on T for certain classes of "nice" solutions ?

Why DG ?

- Curl-conforming Finite Element Method give good results :

$$\text{find } \boldsymbol{E}_h \in V_h^1 \subset H(\mathrm{curl};\Omega), \qquad B_h \in V_h^2 \subset L^2(\Omega),$$

$$\begin{cases} \langle \partial_t \boldsymbol{E}_h, \varphi^1 \rangle - \langle B_h, \mathrm{curl}\, \varphi^1 \rangle = -\langle \boldsymbol{J}, \varphi^1 \rangle, & \varphi^1 \in V_h^1 \\ \langle \partial_t B_h, \varphi^2 \rangle + \langle \mathrm{curl}\, \boldsymbol{E}_h, \varphi^2 \rangle = 0, & \varphi^2 \in V_h^2 \end{cases}$$

- But explicit (leap-frog) time stepping gives

$$\mathbf{M}^1 \mathbf{E}^{n+1} = \mathbf{M}^1 \mathbf{E}^n + \Delta t \big(\mathbf{C}^{2,1} \mathbf{B}^{n+\frac{1}{2}} - \mathbf{J}^{n+\frac{1}{2}} \big)$$
$$\mathbf{M}^2 \mathbf{B}^{n+\frac{1}{2}} = \mathbf{M}^2 \mathbf{B}^{n-\frac{1}{2}} - \Delta t \mathbf{C}^{1,2} \mathbf{E}^n$$

- in FEM : $\mathbf{M}^1 =$ mass matrix in curl-conforming V_h^1
  - different cells are coupled
  - inversion $\Longrightarrow$ global solve,
  - no efficient lumping procedure
- in DG : $\mathbf{M}^1 = \tilde{\mathbf{M}}^1 =$ mass matrix in discontinuous $\tilde{V}_h^1$
  - block diagonal, no coupling
  - trivial parallelization, (much) faster time marching

Outline

Outline

Observation : Gauss laws not satisfied at discrete level

- time-dependent Maxwell eqs :

$$\begin{cases} \partial_t \boldsymbol{E} - \mathbf{curl}\, B = -\boldsymbol{J} & \text{(Ampère)} \\ \partial_t B + \mathrm{curl}\, \boldsymbol{E} = 0 & \text{(Faraday)} \end{cases}$$

- Gauss laws (constraints) :

$$\begin{cases} \mathrm{div}\, \boldsymbol{E} = \rho \\ \mathrm{div}\, B = 0 \end{cases}$$

- data :

$$\begin{cases} \boldsymbol{E}^0, B^0 & \text{(initial fields)} \\ \rho, \boldsymbol{J} & \text{(charge and current densities)} \end{cases}$$

- if Ampère and Faraday hold, then

$$\left\{ \text{Gauss}(t=0) \;\text{ and }\; \partial_t \rho + \mathrm{div}\, \boldsymbol{J} = 0 \right\} \iff \text{Gauss}(t \geq 0)$$

- Pbm : Gauss laws are not preserved by DG solutions (growing errors)

A practical solution : correct the field

- Boris correction (1970) :

$$\begin{cases} \Delta\phi = \operatorname{div} E - \rho \\ E_{\text{corrected}} = E - \nabla\phi \end{cases}$$

- Marder/Langdon correction (1987/1992) :

$$\begin{cases} E^{n+1}_{\text{corrected}} = E^{n+1} + \Delta t \nabla \big[d(\operatorname{div} E^n - \rho^n) \big] \\ E^{n+1}_{\text{corrected}} = E^{n+1} + \Delta t \nabla \big[d(\operatorname{div} E^{n+1} - \rho^{n+1}) \big] \end{cases} \qquad \text{with} \quad d \le \frac{1}{2\Delta t} \left(\frac{\Delta x^2 \Delta y^2}{\Delta x^2 + \Delta y^2} \right)$$

