A general framework for structure-preserving particle approximations to Vlasov-Maxwell equations

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jointwork with

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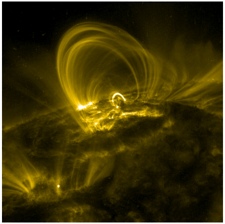
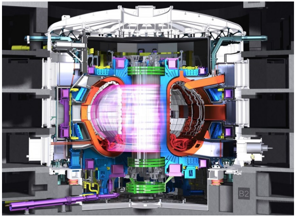
Outline

Outline

Plasmas for controlled nuclear fusion : beautiful, but complex





Advantages :

- no greenhouse gases
- no chain reaction (nuclear accidents)
- harmless fuel (hydrogen isotopes)
- manageable waste

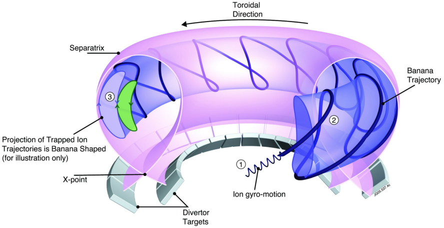
Disadvantages :

- ... no chain reaction !
- ▷ need to heat (about 100 *million* C)
- ▷ need to confine with extreme B fields
- problem complexity :

$$\begin{cases} \text{nb of particles : } N = 10^{22} \\ \text{physical scales : } \rho_e, \lambda_e \sim 10^{-4} \leftrightsquigarrow L \sim 10 \\ \text{time scales : } \omega_{ce}^{-1} \sim 10^{-10} \leftrightsquigarrow T \sim 10 \end{cases}$$

- ▷ brute force grid (space-time) : $\# \sim 10^{26}$

A hierarchy of models (I) : N-body model



- Newton law for a particle $(\boldsymbol{X}_p(t), \boldsymbol{V}_p(t))$, $p = 1 \dots N$, with mass m_p and charge q_p

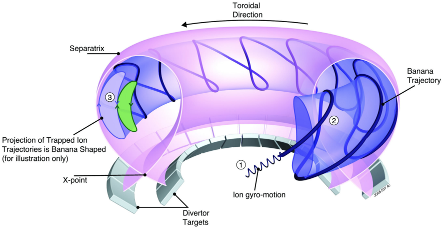
$$\begin{cases} \dfrac{\mathrm{d}\boldsymbol{X}_p}{\mathrm{d}t} = \boldsymbol{V}_p \\ \dfrac{m_p}{q_p}\dfrac{\mathrm{d}\boldsymbol{V}_p}{\mathrm{d}t} = \Big(\boldsymbol{E}_{\mathrm{ext}}(t,\boldsymbol{X}_p) + \boldsymbol{V}_p \times \boldsymbol{B}_{\mathrm{ext}}(t,\boldsymbol{X}_p)\Big) + \sum_{p' \neq p} \Big(\boldsymbol{E}_{p'}(t,\boldsymbol{X}_p) + \boldsymbol{V}_p \times \boldsymbol{B}_{p'}(t,\boldsymbol{X}_p)\Big) \end{cases}$$

- Maxwell equations for the electromagnetic field $(\boldsymbol{E}_p, \boldsymbol{B}_p)$ generated by particle p

$$\begin{cases} \dfrac{1}{c^2}\partial_t \boldsymbol{E}_p - \operatorname{curl} \boldsymbol{B}_p = -\mu_0 \boldsymbol{J}_p \\ \partial_t \boldsymbol{B}_p + \operatorname{curl} \boldsymbol{E}_p = 0 \end{cases}, \qquad \boldsymbol{J}_p(t,\boldsymbol{x}) := q_p \boldsymbol{V}_p \delta_{\boldsymbol{X}_p(t)}(\boldsymbol{x})$$

▷ N trajectories, fully coupled...

A hierarchy of models (II) : Vlasov-Maxwell (mean field)



- Vlasov equation for the particle plasma densities $f_s(t, \boldsymbol{x}, \boldsymbol{v})$ (of species s)

$$\partial_t f_s + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_s + \frac{q_s}{m_s}\Big(\boldsymbol{F}_{\mathrm{ext}}(t, \boldsymbol{x}, \boldsymbol{v}) + \boldsymbol{F}(t, \boldsymbol{x}, \boldsymbol{v})\Big) \cdot \nabla_{\boldsymbol{v}} f_s = 0$$

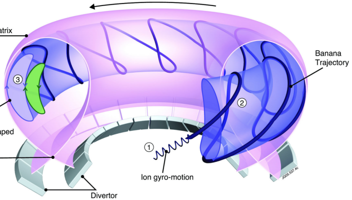
  with $\boldsymbol{F}(t, \boldsymbol{x}, \boldsymbol{v}) := \boldsymbol{E}(t, \boldsymbol{x}) + \boldsymbol{v} \times \boldsymbol{B}(t, \boldsymbol{x})$ the mean-field Lorentz force

- Maxwell equations for the electromagnetic field

$$\begin{cases} \frac{1}{c^2}\partial_t \boldsymbol{E} - \operatorname{curl} \boldsymbol{B} = -\mu_0 \boldsymbol{J} \\ \partial_t \boldsymbol{B} + \operatorname{curl} \boldsymbol{E} = 0 \end{cases}, \qquad \boldsymbol{J}(t, \boldsymbol{x}) := \sum_s q_s \int \boldsymbol{v} f_s(t, \boldsymbol{x}, \boldsymbol{v}) \,\mathrm{d}\boldsymbol{v}$$

▷ simple equations, but very small scales...

A hierarchy of models (III) : Gyrokinetic (electrostatic)



- an excerpt :

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Monte Carlo particle-in-cell methods for the simulation of the Vlasov–Maxwell gyrokinetic equations

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In summary, the GK model used in the following is

$$\frac{\partial f}{\partial t} + \dot{\boldsymbol{R}} \cdot \nabla f + \dot{p}_{\|} \frac{\partial f}{\partial p_{\|}} = 0, \tag{2.43}$$

$$\dot{\boldsymbol{R}} = \frac{p_{\|}}{m} \frac{\boldsymbol{B}^*}{B^*_{\|}} - \frac{c}{eB^*_{\|}} \boldsymbol{b} \times (\mu \nabla B + e \nabla \mathrm{J}_0 \Phi), \tag{2.44}$$

$$\dot{p}_{\|} = -\frac{\boldsymbol{B}^*}{B^*_{\|}} \cdot (\mu \nabla B + e \nabla \mathrm{J}_0 \Phi), \tag{2.45}$$

$$\sum_{sp} \left(\int \mathrm{d}W \, e \mathrm{J}_0^{\dagger} f + \nabla \cdot \left(\frac{n_0 m c^2}{B^2} \nabla_{\perp} \Phi \right) \right) = 0. \tag{2.46}$$

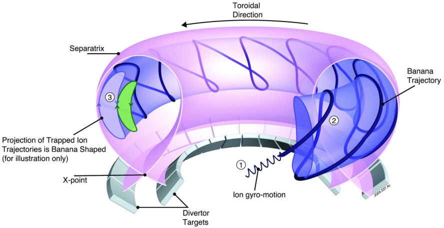
Despite all the approximations made, this model is physically relevant and it can be used to describe a large class of micro-instabilities excited by the density and temperature gradients, like ion temperature gradient (ITG) driven modes or trapped electron modes (TEMs).

- with $(J_0\Phi)(\boldsymbol{R},\mu) = \frac{1}{2\pi}\int_0^{2\pi} \Phi(\boldsymbol{R} + \rho(\alpha))\,\mathrm{d}\alpha$, and $B^* = \nabla \times \boldsymbol{A}^*$, $\boldsymbol{A}^* = \boldsymbol{A} + p_{\|}\frac{c}{e}\boldsymbol{b}, \dots$

▷ equations become increasingly complex !

Outline

Vlasov-Maxwell equations for plasma modelling



- Vlasov equation for the plasma

$$\partial_t f + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f + \boldsymbol{F}(\boldsymbol{x}, \boldsymbol{v}) \cdot \nabla_{\boldsymbol{v}} f = 0$$

▷ Transport structure with trajectories

$$f(t, \boldsymbol{X}(t, \boldsymbol{x}_0, \boldsymbol{v}_0), \boldsymbol{V}(t, \boldsymbol{x}_0, \boldsymbol{v}_0)) = f_0(\boldsymbol{x}_0, \boldsymbol{v}_0)$$

- coupling term : Lorentz force

$$\boldsymbol{F}(t, \boldsymbol{x}, \boldsymbol{v}) = \boldsymbol{E}(t, \boldsymbol{x}) + \boldsymbol{v} \times \boldsymbol{B}(t, \boldsymbol{x})$$

▷ Particle discretization [1]

- Maxwell equations for the field

$$\begin{cases} \partial_t \boldsymbol{E} - \operatorname{curl} \boldsymbol{B} = -\boldsymbol{J} \\ \partial_t \boldsymbol{B} + \operatorname{curl} \boldsymbol{E} = 0 \end{cases}$$

▷ de Rham structure [2] with potentials

$$\boldsymbol{E} = -\partial_t \boldsymbol{A} - \operatorname{grad} \phi, \qquad \boldsymbol{B} = \operatorname{curl} \boldsymbol{A}$$

- coupling term : current density

$$\boldsymbol{J}(t, \boldsymbol{x}) = \int \boldsymbol{v} f(t, \boldsymbol{x}, \boldsymbol{v}) \, \mathrm{d}\boldsymbol{v}$$

▷ Finite Element discretization [2]

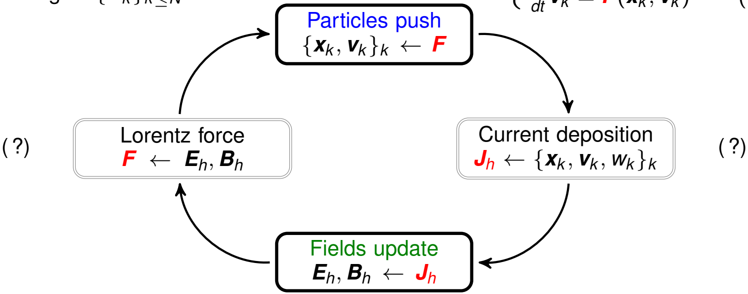
1. Langdon-Birdsall ('70), Hockney-Eastwood ('80s), Markidis-Lapenta ('11), Chacón-Chen-Barnes('13), ...
2. Whitney'57, Bossavit ('88 - '98), Hiptmair ('99), Boffi'00+ Arnold-Falk-Winther ('06), Buffa et al ('11), ...