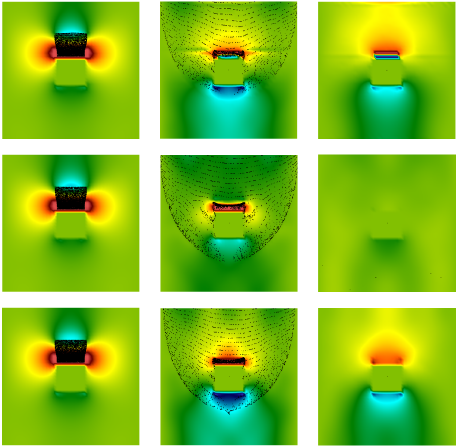
- Hyperbolic correction (2000) :

$$\begin{cases} \partial_t E - \operatorname{curl} B = -J - \nabla\phi \\ \partial_t B + \operatorname{curl} E = 0 \\ \partial_t \phi = \chi^2(\rho - \operatorname{div} E) \end{cases}$$

  - see e.g. (Munz, Omnes, Schneider, Sonnendrücker and Voß '00)

- Satisfactory results, but :
  - non-local corrections or non-physical propagation speeds
  - require additional equations and additional boundary conditions
  - causes of instability maybe not always well understood

Illustration : external impact on a metallic object



electrons leaving a metallic object after short laser impact, $t = 5, 10, 50$ (ns, left to right) with DG-PIC solvers ($\mathbb{Q}_1$ on 60×60 mesh) [sim M. Mounier].

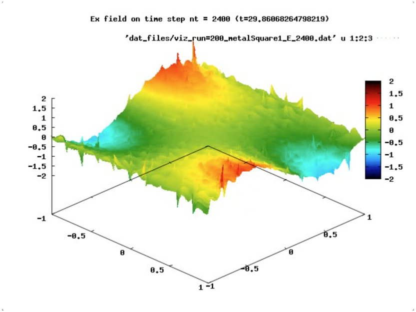
Top to bottom : uncorrected, with hyperbolic field correction, source correction.

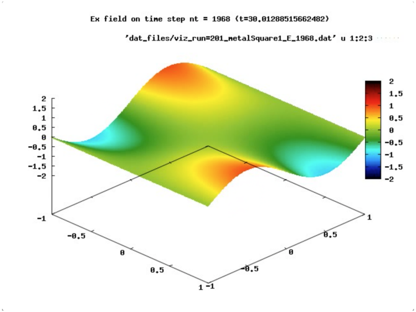
Special case : Maxwell system with exact source

- Model problem with analytical source (Issautier, Poupaud, Cioni and Fezoui '95)

$$\boldsymbol{J}(t,x,y) = (\cos(t) - 1)\begin{pmatrix} \pi\cos(\pi x) + \pi^2 x \sin(\pi y) \\ \pi\cos(\pi y) + \pi^2 y \sin(\pi x) \end{pmatrix} - \cos(t)\begin{pmatrix} x\sin(\pi y) \\ y\sin(\pi x) \end{pmatrix}$$

- Exact continuity equation ($\partial_t \rho + \operatorname{div} \boldsymbol{J} = 0$) satisfied by the sources !
- Numerical test : Centered DG (left) vs curl-conforming FEM (right)





Outline

Gauss-compatible Maxwell schemes with exact source

- Maxwell in "composite" form ($U = \binom{E}{B}$ and $F = \binom{J}{0}$) reads

$$\partial_t U - \mathcal{A} U = -F \qquad \text{with} \qquad \mathcal{A} = \begin{pmatrix} 0 & \text{curl} \\ -\text{curl} & 0 \end{pmatrix}$$

- Definition : a semi-discrete scheme ($U_h = \binom{E_h}{B_h} \in \mathcal{V}_h$) of the form

$$\partial_t U_h - \mathcal{A}_h U_h = -\Pi_h F \qquad \text{with} \qquad \mathcal{A}_h : \mathcal{V}_h \to \mathcal{V}_h, \qquad \mathcal{A}_h = -\mathcal{A}_h^*$$

is **Gauss-compatible** if there exists $\hat{\Pi}_h : \hat{\mathcal{V}} \to \mathcal{V}_h$ such that

$$\boxed{\Pi_h \mathcal{A} V = \mathcal{A}_h \hat{\Pi}_h V \quad \text{for} \quad V \in \hat{\mathcal{V}}}$$