FEM-PIC [1] : main loop

- Numerical particles
  - positions $\{\boldsymbol{x}_k\}_{k\le N}$
  - velocities $\{\boldsymbol{v}_k\}_{k\le N}$
  - weights $\{w_k\}_{k\le N}$

- Particles push

$$\begin{cases} \frac{d}{dt}\boldsymbol{x}_k = \boldsymbol{v}_k & (\text{ in } \mathbb{R}^3 \text{ }) \\ \frac{d}{dt}\boldsymbol{v}_k = \boldsymbol{F}(\boldsymbol{x}_k, \boldsymbol{v}_k) & (\text{ in } \mathbb{R}^3 \text{ }) \end{cases}$$



- Maxwell FEM
  - FEM spaces $\cdots \ V_h^1 \xrightarrow{\text{curl}} V_h^2 \ \cdots$
  - magnetic field $\boldsymbol{B}_h \in V_h^1$
  - electric field $\boldsymbol{E}_h \in V_h^2$

- Fields update

$$\begin{cases} \partial_t \boldsymbol{E}_h - \text{curl } \boldsymbol{B}_h = -\boldsymbol{J}_h & (\text{ in } V_h^2 \text{ }) \\ \partial_t \boldsymbol{B}_h + \text{curl}_h \boldsymbol{E}_h = 0 & (\text{ in } V_h^1 \text{ }) \end{cases}$$

1. Boris ('70), Marder ('87), Eastwood ('91), Villasenor-Buneman ('92), Langdon ('92), Lapenta-Brackbill ('98), Munz-Omnes-Schneider-Sonnendrücker-Voß('00), Weiland ('03), Kim-Chacón-Lapenta ('05), Markidis-Lapenta ('11, '17), Pagès-CP ('20,)...

Variational structure of the continuous Vlasov-Maxwell system

- Action principle : solutions $f(t, \boldsymbol{X}, \boldsymbol{V}) = f_0(\boldsymbol{x}_0, \boldsymbol{v}_0)$, $\boldsymbol{E} = -\partial_t \boldsymbol{A} - \operatorname{grad}\phi$, $\boldsymbol{B} = \operatorname{curl}\boldsymbol{A}$ are extrema of the Action functional

$$\mathcal{S}(\boldsymbol{X}, \boldsymbol{V}, \boldsymbol{A}, \phi) := \int_0^T \mathcal{L}\big((\boldsymbol{X}, \tfrac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{X}, \boldsymbol{V}, \boldsymbol{A}, \tfrac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{A}, \phi)(t)\big)\,\mathrm{d}t$$

▷ with the Lagrangian functional [1]

$$\mathcal{L}(\boldsymbol{X}, \boldsymbol{X}', \boldsymbol{V}, \boldsymbol{A}, \boldsymbol{A}', \phi) = \int f_0(\boldsymbol{x}_0, \boldsymbol{v}_0)\Big(\big(m\boldsymbol{V} + q\boldsymbol{A}(t, \boldsymbol{X})\big)\cdot \boldsymbol{X}' - \Big(\frac{m}{2}\boldsymbol{V}^2 + q\phi(t, \boldsymbol{X})\Big)\Big)\,\mathrm{d}\boldsymbol{x}_0\,\mathrm{d}\boldsymbol{v}_0$$
$$+ \frac{1}{2}\int_\Omega |\operatorname{grad}\phi(t, \boldsymbol{x}) + \boldsymbol{A}'(t, \boldsymbol{x})|^2\,\mathrm{d}\boldsymbol{x} - \frac{1}{2}\int_\Omega |\operatorname{curl}\boldsymbol{A}(t, \boldsymbol{x})|^2\,\mathrm{d}\boldsymbol{x}$$

- Hamiltonian formulation : for an arbitrary functional $\mathcal{F}$ of the solution, it holds

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(f, \boldsymbol{E}, \boldsymbol{B}) = \{\mathcal{F}, \mathcal{H}\}$$

▷ with $\mathcal{H}(f, \boldsymbol{E}, \boldsymbol{B}) = \frac{1}{2}\int_{\Omega\times\mathbb{R}^3}|\boldsymbol{v}|^2 f\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{v} + \frac{1}{2}\int_\Omega(|\boldsymbol{E}|^2 + |\boldsymbol{B}|^2)\,\mathrm{d}\boldsymbol{x}$ and the bracket [2]

$$\{\mathcal{F}, \mathcal{G}\} = \int_{\Omega\times\mathbb{R}^3} f\Big(\Big(\frac{\partial}{\partial\boldsymbol{v}}\frac{\delta\mathcal{F}}{\delta f}\cdot\frac{\partial}{\partial\boldsymbol{x}}\frac{\delta\mathcal{G}}{\delta f} - \frac{\partial}{\partial\boldsymbol{v}}\frac{\delta\mathcal{G}}{\delta f}\cdot\frac{\partial}{\partial\boldsymbol{x}}\frac{\delta\mathcal{F}}{\delta f}\Big) + \boldsymbol{B}\cdot\Big(\frac{\partial}{\partial\boldsymbol{v}}\frac{\delta\mathcal{F}}{\delta f}\times\frac{\partial}{\partial\boldsymbol{v}}\frac{\delta\mathcal{G}}{\delta f}\Big)\Big)\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{v}$$
$$+ \int_{\Omega\times\mathbb{R}^3}\Big(\frac{\delta\mathcal{F}}{\delta\boldsymbol{E}}\cdot\frac{\partial f}{\partial\boldsymbol{v}}\frac{\delta\mathcal{G}}{\delta f} - \frac{\delta\mathcal{G}}{\delta\boldsymbol{E}}\cdot\frac{\partial f}{\partial\boldsymbol{v}}\frac{\delta\mathcal{F}}{\delta f}\Big)\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{v} + \int_\Omega\Big(\frac{\delta\mathcal{F}}{\delta\boldsymbol{E}}\cdot\operatorname{curl}\frac{\delta\mathcal{G}}{\delta\boldsymbol{B}} - \frac{\delta\mathcal{G}}{\delta\boldsymbol{E}}\cdot\operatorname{curl}\frac{\delta\mathcal{F}}{\delta\boldsymbol{B}}\Big)\,\mathrm{d}\boldsymbol{x}$$

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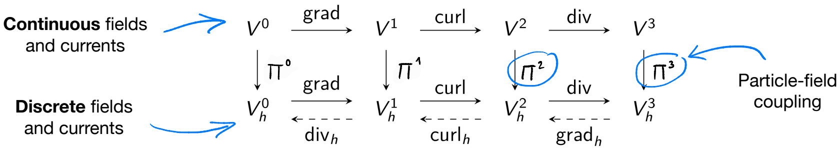
1. Low ('58)
2. Morrison ('80), Marder-Weinstein ('82), Weinstein-Morrison ('81)

Main Result

- Variational particle-field discretization in generic de Rham complex



▷ Action Principle with discrete Lagrangian $\mathcal{L}_h(\boldsymbol{X}_N, \boldsymbol{X}'_N, \boldsymbol{V}_N, \boldsymbol{A}_h, \boldsymbol{A}'_h, \phi_h)$

▷ gauge-free FEM-PIC scheme with

$$\boldsymbol{E}_h = -\,\text{grad}_h\,\phi_h - \partial_t \boldsymbol{A}_h \quad (\text{ in } V_h^2 \,) \qquad \text{and} \qquad \boldsymbol{B}_h = \text{curl}_h\,\boldsymbol{A}_h \quad (\text{ in } V_h^1\,)$$

▷ Hamiltonian structure (semi-disc) : energy stability, discrete Casimirs (Gauss laws)

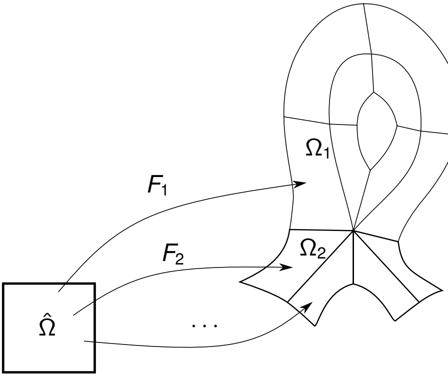
▷ flexible : allows for various field solvers, coupling techniques, (smooth) particles shapes, curvilinear coordinates

- new GEMPIC [2] schemes, with general FEM [3]/DG [4] spaces on complex domains
- with discrete Fourier spaces and gridless projection : Particle-in-Fourier (PIF)
- with discrete Fourier spaces and DFT projections : new Hamiltonian spectral PIC

1. Kraus-Kormann-Morrison-Sonnendrücker ('17)
2. Raviart-Thomas('77), Nedelec('80+), Bossavit('88-'98+), Hiptmair('99+), Arnold-Falk-Winther('02-'10)
3. CP-Sonnendrücker ('16), CP-Güçlü ('21), Güçlü-Hadjout-CP ('22)

Outline

FEEC [1] and broken FEEC on curvilinear/multi-patch domains



- Computational domain : $\Omega = \bigcup_k \Omega_k$
  - ▷ $\Omega_k = F_k(\hat{\Omega})$: mapped patches
  - ▷ $\hat{\Omega} = [0, 1]^D$: reference patch
- FEEC $V_h^\ell = \left(\bigoplus_k V_h^\ell(\Omega_k)\right) \cap V^\ell$
- broken-FEEC : $V_h^\ell = \bigoplus_k V_h^\ell(\Omega_k)$
- Commuting de Rham diagram :

$$\begin{array}{ccccccc} V^0 & \xrightarrow{\text{grad}} & V^1 & \xrightarrow{\text{curl}} & V^2 & \xrightarrow{\text{div}} & V^3 \\ \downarrow \Pi^0 & & \downarrow \Pi^1 & & \downarrow \Pi^2 & & \downarrow \Pi^3 \\ V_h^0 & \xrightarrow{\text{grad}} & V_h^1 & \xrightarrow{\text{curl}} & V_h^2 & \xrightarrow{\text{div}} & V_h^3 \end{array}$$

1. Whitney('57), Bossavit ('88 - '98), Hiptmair ('99), Boffi'00+ Arnold-Falk-Winther ('06), Buffa et al ('11), ...

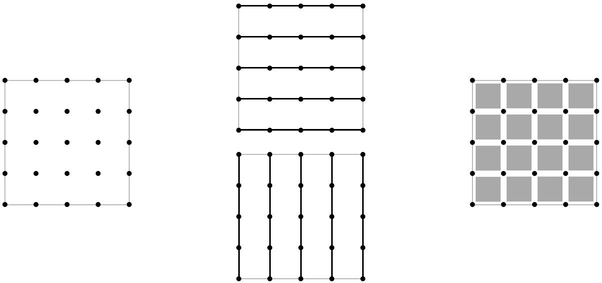
Construction on reference domain (here 2D)