- Theorem (CP and Sonnendrücker '14) : solutions to Gauss-compatible schemes satisfy

$$\|(U_h - \hat{\Pi}_h U)(t)\| \le \|U_h^0 - \hat{\Pi}_h U^0\| + \int_0^t \|(\Pi_h - \hat{\Pi}_h)\partial_t U(s)\| \, \mathrm{d}s$$

▷ long-time stability for the pure Maxwell system

Structure-Preserving schemes : basic criterion

- the semi-discrete Maxwell system

$$\begin{cases} \partial_t \boldsymbol{E}_h - \mathbf{curl}_h B_h = -\dfrac{1}{\varepsilon_0}\boldsymbol{J}_h \\ \partial_t B_h + \mathrm{curl}_h \boldsymbol{E}_h = 0 \end{cases} \qquad \text{preserves} \qquad \mathrm{div}_h \boldsymbol{E}_h = \frac{1}{\varepsilon_0}\rho_h$$

  as long as

$$\partial_t \rho_h + \mathrm{div}_h \boldsymbol{J}_h = 0 \qquad \text{and} \qquad \mathrm{div}_h \mathbf{curl}_h = 0$$

  ... but what should one take for div_h ?

- example 1 (FEM = curl-conforming V_h^1) : take $V_h^0 \xrightarrow{\mathbf{grad}} V_h^1$, then

$$\mathrm{div}_h = (-\mathbf{grad}_h)^* : V_h^1 \to V_h^0$$

  is a proper discrete divergence

- example 2 (DG = discontinuous $\tilde{V}_h^1$) : again, take $V_h^0 \xrightarrow{\mathbf{grad}} \tilde{V}_h^1$, then

$$\mathrm{div}_h = (-\mathbf{grad}_h)^* : \tilde{V}_h^1 \to V_h^0$$

  satisfies $\mathrm{div}_h \mathbf{curl}_h = 0$ but is not a proper discrete divergence

Structure-Preserving scheme : one definition

- Def : the semi-discrete Maxwell system

$$\begin{cases} \partial_t \boldsymbol{E}_h - \mathbf{curl}_h B_h = -\boldsymbol{J}_h \\ \partial_t B_h + \mathrm{curl}_h \boldsymbol{E}_h = 0 \\ \mathrm{div}_h \boldsymbol{E}_h = \rho_h \end{cases} \qquad \text{with} \qquad \begin{cases} \mathbf{curl}_h := (\mathrm{curl}_h)^* \\ \mathrm{curl}_h : V_h^1 \to V_h^2 \\ \mathrm{div}_h : V_h^1 \to V_h^0 \end{cases}$$

(and $\int B_h = \int B_h^0$) is **structure-preserving** if the following holds :

▷ Exact sequence property : the sequence

$$V_h^0 \xrightarrow{\mathbf{grad}_h := (\mathrm{div}_h)^*} V_h^1 \xrightarrow{\mathrm{curl}_h} V_h^2 \xrightarrow{\int} \mathbb{R}$$

is exact in the sense that $\mathbf{grad}_h V_h^0 = \ker \mathrm{curl}_h$ and $\mathrm{curl}_h V_h^1 = \ker(\int_{|V_h^2})$.

▷ Uniform stability : the above operators satisfy

$$\begin{aligned} \|u\| &\le c_P \|\mathbf{grad}_h u\|, \qquad & u &\in V_h^0 \cap (\ker \mathbf{grad}_h)^\perp \\ \|\boldsymbol{u}\| &\le c_P \|\mathrm{curl}_h \boldsymbol{u}\|, \qquad & \boldsymbol{u} &\in V_h^1 \cap (\ker \mathrm{curl}_h)^\perp \end{aligned}$$

with a constant c_P independent of h.