- Polynomial (order p) de Rham sequence :

$$\hat{V}_h^0 = \mathbb{P}_{p,p} \quad \xrightarrow{\text{grad}} \quad \hat{V}_h^1 = \begin{pmatrix} \mathbb{P}_{p-1,p} \\ \mathbb{P}_{p,p-1} \end{pmatrix} \quad \xrightarrow{\text{curl}} \quad \hat{V}_h^3 = \mathbb{P}_{p-1,p-1}$$

- Geometric degrees of freedom [1] :

$$\sigma^0_{\boldsymbol{m}}(u) = u(\boldsymbol{x_m}), \qquad \sigma^1_{\alpha,\boldsymbol{m}}(\boldsymbol{u}) = \int_{\mathtt{e}_{\alpha,\boldsymbol{m}}} \boldsymbol{e}_\alpha \cdot \boldsymbol{u} \qquad \sigma^2_{\alpha,\boldsymbol{m}}(\boldsymbol{u}) = \int_{\mathtt{f}_{\alpha,\boldsymbol{m}}} \boldsymbol{e}_\alpha \cdot \boldsymbol{u}$$



1. Whitney('57), Robidoux('08), Bossavit-Rapetti('09), Kreeft-Palha-Gerritsma('11), Sonnendrücker('19) ...

Construction on mapped patches $\Omega_k = F_k(\hat{\Omega})$

- push-forward operators

$$\mathcal{F}^0_k \hat{u} = \hat{u} \circ F_k^{-1}, \quad \mathcal{F}^1_k \hat{\boldsymbol{u}} = (DF_k^{-T} \hat{\boldsymbol{u}}) \circ F_k^{-1}, \quad \mathcal{F}^2_k \hat{\boldsymbol{u}} = (\frac{DF_k}{J_{F_k}} \hat{\boldsymbol{u}}) \circ F_k^{-1}, \quad \mathcal{F}^3_k \hat{u} = (\frac{1}{J_{F_k}} \hat{u}) \circ F_k^{-1}$$

  with DF and J_F the Jacobian matrix and determinant of F

- local FEM spaces $V^\ell_h(\Omega_k) = \mathcal{F}^\ell_k \hat{V}^\ell_h$

▷ commutation property $d^\ell \mathcal{F}^\ell = \mathcal{F}^{\ell+1} \hat{d}^\ell \implies$ local de Rham sequences :

$$V^0_h(\Omega_k) \xrightarrow{d^0} V^1_h(\Omega_k) \xrightarrow{d^1} V^2_h(\Omega_k) \xrightarrow{d^2} V^3_h(\Omega_k)$$

- degrees of freedom $\sigma^\ell_{k,i}(u) := \hat{\sigma}^\ell_i((\mathcal{F}^\ell)^{-1} u)$

▷ geometric nature

$$\sigma^0_{k,\hat{\boldsymbol{x}}}(u) = u(F_k(\hat{\boldsymbol{x}})), \quad \sigma^1_{k,\hat{\mathtt{e}}}(\boldsymbol{u}) = \int_{F_k(\hat{\mathtt{e}})} \boldsymbol{\tau}_{F_k(\hat{\mathtt{e}})} \cdot \boldsymbol{u}, \quad \sigma^2_{k,\hat{\mathtt{f}}}(\boldsymbol{u}) = \int_{F_k(\hat{\mathtt{f}})} \boldsymbol{n}_{F_k(\hat{\mathtt{f}})} \cdot \boldsymbol{u}, \quad \sigma^3_{k,\hat{\mathtt{c}}}(u) = \int_{F_k(\hat{\mathtt{c}})} u$$

▷ local basis functions

$$\Lambda^\ell_{k,i} = \mathcal{F}^\ell_k \hat{\Lambda}^\ell_i \qquad \text{with} \qquad \sigma^\ell_{k,j}(\Lambda^\ell_{k,i}) = \hat{\sigma}^\ell_j(\hat{\Lambda}^\ell_i) = \delta_{i,j}$$

▷ Finite Element projections

$$\Pi^\ell : u \mapsto \sum_{k,i} \sigma^\ell_{k,i}(u) \Lambda^\ell_{k,i} \qquad \Big(= \sum_k \mathcal{F}^\ell_k \hat{\Pi}^\ell (\mathcal{F}^\ell_k)^{-1} u \Big)$$

Commuting diagram follows from geometrical relations

$$\begin{array}{ccccccc} V^0 & \xrightarrow{\text{grad}} & V^1 & \xrightarrow{\text{curl}} & V^2 & \xrightarrow{\text{div}} & V^3 \\ \downarrow \Pi^0 & & \downarrow \Pi^1 & & \downarrow \Pi^2 & & \downarrow \Pi^3 \\ V^0_h & \xrightarrow{\text{grad}} & V^1_h & \xrightarrow{\text{curl}} & V^2_h & \xrightarrow{\text{div}} & V^3_h \end{array}$$

- projection Π^ℓ characterized by : $\Pi^\ell u \in V_h^\ell$ and $\sigma_i^\ell(\Pi^\ell u) = \sigma_i^\ell(u)$ for all i
  - ▷ given faces $\mathtt{f}_i \in \mathcal{F}_h$ with normals $\boldsymbol{n}_{\mathtt{f}_i}$ and edges $\mathtt{e}_j \in \mathcal{E}_h$ with tangents $\boldsymbol{\tau}_{\mathtt{e}_j}$ we have

$$\sigma_i^2(\operatorname{curl} \boldsymbol{u}) = \int_{\mathtt{f}_i} \boldsymbol{n}_{\mathtt{f}_i} \cdot \operatorname{curl} \boldsymbol{u} = \int_{\partial \mathtt{f}_i} \boldsymbol{\tau}_{\mathtt{e}}^{\mathtt{f}_i} \cdot \boldsymbol{u} = \sum_{\mathtt{e}_j \in \mathcal{E}_h} C_{ij} \int_{\mathtt{e}_j} \boldsymbol{\tau}_{\mathtt{e}_j} \cdot \boldsymbol{u} = \sum_{\mathtt{e}_j \in \mathcal{E}_h} C_{ij} \sigma_j^1(\boldsymbol{u})$$

  where $C_{ij} \in \{-1, 0, +1\}$ is the orientation of the edge $\mathtt{e}_j$ in the face $\mathtt{f}_i$.
  - ▷ in particular,

$$\sigma_i^2(\Pi^2 \operatorname{curl} \boldsymbol{u}) = \sigma_i^2(\operatorname{curl} \boldsymbol{u}) = \sum_{e_j \in \mathcal{E}_h} C_{ij} \sigma_j^1(\boldsymbol{u})$$

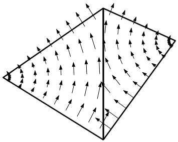
and $$\sigma_i^2(\operatorname{curl} \Pi^1 \boldsymbol{u}) = \sum_{e_j \in \mathcal{E}_h} C_{ij} \sigma_j^1(\Pi^1 \boldsymbol{u}) = \sum_{e_j \in \mathcal{E}_h} C_{ij} \sigma_j^1(\boldsymbol{u})$$

  - ▷ this shows $\Pi^2 \operatorname{curl} = \operatorname{curl} \Pi^1$
  - ▷ and that C (the curl operator matrix) is mapping-independent
  - ▷ similar relations for grad and div follow with same arguments
- smoothed “projections” Π_S^ℓ characterized by : $\sigma_i^\ell(\Pi_S^\ell u) = \sigma_i^\ell(u * S)$ also commute

Extension to broken FEEC

- start from a conforming sequence [1]

$$V_h^{0,c} \xrightarrow{\text{grad}} V_h^{1,c} \xrightarrow{\text{curl}} V_h^{2,c} \xrightarrow{\text{div}} V_h^{3,c} \tag{1}$$



1. Bossavit ('88), Hiptmair ('02), Arnold + Falk + Winther ('06, '10), Brezzi + Boffi + Fortin ('13)
2. CP + Sonnendrücker (15, 16), Ern + Guermond (15)

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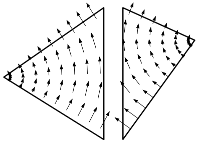
- relax interface constraints : use fully discontinuous V_h^ℓ

$$V_h^{\ell,c} \subset V_h^\ell \not\subset V^\ell$$



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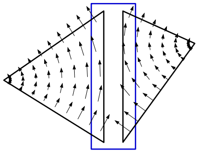

- define local conforming projection operators [2]

$$P_h^\ell : V_h^\ell \to V_h^{\ell,c}$$

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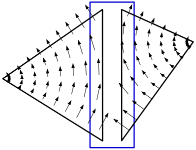
$$V_h^{0,c} \xrightarrow{\text{grad}} V_h^{1,c} \xrightarrow{\text{curl}} V_h^{2,c} \xrightarrow{\text{div}} V_h^{3,c} \tag{1}$$

- relax interface constraints : use fully discontinuous V_h^ℓ

$$V_h^{\ell,c} \subset V_h^\ell \not\subset V^\ell$$



- define local conforming projection operators [2]

$$P_h^\ell : V_h^\ell \to V_h^{\ell,c}$$

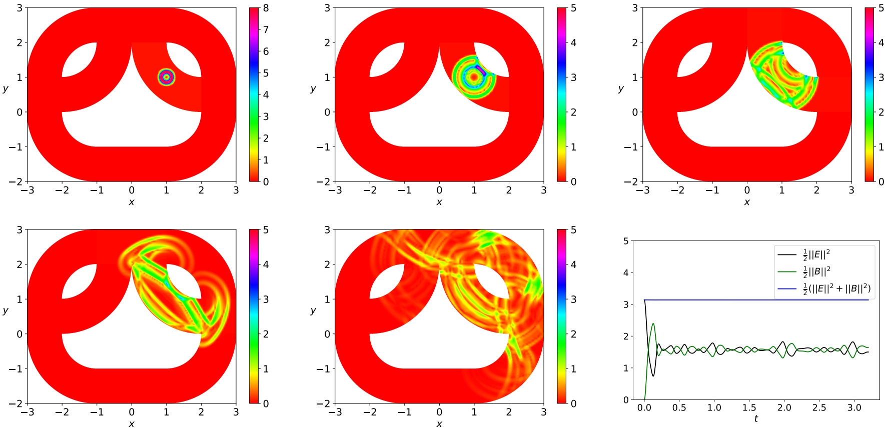
- broken-FEEC diagram

$$\begin{array}{ccccccc}
V^0 & \xrightarrow{\text{grad}} & V^1 & \xrightarrow{\text{curl}} & V^2 & \xrightarrow{\text{div}} & V^3 \\
\downarrow \Pi_h^0 & & \downarrow \Pi_h^1 & & \downarrow \Pi_h^2 & & \downarrow \Pi_h^3 \\
V_h^{0,c} & \xrightarrow{\text{grad}} & V_h^{1,c} & \xrightarrow{\text{curl}} & V_h^{2,c} & \xrightarrow{\text{div}} & V_h^{3,c} \\
\uparrow P_h^0 & & \uparrow P_h^1 & & \uparrow P_h^2 & & \uparrow P_h^3 \\
V_h^0 & \xrightarrow{\text{grad } P_h^0} & V_h^1 & \xrightarrow{\text{curl } P_h^1} & V_h^2 & \xrightarrow{\text{div } P_h^2} & V_h^3
\end{array}$$

  ▷ Conforming/Non-conforming Galerkin (CONGA) schemes

1. Bossavit ('88), Hiptmair ('02), Arnold + Falk + Winther ('06, '10), Brezzi + Boffi + Fortin ('13)
2. CP + Sonnendrücker (15, 16), Ern + Guermond (15)
3. CP (15), CP + Sonnendrücker (16), CP + Güçlü (21), Güçlü + Hadjout + CP (22)

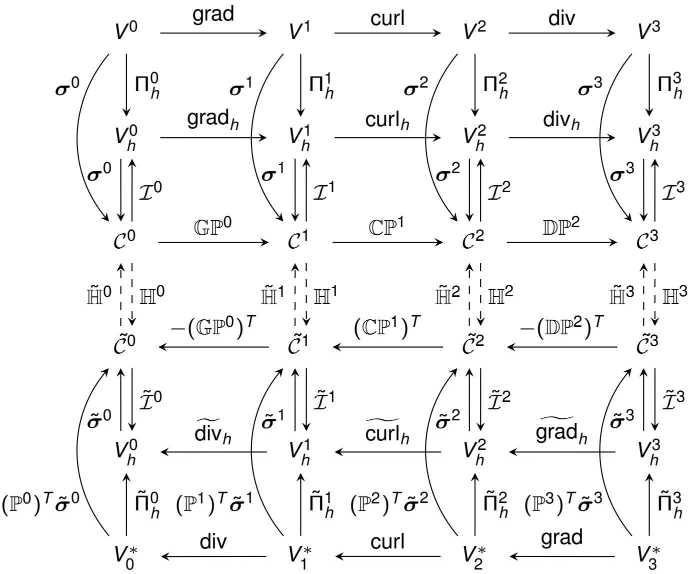
CONGA simulation of an EM pulse propagating in a metallic cavity



$$\begin{cases} \mathbf{B}^{n+\frac{1}{2}} = \mathbf{B}^n - \frac{\Delta t}{2}\mathbb{CP}^1\mathbf{E}^n \\ \mathbf{E}^{n+1} = \mathbf{E}^n + \Delta t\tilde{\mathbb{H}}^1\left((\mathbb{CP}^1)^T\mathbb{H}^2\mathbf{B}^{n+\frac{1}{2}} - (\mathbb{P}^1)^T\tilde{\boldsymbol{\sigma}}^1(J^{n+\frac{1}{2}})\right) \\ \mathbf{B}^{n+1} = \mathbf{B}^{n+\frac{1}{2}} - \frac{\Delta t}{2}\mathbb{CP}^1\mathbf{E}^{n+1} \end{cases}$$

- curl matrices : block-diagonal
- Hodge matrices : block-diag.
- projection matrices : local
- dual dofs $\boldsymbol{\sigma}^1$: local

Full broken-FEEC diagram[1] : $V_h^\ell := \{v \in L^2(\Omega) : v|_{\Omega_k} \in V_h^\ell(\Omega_k)\}$



1. *A broken-FEEC framework for EM pbms on mapped multipatch domains*, Güçlü-Hadjout-CP ('22)

Outline

Spectral solvers : Particle-in-Fourier (PIF) vs. spectral PIC

- fields in Fourier spaces

$$\boldsymbol{E}_h(t, \boldsymbol{x}) = \sum_{-K \le k_1, k_2, k_3 \le K} \boldsymbol{E}_{\boldsymbol{k}}(t) \mathrm{e}^{\frac{2\mathrm{i}\pi \boldsymbol{k}\cdot\boldsymbol{x}}{L}}$$

$$\boldsymbol{B}_h(t, \boldsymbol{x}) = \quad \cdots \quad \text{(same form)}$$

- particle densities, smoothing kernel S

$$\boldsymbol{J}_N(t, \boldsymbol{x}) = \sum_{1 \le p \le N} w_p \mathbf{v}_p(t) S(\boldsymbol{x} - \mathbf{x}_p(t))$$

▷ coupled solver

$$\begin{cases} -\partial_t \boldsymbol{E}_{\boldsymbol{k}} + \left(\frac{2\mathrm{i}\pi \boldsymbol{k}}{L}\right) \times \boldsymbol{B}_{\boldsymbol{k}} = \boldsymbol{J}_{\boldsymbol{k}}, \\ \partial_t \boldsymbol{B}_{\boldsymbol{k}} + \left(\frac{2\mathrm{i}\pi \boldsymbol{k}}{L}\right) \times \boldsymbol{E}_{\boldsymbol{k}} = 0 \end{cases}$$

$$\begin{cases} \partial_t \mathbf{x}_p = \mathbf{v}_p, \\ \partial_t \mathbf{v}_p = \boldsymbol{E}_h^S(\mathbf{x}_p) + \mathbf{v}_p \times \boldsymbol{B}_h^S(\mathbf{x}_p) \end{cases}$$

- PIF is gridless [1]

$$\boldsymbol{J}_{\boldsymbol{k}} := \left(\tfrac{1}{L}\right)^3 \int_{[0,L^3]} \boldsymbol{J}_N(\boldsymbol{x}) \mathrm{e}^{-\frac{2\mathrm{i}\pi \boldsymbol{k}\cdot\boldsymbol{x}}{L}} \,\mathrm{d}\boldsymbol{x}$$

$$\boldsymbol{E}_h^S(\mathbf{x}_p) := \int_{[0,L]^3} \boldsymbol{E}_h(\boldsymbol{x}) S(\boldsymbol{x} - \mathbf{x}_p) \,\mathrm{d}\boldsymbol{x}$$

- conservation properties [2] (charge, energy, momentum)
- well-defined for point particles
- complexity : $\sim NK^3$

- PIC [1] : DFT grid, $\Delta x = \frac{L}{M}$, $M \ge 2K + 1$

$$\boldsymbol{J}_{\boldsymbol{k}} := \left(\tfrac{1}{M}\right)^3 \sum_{1 \le j_1, j_2, j_3 \le M} \boldsymbol{J}_N(\boldsymbol{j}\Delta x) \mathrm{e}^{-\frac{2\mathrm{i}\pi \boldsymbol{k}\cdot\boldsymbol{j}}{M}}$$

$$\boldsymbol{E}_h^S(\mathbf{x}_p) := \left(\tfrac{L}{M}\right)^3 \sum_{1 \le j_1, j_2, j_3 \le M} \boldsymbol{E}_h(\boldsymbol{j}\Delta x) S(\boldsymbol{j}\Delta x - \mathbf{x}_p)$$

- complexity : $\sim Nq^3 + M^3 \log M$ (for $S(\boldsymbol{x}) = (\Delta x)^{-3} \mathcal{B}_q(\boldsymbol{x}/\Delta x)$)
- aliasing errors, invariants ?
- ill-defined for point particles

1. Langdon-Birdsall ('70), Vlad Briguglio et al ('01), Lifschitz et al ('09), Decyk ('11), Ohana et al ('17),
2. Evstatiev-Shadwick ('13), Shadwick-Stamm-Evstatiev ('14), Ameres ('18)

Spectral solvers : Particle-in-Fourier (PIF) vs. spectral PIC

- here, the Hamiltonian framework allows to

  - ▷ distinguish PIF and spectral PIC by the projections Π^ℓ
  - ▷ better understand the conservation properties of spectral PIC
  - ▷ extend to hybrid field solvers and curvilinear geometries
  - ▷ handle anti-aliasing techniques and Fourier back-filtering

---

- PIF is gridless [1]

$$\boldsymbol{J_k} := \left(\tfrac{1}{L}\right)^3 \int_{[0,L^3]} \boldsymbol{J}_N(\boldsymbol{x}) \mathrm{e}^{-\frac{2\mathrm{i}\pi \boldsymbol{k}\cdot\boldsymbol{x}}{L}} \,\mathrm{d}\boldsymbol{x}$$

$$\boldsymbol{E}_h^S(\mathbf{x}_p) := \int_{[0,L]^3} \boldsymbol{E}_h(\boldsymbol{x}) S(\boldsymbol{x} - \mathbf{x}_p) \,\mathrm{d}\boldsymbol{x}$$

- conservation properties [2] (charge, energy, momentum)
- well-defined for point particles
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- PIC [1] : DFT grid, $\Delta x = \frac{L}{M}$, $M \geq 2K + 1$

$$\boldsymbol{J_k} := \left(\tfrac{1}{M}\right)^3 \sum_{1 \leq j_1, j_2, j_3 \leq M} \boldsymbol{J}_N(\boldsymbol{j}\Delta x) \mathrm{e}^{-\frac{2\mathrm{i}\pi \boldsymbol{k}\cdot\boldsymbol{j}}{M}}$$

$$\boldsymbol{E}_h^S(\mathbf{x}_p) := \left(\tfrac{L}{M}\right)^3 \sum_{1 \leq j_1, j_2, j_3 \leq M} \boldsymbol{E}_h(\boldsymbol{j}\Delta x) S(\boldsymbol{j}\Delta x - \mathbf{x}_p)$$

- complexity : $\sim Nq^3 + M^3 \log M$ (for $S(\boldsymbol{x}) = (\Delta x)^{-3} \mathcal{B}_q(\boldsymbol{x}/\Delta x)$)
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2. Evstatiev-Shadwick ('13), Shadwick-Stamm-Evstatiev ('14), Ameres ('18)