Equivalent definition in “composite” form

- Let
$$\mathcal{A}_h = \begin{pmatrix} 0 & (\mathrm{curl}_h)^* \\ -\mathrm{curl}_h & 0 \end{pmatrix} : (V_h^1 \times V_h^2) \to (V_h^1 \times V_h^2)$$
and
$$\mathcal{D}_h = \begin{pmatrix} \mathrm{div}_h & 0 \\ 0 & \int_{|V_h^2} \end{pmatrix} : (V_h^1 \times V_h^2) \to (V_h^0 \times \mathbb{R})$$
- Then the semi-discrete Maxwell system reads
$$\partial_t U_h - \mathcal{A}_h U_h = \begin{pmatrix} -\boldsymbol{J}_h \\ 0 \end{pmatrix} \qquad \text{and} \qquad \mathcal{D}_h U_h = \begin{pmatrix} \rho_h \\ \int B_h^0 \end{pmatrix}$$
$(U_h := \left(\begin{smallmatrix} \boldsymbol{E}_h \\ B_h \end{smallmatrix}\right))$ and it is structure-preserving iff

$$\begin{cases} \ker \mathcal{D}_h = (\ker \mathcal{A}_h)^\perp & \textit{(Compatibility of the kernels)} \\ \|Z\| \le c_P \|\mathcal{A}_h Z\|, \quad Z \in (\ker \mathcal{A}_h)^\perp & \textit{(Stability of the composite curl)} \\ \|Z\| \le c_P \|\mathcal{D}_h Z\|, \quad Z \in (\ker \mathcal{D}_h)^\perp & \textit{(Stability of the composite divergence)} \end{cases}$$

Long-time stability

- Lemma (long-time stability) : let U_h be a solution to $\partial_t U_h - \mathcal{A}_h U_h = -F_h := \begin{pmatrix} -\boldsymbol{J}_h \\ 0 \end{pmatrix}$ with $\mathcal{A}_h$ and $\mathcal{D}_h$ as above. Then
  - the discrete Gauss laws

    $$\mathcal{D}_h U_h = \begin{pmatrix} \rho_h \\ \int B_h^0 \end{pmatrix}$$

    are preserved, provided the sources satisfy the discrete continuity equation

    $$\partial_t \rho_h + \mathrm{div}_h \boldsymbol{J}_h = 0$$

  - and we have a long-time stability estimate

    $$\|U_h(t)\| \lesssim (\text{initial terms}) + \|\rho_h(t)\| + \|\boldsymbol{J}_h(t)\| + \Big\| \int_0^t e^{(t-s)\mathcal{A}_h} \partial_t F_h(s)\,\mathrm{d}s \Big\|$$

- Proof : Gauss laws follows from $\mathcal{D}_h \mathcal{A}_h = 0$. For the estimate, write $U_h = U_{(0)} + U_\perp \in \ker \mathcal{A}_h \oplus (\ker \mathcal{A}_h)^\perp = (\ker \mathcal{D}_h)^\perp \oplus (\ker \mathcal{A}_h)^\perp$, so that

$$\|U_h\| \le \|U_{(0)}\| + \|U_\perp\| \le c_P(\|\mathcal{D}_h U_{(0)}\| + \|\mathcal{A}_h U_\perp\|) = c_P(\|\mathcal{D}_h U_h\| + \|\mathcal{A}_h U_h\|)$$

then control $\mathcal{D}_h U_h$ with the sources and $\mathcal{A}_h U_h$ with the evolution equation

$$\partial_t(\mathcal{A}_h U_h - F_h) = \mathcal{A}_h \partial_t U_h - \partial_t F_h = \mathcal{A}_h(\mathcal{A}_h U_h - F_h) - \partial_t F_h$$

Outline

Application to DG

- Preliminary step : observe that in 2D, the DG curl satisfies

$$\mathrm{curl}_h = \mathrm{curl}\,\mathcal{P}_h^1 : \tilde{V}_h^1 \to V_h^2$$

  with $\mathcal{P}_h^1 : \tilde{V}_h^1 \to V_h^1$ averaged Nedelec interpolation (smoothing)
- Step 1. Identify

$$\mathrm{curl}_h\,\tilde{V}_h^1 = \mathrm{curl}\,V_h^1 = \ker(\textstyle\int_{|V_h^2}) \quad \text{and} \quad \ker \mathrm{curl}_h = \underbrace{\ker \mathrm{curl}|_{V_h^1}}_{= \mathbf{grad}\,V_h^0} \oplus (I - \mathcal{P}_h^1)\,\tilde{V}_h^1$$

- Step 2. Let $\mathbf{grad}_h : (V_h^0 \times \tilde{V}_h^1) \ni (\psi, \tilde{\varphi}) \to \mathbf{grad}\,\psi + (I - \mathcal{P}_h^1)\tilde{\varphi} \in \tilde{V}_h^1$ so that

$$(V_h^0 \times \tilde{V}_h^1) \xrightarrow{\mathbf{grad}_h} \tilde{V}_h^1 \xrightarrow{\mathrm{curl}_h} V_h^2 \xrightarrow{\int} \mathbb{R}$$

  is exact (and prove the uniform stability of these operators)
- Step 3. State the resulting discrete continuity equation :

$$\langle \partial_t \rho_h, \varphi \rangle + \langle \tilde{\boldsymbol{J}}_h, -\mathbf{grad}\,\psi \rangle + \langle \tilde{\boldsymbol{J}}_h, (I - \mathcal{P}_h^1)\tilde{\varphi} \rangle = 0 \qquad \text{for } (\psi, \tilde{\varphi}) \in V_h^0 \times \tilde{V}_h^1$$

Application to DG-PIC

- N-particle approximation for f (with smooth shapes of radius $\varepsilon > 0$)

$$f_N(t, \boldsymbol{x}, \boldsymbol{v}) := \sum_{k=1}^{N} q_k \zeta_\varepsilon(\boldsymbol{x} - \boldsymbol{x}_k(t))\zeta_\varepsilon(\boldsymbol{v} - \boldsymbol{v}_k(t))$$

- Associated particle approximations for ρ and $\boldsymbol{J}$:

$$\rho_N(t, \boldsymbol{x}) := \sum_{k=1}^{N} q_k \zeta_\varepsilon(\boldsymbol{x} - \boldsymbol{x}_k(t)), \qquad \boldsymbol{J}_N(t, \boldsymbol{x}) := \sum_{k=1}^{N} q_k \boldsymbol{v}_k(t) \zeta_\varepsilon(\boldsymbol{x} - \boldsymbol{x}_k(t))$$

Note : they satisfy an exact continuity equation $\partial_t \rho_N + \operatorname{div} \boldsymbol{J}_N = 0$

- Current deposition scheme : from $\boldsymbol{J}_N$, define the DG source $\tilde{\boldsymbol{J}}_h \in \tilde{V}_h^1$ by

$$\langle \tilde{\boldsymbol{J}}_h, \tilde{\varphi} \rangle = \langle \boldsymbol{J}_N, \mathcal{P}_h^1 \tilde{\varphi} \rangle, \qquad \tilde{\varphi} \in \tilde{V}_h^1$$

  - RHS computed as in FEM-PIC, and $\tilde{\boldsymbol{J}}_h$ given by a local inversion of $\tilde{\mathbf{M}}^1$
  - Note : applying $\mathcal{P}_h^1$ is local, so this can be seen as a local correction of standard DG curent deposition

- Then : check that the proper DG continuity equation holds (in $V_h^0 \times \tilde{V}_h^1$)

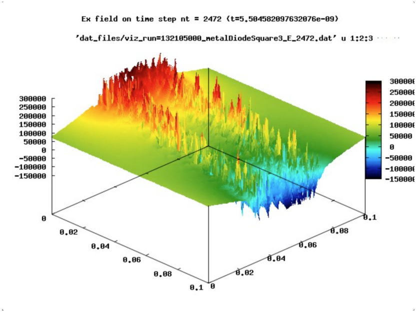
$$\partial_t \rho_h + \operatorname{div}_h \tilde{\boldsymbol{J}}_h = 0 \qquad \text{where} \quad \langle \rho_h, (\psi, \tilde{\varphi}) \rangle := \langle \rho_N, \psi \rangle, \quad (\psi, \tilde{\varphi}) \in V_h^0 \times \tilde{V}_h^1$$