Compatible Finite Elements meet Fourier spaces

- functional de Rham structure [1]

$$\begin{array}{ccccccc} V^0 & \xrightarrow{\text{grad}} & V^1 & \xrightarrow{\text{curl}} & V^2 & \xrightarrow{\text{div}} & V^3 \\ \downarrow \Pi^0 & & \downarrow \Pi^1 & & \downarrow \Pi^2 & & \downarrow \Pi^3 \\ V_h^0 & \underset{\text{div}_h}{\overset{\text{grad}}{\rightleftarrows}} & V_h^1 & \underset{\text{curl}_h}{\overset{\text{curl}}{\rightleftarrows}} & V_h^2 & \underset{\text{grad}_h}{\overset{\text{div}}{\rightleftarrows}} & V_h^3 \end{array}$$

- commuting diagram operators

$$\text{grad}\,\Pi^0 = \Pi^1\,\text{grad}, \ \ \text{curl}\,\Pi^1 = \Pi^2\,\text{curl}, \ \ \text{div}\,\Pi^2 = \Pi^3\,\text{div}$$

- continuous fields

$$\boldsymbol{B}(t) \in V^1, \qquad \boldsymbol{E}(t), \ \boldsymbol{J}(t) \in V^2$$

- discrete fields

$$\boldsymbol{B}_h(t) \in V_h^1, \qquad \boldsymbol{E}_h(t), \ \boldsymbol{J}_h(t) \in V_h^2$$

- discrete Maxwell equations

$$\begin{cases} \partial_t \boldsymbol{E}_h - \text{curl}\,\boldsymbol{B}_h = -\Pi^2 \boldsymbol{J} \\ \partial_t \boldsymbol{B}_h + \text{curl}_h\,\boldsymbol{E}_h = 0 \end{cases}$$

- for spectral solvers : V_h^ℓ = Fourier spaces

▷ gridless setting : L^2 projections, truncated Fourier series

$$PG = \sum_{|k| \le K} \mathcal{F}_k(G) e^{\frac{2i\pi kx}{L}} \qquad \text{with} \qquad \mathcal{F}_k(G) = \frac{1}{L}\int G(x) e^{-\frac{2i\pi kx}{L}}\,dx$$

▷ with a grid : DFT with $M \ge 2K + 1$ points, pseudo differentials, Fourier filtering

$$(\tilde{P}G)_k = \gamma_{\boldsymbol{k}} \Big(\frac{2i\pi k}{L}\Big)^{-1} \mathcal{F}_{M,k}(\partial G) \qquad \text{with} \qquad \mathcal{F}_{M,k}(G) = \frac{1}{M}\sum_{j=1}^{M} G(j\Delta x) e^{-\frac{2i\pi kj}{M}}$$

1. Bossavit ('88 - '98), Hiptmair ('99), Arnold-Falk-Winther ('06), Buffa-Rivas-Sangalli-Vázquez ('11), CP-Sonnendrücker ('17), Kraus-Kormann-Morrison-Sonnendrücker ('17), CP-Güçlü ('21), ...

Outline

Discrete action principle

- continuous Lagrangian [1] (Vlasov-Maxwell)

$$\mathcal{L} = \int f(t_0, \boldsymbol{x}_0, \boldsymbol{v}_0) \left((m\boldsymbol{V} + q\boldsymbol{A}(t, \boldsymbol{X})) \cdot \boldsymbol{X}' - \left(\frac{m}{2} \boldsymbol{V}^2 + q\phi(t, \boldsymbol{X}) \right) \right) \mathrm{d}\boldsymbol{x}_0 \, \mathrm{d}\boldsymbol{v}_0 + \frac{1}{2} \int_\Omega |\operatorname{grad} \phi(t, \boldsymbol{x}) + \boldsymbol{A}'(t, \boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x} - \frac{1}{2} \int_\Omega |\operatorname{curl} \boldsymbol{A}(t, \boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x}$$

- discrete Lagrangian (Particle-Field)

$$\mathcal{L}_h = \sum_{p=1}^{N} w_p \left((m\boldsymbol{V}_p + q\boldsymbol{A}^S(\boldsymbol{X}_p)) \cdot \boldsymbol{X}_p' - \left(\frac{m}{2} \boldsymbol{V}_p^2 + q\phi^S(\boldsymbol{X}_p) \right) \right) + \frac{1}{2} \int_\Omega |\operatorname{grad}_h \phi_h(\boldsymbol{x}) + \boldsymbol{A}_h'(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x} - \frac{1}{2} \int_\Omega |\operatorname{curl}_h \boldsymbol{A}_h(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x}.$$

- $\mathbf{X}_N, \mathbf{V}_N$: collections of particle trajectories
- $\boldsymbol{A}_h \in V_h^2$, $\phi_h \in V_h^3$: discrete (FEM) potential fields
- coupling potentials

$$\begin{cases} \boldsymbol{A}^S(\boldsymbol{X}_p) := \sum_{\alpha=1}^{3} \boldsymbol{e}_\alpha \int_\Omega \left(\boldsymbol{A}_h \cdot \Pi^2(\boldsymbol{e}_\alpha S_{\boldsymbol{X}_p}) \right) \mathrm{d}\boldsymbol{x}, \\ \phi^S(\boldsymbol{X}_p) := \int_\Omega \left(\phi_h \Pi^3(S_{\boldsymbol{X}_p}) \right) \mathrm{d}\boldsymbol{x} \end{cases}$$

with smoothing kernels $S_{\boldsymbol{X}_p}(\boldsymbol{x}) = S(\boldsymbol{x} - \boldsymbol{X}_p)$

1. Low ('58)

Variational principle with commuting diagrams

- Variational principle[1] leads to Euler-Lagrange equations, eg : $\boxed{\dfrac{\partial}{\partial t}\dfrac{\delta \mathcal{L}_h}{\delta \mathbf{X}'_N} = \dfrac{\delta \mathcal{L}_h}{\delta \mathbf{X}_N}}$
  - ▷ this gives

$$
\begin{aligned}
\frac{m_p}{q_p}\frac{\mathrm{d}\boldsymbol{V}_p}{\mathrm{d}t}\cdot\boldsymbol{e}_\alpha &= \int_\Omega \boldsymbol{A}_h\cdot\Pi^2\big(\boldsymbol{e}_\alpha(\boldsymbol{V}_p\cdot\operatorname{grad} S_{\boldsymbol{X}_p}) - \boldsymbol{V}_p(\boldsymbol{e}_\alpha\cdot\operatorname{grad} S_{\boldsymbol{X}_p})\big)\\
&\qquad - \int_\Omega \partial_t\boldsymbol{A}_h\cdot\Pi^2(\boldsymbol{e}_\alpha S_{\boldsymbol{X}_p}) + \int_\Omega \phi_h\Pi^3(\boldsymbol{e}_\alpha\cdot\operatorname{grad} S_{\boldsymbol{X}_p})\\
&= \int_\Omega \boldsymbol{A}_h\cdot\Pi^2\operatorname{curl}(\boldsymbol{e}_\alpha\times\boldsymbol{V}_p S_{\boldsymbol{X}_p}) - \int_\Omega \partial_t\boldsymbol{A}_h\cdot\Pi^2(\boldsymbol{e}_\alpha S_{\boldsymbol{X}_p}) + \int_\Omega \phi_h\Pi^3\operatorname{div}(\boldsymbol{e}_\alpha S_{\boldsymbol{X}_p})\\
&= \int_\Omega \boldsymbol{A}_h\cdot\operatorname{curl}\Pi^1(\boldsymbol{e}_\alpha\times\boldsymbol{V}_p S_{\boldsymbol{X}_p}) - \int_\Omega \partial_t\boldsymbol{A}_h\cdot\Pi^2(\boldsymbol{e}_\alpha S_{\boldsymbol{X}_p}) + \int_\Omega \phi_h\operatorname{div}\Pi^3(\boldsymbol{e}_\alpha S_{\boldsymbol{X}_p})\\
&= \int_\Omega \operatorname{curl}_h\boldsymbol{A}_h\cdot\Pi^1(\boldsymbol{e}_\alpha\times\boldsymbol{V}_p S_{\boldsymbol{X}_p}) - \int_\Omega (\partial_t\boldsymbol{A}_h + \operatorname{grad}_h\phi_h)\cdot\Pi^2(\boldsymbol{e}_\alpha S_{\boldsymbol{X}_p})\\
&= \int_\Omega \boldsymbol{B}_h\cdot\Pi^1(\boldsymbol{e}_\alpha\times\boldsymbol{V}_p S_{\boldsymbol{X}_p}) + \int_\Omega \boldsymbol{E}_h\cdot\Pi^2(\boldsymbol{e}_\alpha S_{\boldsymbol{X}_p})
\end{aligned}
$$

  - ▷ hence, $\boxed{\dfrac{m_p}{q_p}\dfrac{\mathrm{d}\boldsymbol{V}_p}{\mathrm{d}t} = \boldsymbol{V}_p\times\boldsymbol{B}^S(\boldsymbol{X}_p) + \boldsymbol{E}^S(\boldsymbol{X}_p)}$, with coupling fields

$$
\boldsymbol{B}^S(\boldsymbol{X}_p) := \sum_{\alpha=1}^{3}\boldsymbol{e}_\alpha\int_\Omega \boldsymbol{B}_h\cdot\Pi^1(\boldsymbol{e}_\alpha S_{\boldsymbol{X}_p}) \quad \text{and} \quad \boldsymbol{E}^S(\boldsymbol{X}_p) := \sum_{\alpha=1}^{3}\boldsymbol{e}_\alpha\int_\Omega \boldsymbol{E}_h\cdot\Pi^2(\boldsymbol{e}_\alpha S_{\boldsymbol{X}_p})
$$

1. Lewis ('70), Morrison ('80-'16), Eastwood ('91), Kraus ('13), Turchetti-Sinigardi-Londrillo ('14), ...

Resulting variational FEM-PIC system

- Field equations

$$\begin{cases} -\partial_t \boldsymbol{E}_h + \operatorname{curl} \boldsymbol{B}_h = \Pi^2 \boldsymbol{J}_N^S \\ \partial_t \boldsymbol{B}_h + \operatorname{curl}_h \boldsymbol{E}_h = 0 \end{cases} \quad \text{with} \quad \Pi^2 \boldsymbol{J}_N^S = \sum_{p=1\cdots N} q_p \Pi^2 (\boldsymbol{V}_p S_{\boldsymbol{X}_p})$$

  with the discrete weak operator $\operatorname{curl}_h : V_h^2 \to V_h^1$

- trajectory equations

$$\begin{cases} \dfrac{\mathrm{d}\boldsymbol{X}_p}{\mathrm{d}t} = \boldsymbol{V}_p \\ \dfrac{\mathrm{d}\boldsymbol{V}_p}{\mathrm{d}t} = \dfrac{q_p}{m_p} (\boldsymbol{E}^S(\boldsymbol{X}_p) + \boldsymbol{V}_p \times \boldsymbol{B}^S(\boldsymbol{X}_p)) \end{cases} \quad \text{for } p = 1, \dots, N$$

- coupling fields

$$\boldsymbol{B}^S(\boldsymbol{X}_p) = \sum_{\alpha=1}^{3} \boldsymbol{e}_\alpha \int_\Omega \boldsymbol{B}_h \cdot \Pi^1(\boldsymbol{e}_\alpha S_{\boldsymbol{X}_p}) \qquad \boldsymbol{E}^S(\boldsymbol{X}_p) = \sum_{\alpha=1}^{3} \boldsymbol{e}_\alpha \int_\Omega \boldsymbol{E}_h \cdot \Pi^2(\boldsymbol{e}_\alpha S_{\boldsymbol{X}_p}),$$

- variational Gauss laws (exact invariant)

$$\begin{cases} \operatorname{div} \boldsymbol{E}_h = \Pi^3 \rho_N^S \\ \operatorname{div}_h \boldsymbol{B}_h = 0 \end{cases} \quad \text{with} \quad \Pi^3 \rho_N^S = \sum_{p=1\cdots N} q_p \Pi^3 (S_{\boldsymbol{X}_p})$$

  with the discrete weak operator $\operatorname{div}_h : V_h^1 \to V_h^0$

- extends GEMPIC scheme (spline FEM, strong Faraday equation, $S = \delta$)

1. Kraus-Kormann-Morrison-Sonnendrücker ('17)

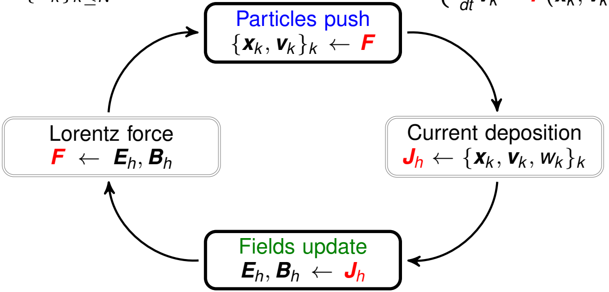
FEM-PIC loop [1] : reminder

- **Numerical particles**
  - positions $\{\boldsymbol{x}_k\}_{k \le N}$
  - velocities $\{\boldsymbol{v}_k\}_{k \le N}$
  - weights $\{w_k\}_{k \le N}$

- **Particles push**

$$\begin{cases} \frac{d}{dt}\boldsymbol{x}_k = \boldsymbol{v}_k & (\text{ in } \mathbb{R}^3 \text{ }) \\ \frac{d}{dt}\boldsymbol{v}_k = \boldsymbol{F}(\boldsymbol{x}_k, \boldsymbol{v}_k) & (\text{ in } \mathbb{R}^3 \text{ }) \end{cases}$$

(?)



(?)

- **Maxwell FEM**
  - FEM spaces $\cdots \ V_h^1 \xrightarrow{\text{curl}} V_h^2 \ \cdots$
  - magnetic field $\boldsymbol{B}_h \in V_h^1$
  - electric field $\boldsymbol{E}_h \in V_h^2$

- **Fields update**

$$\begin{cases} \partial_t \boldsymbol{E}_h - \text{curl } \boldsymbol{B}_h = -\boldsymbol{J}_h & (\text{ in } V_h^2 \text{ }) \\ \partial_t \boldsymbol{B}_h + \text{curl}_h \boldsymbol{E}_h = 0 & (\text{ in } V_h^1 \text{ }) \end{cases}$$

1. Boris ('70), Marder ('87), Eastwood ('91), Villasenor-Buneman ('92), Langdon ('92), Lapenta-Brackbill ('98), Munz-Omnes-Schneider-Sonnendrücker-Voß('00), Weiland ('03), Kim-Chacón-Lapenta ('05), Markidis-Lapenta ('11, '17), Pagès-CP ('20,)...

Hamiltonian structure

- continuous VM system [1] :

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(f,\boldsymbol{E},\boldsymbol{B}) = \{\mathcal{F},\mathcal{H}\}$$

▷ with $\mathcal{H}(f,\boldsymbol{E},\boldsymbol{B}) = \frac{1}{2}\int_{\Omega\times\mathbb{R}^3}|\boldsymbol{v}|^2 f\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{v} + \frac{1}{2}\int_\Omega(|\boldsymbol{E}|^2+|\boldsymbol{B}|^2)\,\mathrm{d}\boldsymbol{x}$ and

$$\{\mathcal{F},\mathcal{G}\} = \int_{\Omega\times\mathbb{R}^3} f\left(\left(\frac{\partial}{\partial\boldsymbol{v}}\frac{\delta\mathcal{F}}{\delta f}\cdot\frac{\partial}{\partial\boldsymbol{x}}\frac{\delta\mathcal{G}}{\delta f} - \frac{\partial}{\partial\boldsymbol{v}}\frac{\delta\mathcal{G}}{\delta f}\cdot\frac{\partial}{\partial\boldsymbol{x}}\frac{\delta\mathcal{F}}{\delta f}\right) + \boldsymbol{B}\cdot\left(\frac{\partial}{\partial\boldsymbol{v}}\frac{\delta\mathcal{F}}{\delta f}\times\frac{\partial}{\partial\boldsymbol{v}}\frac{\delta\mathcal{G}}{\delta f}\right)\right)\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{v}$$
$$+\int_{\Omega\times\mathbb{R}^3}\left(\frac{\delta\mathcal{F}}{\delta\boldsymbol{E}}\cdot\frac{\partial f}{\partial\boldsymbol{v}}\frac{\delta\mathcal{G}}{\delta f} - \frac{\delta\mathcal{G}}{\delta\boldsymbol{E}}\cdot\frac{\partial f}{\partial\boldsymbol{v}}\frac{\delta\mathcal{F}}{\delta f}\right)\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{v} + \int_\Omega\left(\frac{\delta\mathcal{F}}{\delta\boldsymbol{E}}\cdot\operatorname{curl}\frac{\delta\mathcal{G}}{\delta\boldsymbol{B}} - \frac{\delta\mathcal{G}}{\delta\boldsymbol{E}}\cdot\operatorname{curl}\frac{\delta\mathcal{F}}{\delta\boldsymbol{B}}\right)\mathrm{d}\boldsymbol{x}$$

- discrete VM system [2] :

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}_h(\mathbf{X}_N,\mathbf{V}_N,\boldsymbol{E}_h,\boldsymbol{B}_h) = \{\mathcal{F}_h,\mathcal{H}_h\}_h$$

▷ with $\mathcal{H}_h(\mathbf{X}_N,\mathbf{V}_N,\boldsymbol{E}_h,\boldsymbol{B}_h) = \frac{1}{2}\sum_p w_p|\boldsymbol{V}_p|^2 + \frac{1}{2}\int(|\boldsymbol{E}_h|^2+|\boldsymbol{B}_h|^2)$ and

$$\{\mathcal{F}_h,\mathcal{G}_h\}_h = \sum_{p=1}^N\left[\frac{1}{w_p}\left(\left(\frac{\delta\mathcal{F}_h}{\delta\boldsymbol{X}_p}\cdot\frac{\delta\mathcal{G}_h}{\delta\boldsymbol{V}_p} - \frac{\delta\mathcal{F}_h}{\delta\boldsymbol{V}_p}\cdot\frac{\delta\mathcal{G}_h}{\delta\boldsymbol{X}_p}\right) + \boldsymbol{B}^S(\boldsymbol{X}_p)\cdot\left(\frac{\delta\mathcal{F}_h}{\delta\boldsymbol{V}_p}\times\frac{\delta\mathcal{G}_h}{\delta\boldsymbol{V}_p}\right)\right)\right.$$
$$\left.-\int_\Omega\left(\frac{\delta\mathcal{F}_h}{\delta\boldsymbol{E}_h}\cdot\Pi^2\left(S_{\boldsymbol{X}_p}\frac{\delta\mathcal{G}_h}{\delta\boldsymbol{V}_p}\right) - \frac{\delta\mathcal{G}_h}{\delta\boldsymbol{E}_h}\cdot\Pi^2\left(S_{\boldsymbol{X}_p}\frac{\delta\mathcal{F}_h}{\delta\boldsymbol{V}_p}\right)\right)\right] + \int_\Omega\left(\frac{\delta\mathcal{F}_h}{\delta\boldsymbol{E}_h}\cdot\operatorname{curl}\frac{\delta\mathcal{G}_h}{\delta\boldsymbol{B}_h} - \frac{\delta\mathcal{G}_h}{\delta\boldsymbol{E}_h}\cdot\operatorname{curl}\frac{\delta\mathcal{F}_h}{\delta\boldsymbol{B}_h}\right)$$

1. Morrison ('80), Marder-Weinstein ('82), Weinstein-Morrison ('81)
2. CP-Kormann-Sonnendrücker ('21)

Outline

Resulting variational scheme : Fourier-GEMPIC

- Abstract variational scheme (Hamiltonian)

▷ particle push

$$\begin{cases} \partial_t \mathbf{x}_p = \mathbf{v}_p \\ \partial_t \mathbf{v}_p = \boldsymbol{E}_h^S(\mathbf{x}_p) + \mathbf{v}_p \times \boldsymbol{B}_h^S(\mathbf{x}_p) \end{cases} \quad \text{with} \quad \begin{cases} \boldsymbol{E}_{h,\alpha}^S(\mathbf{x}_p) := \int \boldsymbol{E}_{h,\alpha}(\boldsymbol{x})(\Pi_\alpha^2 S_{\mathbf{x}_p})(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \\ \boldsymbol{B}_{h,\alpha}^S(\mathbf{x}_p) := \int \boldsymbol{B}_{h,\alpha}(\boldsymbol{x})(\Pi_\alpha^1 S_{\mathbf{x}_p})(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \end{cases}$$

▷ field solve

$$\begin{cases} -\partial_t \boldsymbol{E}_h + \operatorname{curl} \boldsymbol{B}_h = \boldsymbol{J}_h^S \\ \partial_t \boldsymbol{B}_h + \operatorname{curl} \boldsymbol{E}_h = 0 \end{cases} \quad \text{with} \quad \boldsymbol{J}_h^S = \Pi^2(S * \boldsymbol{J}_N^\delta) = \sum_{p=1\cdots N} w_p \Pi^2(\mathbf{v}_p S_{\mathbf{x}_p})$$