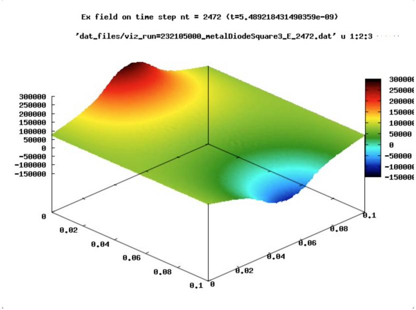
Summary and numerical validation

- The (semi-discrete) DG scheme

$$\begin{cases} \langle \partial_t \tilde{\boldsymbol{E}}_h, \tilde{\varphi}^1 \rangle - \langle B_h, \operatorname{curl}_h \tilde{\varphi}^1 \rangle - \langle \{B_h\}, [\tilde{\varphi}^1] \rangle_{\mathcal{F}_h} = -\langle \tilde{\boldsymbol{J}}_h, \tilde{\varphi}^1 \rangle, & \tilde{\varphi}^1 \in \tilde{V}_h^1 \\ \langle \partial_t B_h, \varphi^2 \rangle + \langle \tilde{\boldsymbol{E}}_h, \mathbf{curl}_h \varphi^2 \rangle + \langle \{\tilde{\boldsymbol{E}}_h\}, [\varphi^2] \rangle_{\mathcal{F}_h} = 0, & \varphi^2 \in V_h^2 \end{cases}$$

  coupled with the current deposition $\langle \tilde{\boldsymbol{J}}_h, \tilde{\varphi} \rangle = \langle \boldsymbol{J}_N, \mathcal{P}_h^1 \tilde{\varphi} \rangle$ for all $\tilde{\varphi} \in \tilde{V}_h^1$ preserves the discrete Gauss law $\operatorname{div}_h \tilde{\boldsymbol{E}}_h = \rho_h$ (in $V_h^0 \times \tilde{V}_h^1$) that makes the whole system structure-preserving, and hence is long-time stable.
- Validation : DG with standard (left) and corrected deposition (right)





Some references on conforming solvers

A. Bossavit
Solving Maxwell equations in a closed cavity, and the question of 'spurious modes' (IEEE Transactions on Magnetics 1990)

P. Monk
An analysis of Nédélec's method for the spatial discretization of Maxwell's equations (JCAM 1993)

S. Caorsi, P. Fernandes and M. Raffetto
On the convergence of Galerkin finite element approximations of electromagnetic eigenproblems (SINUM 2000)

P. Monk and L. Demkowicz
Discrete compactness and the approximation of Maxwell's equations in $\mathbb{R}^3$ (Math of Comp 2001)

R. Hiptmair
Finite elements in computational electromagnetism (Acta Numerica 2002)

M. Costabel and M. Dauge
Computation of resonance frequencies for Maxwell equations in non-smooth domains (Topics in computational wave propagation 2003)

D. Boffi
Compatible Discretizations for Eigenvalue Problems (Compatible Spatial Discretizations 2006)

D.N. Arnold, R.S. Falk and R. Winther
Finite element exterior calculus, homological techniques, and applications (Acta Numerica 2006)

Conclusion

- Some new results
  - unified analysis for conforming and nonconforming Galerkin approximations
  - problem of large deviations solved in many practical cases
  - Faraday (E/B) and Ampere (D/H) schemes treated
  - Raviart-Thomas interpolation for current densities
  - deposition schemes for point and finite-size particles
  - exact sequences for DG spaces and compatible Gauss laws
  - Conga : new DG method, free of spurious oscillations + strong Gauss law
- see `www.ljll.math.upmc.fr/~campos` for preprints

Thank you !