- Application to Fourier spaces :

▷ particle push

$$\begin{cases} \partial_t \mathbf{x}_p = \mathbf{v}_p \\ \partial_t \mathbf{v}_p = \boldsymbol{E}_h^S(\mathbf{x}_p) + \mathbf{v}_p \times \boldsymbol{B}_h^S(\mathbf{x}_p) \end{cases} \quad \text{with} \quad \begin{cases} \boldsymbol{E}_{h,\alpha}^S(\mathbf{x}_p) = L^3 \sum_{\boldsymbol{k}} \overline{\boldsymbol{E}_{\boldsymbol{k},\alpha}} (\Pi_\alpha^2 S_{\mathbf{x}_p})_{\boldsymbol{k}} \\ \boldsymbol{B}_{h,\alpha}^S(\mathbf{x}_p) = L^3 \sum_{\boldsymbol{k}} \overline{\boldsymbol{B}_{\boldsymbol{k},\alpha}} (\Pi_\alpha^1 S_{\mathbf{x}_p})_{\boldsymbol{k}} \end{cases}$$

▷ field solve

$$\begin{cases} -\partial_t \boldsymbol{E}_{\boldsymbol{k}} + \frac{2\mathrm{i}\pi \boldsymbol{k}}{L} \times \boldsymbol{B}_{\boldsymbol{k}} = \sum_p w_p \Pi^2(\mathbf{v}_p S_{\mathbf{x}_p})_{\boldsymbol{k}} \\ \partial_t \boldsymbol{B}_{\boldsymbol{k}} + \frac{2\mathrm{i}\pi \boldsymbol{k}}{L} \times \boldsymbol{E}_{\boldsymbol{k}} = 0 \end{cases}$$

Fourier-GEMPIC : discrete Hamiltonian system

- discrete variables

$$\boldsymbol{u}(t) = \begin{pmatrix} \mathbf{X} \\ \mathbf{V} \\ \boldsymbol{e} \\ \boldsymbol{b} \end{pmatrix}(t) = \begin{pmatrix} (\mathbf{x}_p)_{p\le N} \\ (\mathbf{v}_p)_{p\le N} \\ (\boldsymbol{E}_{\boldsymbol{k}})_{|\boldsymbol{k}|_\infty \le K} \\ (\boldsymbol{B}_{\boldsymbol{k}})_{|\boldsymbol{k}|_\infty \le K} \end{pmatrix}(t)$$

- discrete Hamiltonian

$$\mathcal{H} = \frac{1}{2}\mathbf{V}^T \mathbb{W}_m \mathbf{V} + \frac{1}{2}\mathbf{e}^T \mathbb{M}^2 \mathbf{e} + \frac{1}{2}\boldsymbol{b}^T \mathbb{M}^1 \boldsymbol{b}$$

with $\mathbb{W}_m$: particle weighting matrix, $\mathbb{M}^1$, $\mathbb{M}^2$: FEM mass matrices

- Hamiltonian system

$$\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} = \mathbb{J}(\boldsymbol{u})\nabla_{\boldsymbol{u}}\mathcal{H}(\boldsymbol{u})$$

- Poisson matrix (antisymmetric, Jacobi identity)

$$\mathbb{J}(\boldsymbol{u}) = \begin{pmatrix} 0 & \mathbb{W}_{1/m} & 0 & 0 \\ -\mathbb{W}_{1/m} & \mathbb{W}_{q/m}\mathbb{B}^1(\mathbf{X}, \boldsymbol{b})\mathbb{W}_{1/m} & \mathbb{W}_{q/m}\mathbb{S}^2(\mathbf{X})(\mathbf{X}) & 0 \\ 0 & -\mathbb{S}^2(\mathbf{X})^T\mathbb{W}_{q/m} & 0 & \mathbb{C}(\mathbb{M}^1)^{-1} \\ 0 & 0 & -(\mathbb{M}^1)^{-1}\mathbb{C}^T & 0 \end{pmatrix}$$

with
$$\begin{cases} \mathbb{C} \equiv \text{discrete curl matrix} \\ \mathbb{S}^2(\mathbf{X})_{p,k} \equiv \Pi^2 \text{ coupling of } p\text{-th particle with mode } k \\ \mathbb{B}^1(\mathbf{X}, \boldsymbol{b})_{p,p} \equiv \text{magnetic rotation of } p\text{-th trajectory with } \Pi^1 \text{ coupling} \end{cases}$$

Fourier-GEMPIC scheme : conservation properties

- conservation of Gauss laws : ok

$$\begin{cases} \partial_t(\mathrm{div}\, \boldsymbol{E}_h) = -\,\mathrm{div}\, \Pi^2 \boldsymbol{J}_N = -\Pi^3\, \mathrm{div}\, \boldsymbol{J}_N = \partial_t(\Pi^3 \rho_N) \\ \partial_t(\mathrm{div}\, \boldsymbol{B}_h) = -\,\mathrm{div}(\mathrm{curl}\, \boldsymbol{E}_h) = 0 \end{cases}$$

- conservation of energy : ok

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\tfrac{1}{2}\int |\boldsymbol{E}_h|^2 + |\boldsymbol{B}_h|^2\Big) = \int \boldsymbol{E}_h \cdot (\mathrm{curl}\, \boldsymbol{B}_h - \Pi^2 \boldsymbol{J}_N) - \boldsymbol{B}_h \cdot \mathrm{curl}\, \boldsymbol{E}_h = -\int \boldsymbol{E}_h \cdot \Pi^2 \boldsymbol{J}_N$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\tfrac{1}{2}\sum_p w_p |\mathbf{v}_p|^2\Big) = \sum_p w_p \mathbf{v}_p \cdot \big(\mathbf{v}_p \times \boldsymbol{B}_h^S(\mathbf{x}_p) + \boldsymbol{E}_h^S(\mathbf{x}_p)\big) = \sum_p w_p \int \Pi^2(\mathbf{v}_p S(\boldsymbol{x} - \mathbf{x}_p)) \cdot \boldsymbol{E}_h(\mathbf{x})$$

- conservation of momentum ? $\mathcal{P} = \sum_p w_p \mathbf{v}_p + L^3 \sum_{\boldsymbol{k}} \mathbf{E}_{\boldsymbol{k}} \times \overline{\mathbf{B}_{\boldsymbol{k}}}$

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\sum_p w_p \mathbf{v}_p\Big)_\alpha = \sum_{p,\boldsymbol{k}} w_p L^3 \Big(\overline{\boldsymbol{E}_{\boldsymbol{k},\alpha}}(\Pi^2 S_{\mathbf{x}_p})_{\boldsymbol{k},\alpha} \pm \mathbf{v}_{p,\alpha\pm 1} \overline{\boldsymbol{B}_{\boldsymbol{k},\alpha\mp 1}}(\Pi^1 S_{\mathbf{x}_p})_{\boldsymbol{k},\alpha\mp 1}\Big)$$

and, using that $\sum_{\boldsymbol{k}} (\boldsymbol{k} \times \boldsymbol{C}_{\boldsymbol{k}}) \times \overline{\boldsymbol{C}_{\boldsymbol{k}}} = -\sum_{\boldsymbol{k}} (\boldsymbol{k} \cdot \boldsymbol{C}_{\boldsymbol{k}}) \overline{\boldsymbol{C}_{\boldsymbol{k}}}$,

$$\frac{\mathrm{d}}{\mathrm{d}t} L^3 \sum_{\boldsymbol{k}} \mathbf{E}_{\boldsymbol{k}} \times \overline{\mathbf{B}_{\boldsymbol{k}}} = L^3 \sum_{\boldsymbol{k}} \boldsymbol{E}_{\boldsymbol{k}} \times \Big(-\overline{\tfrac{2\mathrm{i}\pi \boldsymbol{k}}{L} \times \mathbf{E}_{\boldsymbol{k}}}\Big) + \Big(\tfrac{2\mathrm{i}\pi \boldsymbol{k}}{L} \times \boldsymbol{B}_{\boldsymbol{k}} - (\Pi^2 \boldsymbol{J}_N)_{\boldsymbol{k}}\Big) \times \overline{\mathbf{B}_{\boldsymbol{k}}}$$

$$= L^3 \sum_{\boldsymbol{k}} -(\Pi^3 \rho_N)_{\boldsymbol{k}} \overline{\boldsymbol{E}_{\boldsymbol{k}}} - (\Pi^2 \boldsymbol{J}_N)_{\boldsymbol{k}} \times \overline{\mathbf{B}_{\boldsymbol{k}}}$$

▷ ok if $\Pi^0 = \Pi^1_\alpha = \Pi^2_\alpha = \Pi^3$ (eg, L^2 projections)

Outline

Hamiltonian time splitting [1] : preserving the Poisson structure

- Step $\mathcal{H}_{E,B}$:

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}_p = 0 \\ \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{v}_p = \boldsymbol{E}_h^S(\mathbf{x}_p) \\ \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{E}_h = \mathrm{curl}\, \boldsymbol{B}_h \\ \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{B}_h = -\,\mathrm{curl}\, \boldsymbol{E}_h \end{cases} \quad \text{i.e.,} \quad \begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}_p = 0 \\ \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{v}_{p,\alpha} = L^3 \sum_{\boldsymbol{k}} \overline{E_{\boldsymbol{k},\alpha}}(\Pi^2_\alpha S_{\mathbf{x}_p})_{\boldsymbol{k}} \\ \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{E}_{\boldsymbol{k}} = \frac{2\mathrm{i}\pi\boldsymbol{k}}{L} \times \boldsymbol{B}_{\boldsymbol{k}} \\ \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{B}_{\boldsymbol{k}} = -\frac{2\mathrm{i}\pi\boldsymbol{k}}{L} \times \boldsymbol{E}_{\boldsymbol{k}} \end{cases} \quad \text{for} \quad \begin{cases} 1 \le \alpha \le 3 \\ p = 1 \cdots N \\ |\boldsymbol{k}|_\infty \le K \end{cases}$$

- Step $\mathcal{H}_{p,\alpha}$, for $1 \le \alpha \le 3$:

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}_p = \mathbf{v}_p^{[\alpha]} \\ \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{v}_p = \mathbf{v}_p^{[\alpha]} \times \boldsymbol{B}_h^S(\mathbf{x}_p) \\ \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{E}_h = -\Pi^2(\boldsymbol{J}_N^{[\alpha]}) \\ \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{B}_h = 0 \end{cases} \quad \text{i.e.,} \quad \begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x}_{p,\alpha} = \mathrm{v}_{p,\alpha} \\ \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x}_{p,\alpha\pm1} = \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{v}_{p,\alpha} = 0 \\ \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{v}_{p,\alpha\pm1} = \mp L^3 \sum_{\boldsymbol{k}} \mathrm{v}_{p,\alpha}\overline{B_{\boldsymbol{k},\alpha\mp1}}(\Pi^1_{\alpha\mp1} S_{\mathbf{x}_p})_{\boldsymbol{k}} \\ \frac{\mathrm{d}}{\mathrm{d}t}E_{\boldsymbol{k},\alpha} = -\sum_p w_p \mathrm{v}_{p,\alpha}(\Pi^2_\alpha S_{\mathbf{x}_p})_{\boldsymbol{k}} \\ \frac{\mathrm{d}}{\mathrm{d}t}E_{\boldsymbol{k},\alpha\pm1} = \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{B}_{\boldsymbol{k}} = 0 \end{cases}$$

where $\boldsymbol{G}^{[\alpha]} := \hat{\boldsymbol{e}}_\alpha(\hat{\boldsymbol{e}}_\alpha \cdot \boldsymbol{G})$

- exact solutions, explicit formulas $\rightsquigarrow$ spectral PIC with non-standard DFT

1. Crouseilles, Einkemmer, Faou ('15), Kraus, Kormann, Morrison, Sonnendrücker ('17)

Hamiltonian time splitting : conservation properties

- Discrete Gauss laws and Hamiltonian structure : preserved
- Energy : preserved within bounds, by backward error analysis
- Momentum ? Step $\mathcal{H}_{E,B}$:

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\Big(\sum_p w_p \mathbf{v}_p\Big)_\alpha = \sum_{p,\boldsymbol{k}} w_p L^3 \Big(\overline{E_{\alpha,\boldsymbol{k}}}(\Pi^2_\alpha S_{\mathbf{x}_p})_{\boldsymbol{k}}\Big) \\ \frac{\mathrm{d}}{\mathrm{d}t} L^3 \Big(\sum_{\boldsymbol{k}} \mathbf{E}_{\boldsymbol{k}} \times \overline{\mathbf{B}_{\boldsymbol{k}}}\Big)_\alpha = L^3 \sum_{\boldsymbol{k}} -(\Pi^3 \rho_N)_{\boldsymbol{k}} \overline{E_{\alpha,\boldsymbol{k}}} \end{cases} \quad \text{for} \quad 1 \le \alpha \le 3$$

Step $\mathcal{H}_{p,\alpha}$, for $1 \le \alpha \le 3$:

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\Big(\sum_p w_p \mathbf{v}_p\Big)_{\alpha\pm1} = \mp \sum_{p,\boldsymbol{k}} w_p L^3 \Big(\mathrm{v}_{p,\alpha} \overline{B_{\boldsymbol{k},\alpha\mp1}}(\Pi^1_{\alpha\mp1} S_{\mathbf{x}_p})_{\boldsymbol{k}}\Big) \\ \frac{\mathrm{d}}{\mathrm{d}t} L^3 \Big(\sum_{\boldsymbol{k}} \mathbf{E}_{\boldsymbol{k}} \times \overline{B_{\boldsymbol{k}}}\Big)_{\alpha\pm1} = \pm L^3 \sum_{p,\boldsymbol{k}} w_p \mathrm{v}_{p,\alpha} (\Pi^2_\alpha S_{\mathbf{x}_p})_{\boldsymbol{k}} \times \overline{B_{\alpha\mp1,\boldsymbol{k}}} \end{cases}$$

▷ Projection discrepancy, solved with momentum-preserving velocity kicks

$$(\mathcal{H}_{E,B}) \quad \tfrac{\mathrm{d}}{\mathrm{d}t}\mathrm{v}_{p,\alpha} = L^3 \sum_{\boldsymbol{k}} \overline{E_{\boldsymbol{k},\alpha}}(\Pi^3 S_{\mathbf{x}_p})_{\boldsymbol{k}}, \quad (\mathcal{H}_{p,\alpha}) \quad \tfrac{\mathrm{d}}{\mathrm{d}t}\mathrm{v}_{p,\alpha\pm1} = \mp L^3 \sum_{\boldsymbol{k}} \mathrm{v}_{p,\alpha} \overline{B_{\boldsymbol{k},\alpha\mp1}}(\Pi^2_\alpha S_{\mathbf{x}_p})_{\boldsymbol{k}}$$

- variational scheme and momentum-preserving variant coincide in gridless PIF

Hamiltonian time splitting [1] : variational scheme (again)

- Step $\mathcal{H}_{E,B}$:

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}_p = 0 \\ \dfrac{\mathrm{d}}{\mathrm{d}t}\mathbf{v}_p = \boldsymbol{E}_h^S(\mathbf{x}_p) \\ \dfrac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{E}_h = \operatorname{curl} \boldsymbol{B}_h \\ \dfrac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{B}_h = -\operatorname{curl} \boldsymbol{E}_h \end{cases} \quad \text{i.e.,} \quad \begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}_p = 0 \\ \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{v}_{p,\alpha} = L^3 \sum_{\boldsymbol{k}} \overline{E_{\boldsymbol{k},\alpha}}(\Pi^2_\alpha S_{\mathbf{x}_p})_{\boldsymbol{k}} \\ \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{E}_{\boldsymbol{k}} = \frac{2\mathrm{i}\pi\boldsymbol{k}}{L} \times \boldsymbol{B}_{\boldsymbol{k}} \\ \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{B}_{\boldsymbol{k}} = -\frac{2\mathrm{i}\pi\boldsymbol{k}}{L} \times \boldsymbol{E}_{\boldsymbol{k}} \end{cases} \quad \text{for} \quad \begin{cases} 1 \le \alpha \le 3 \\ p = 1 \cdots N \\ |\boldsymbol{k}|_\infty \le K \end{cases}$$

- Step $\mathcal{H}_{p,\alpha}$, for $1 \le \alpha \le 3$:

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}_p = \mathbf{v}_p^{[\alpha]} \\ \dfrac{\mathrm{d}}{\mathrm{d}t}\mathbf{v}_p = \mathbf{v}_p^{[\alpha]} \times \boldsymbol{B}_h^S(\mathbf{x}_p) \\ \dfrac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{E}_h = -\Pi^2(\boldsymbol{J}_N^{[\alpha]}) \\ \dfrac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{B}_h = 0 \end{cases} \quad \text{i.e.,} \quad \begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x}_{p,\alpha} = \mathrm{v}_{p,\alpha} \\ \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x}_{p,\alpha\pm1} = \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{v}_{p,\alpha} = 0 \\ \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{v}_{p,\alpha\pm1} = \mp L^3 \sum_{\boldsymbol{k}} \mathrm{v}_{p,\alpha}\overline{B_{\boldsymbol{k},\alpha\mp1}}(\Pi^1_{\alpha\mp1} S_{\mathbf{x}_p})_{\boldsymbol{k}} \\ \frac{\mathrm{d}}{\mathrm{d}t}E_{\boldsymbol{k},\alpha} = -\sum_p w_p \mathrm{v}_{p,\alpha}(\Pi^2_\alpha S_{\mathbf{x}_p})_{\boldsymbol{k}} \\ \frac{\mathrm{d}}{\mathrm{d}t}E_{\boldsymbol{k},\alpha\pm1} = \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{B}_{\boldsymbol{k}} = 0 \end{cases}$$

where $\boldsymbol{G}^{[\alpha]} := \hat{\boldsymbol{e}}_\alpha(\hat{\boldsymbol{e}}_\alpha \cdot \boldsymbol{G})$

- exact solutions, explicit formulas $\rightsquigarrow$ spectral PIC with non-standard DFT

1. Crouseilles, Einkemmer, Faou ('15), Kraus, Kormann, Morrison, Sonnendrücker ('17)

Hamiltonian time splitting [1] : momentum-preserving variant

- Step $\mathcal{H}_{E,B}$:

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}_p = 0 \\ \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{v}_p = \boldsymbol{E}_h^S(\mathbf{x}_p) \\ \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{E}_h = \mathrm{curl}\, \boldsymbol{B}_h \\ \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{B}_h = -\,\mathrm{curl}\, \boldsymbol{E}_h \end{cases} \quad \text{i.e.,} \quad \begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}_p = 0 \\ \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{v}_{p,\alpha} = L^3 \sum_{\boldsymbol{k}} \overline{E_{\boldsymbol{k},\alpha}}(\Pi^3 S_{\mathbf{x}_p})_{\boldsymbol{k}} \\ \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{E}_{\boldsymbol{k}} = \frac{2i\pi\boldsymbol{k}}{L} \times \boldsymbol{B}_{\boldsymbol{k}} \\ \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{B}_{\boldsymbol{k}} = -\frac{2i\pi\boldsymbol{k}}{L} \times \boldsymbol{E}_{\boldsymbol{k}} \end{cases} \quad \text{for} \quad \begin{cases} 1 \le \alpha \le 3 \\ p = 1 \cdots N \\ |\boldsymbol{k}|_\infty \le K \end{cases}$$

- Step $\mathcal{H}_{p,\alpha}$, for $1 \le \alpha \le 3$:

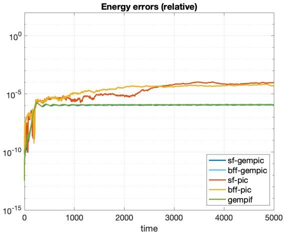
$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}_p = \mathbf{v}_p^{[\alpha]} \\ \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{v}_p = \mathbf{v}_p^{[\alpha]} \times \boldsymbol{B}_h^S(\mathbf{x}_p) \\ \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{E}_h = -\Pi^2(\boldsymbol{J}_N^{[\alpha]}) \\ \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{B}_h = 0 \end{cases} \quad \text{i.e.,} \quad \begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}x_{p,\alpha} = v_{p,\alpha} \\ \frac{\mathrm{d}}{\mathrm{d}t}x_{p,\alpha\pm1} = \frac{\mathrm{d}}{\mathrm{d}t}v_{p,\alpha} = 0 \\ \frac{\mathrm{d}}{\mathrm{d}t}v_{p,\alpha\pm1} = \mp L^3 \sum_{\boldsymbol{k}} v_{p,\alpha}\overline{B_{\boldsymbol{k},\alpha\mp1}}(\Pi^2_\alpha S_{\mathbf{x}_p})_{\boldsymbol{k}} \\ \frac{\mathrm{d}}{\mathrm{d}t}E_{\boldsymbol{k},\alpha} = -\sum_p w_p v_{p,\alpha}(\Pi^2_\alpha S_{\mathbf{x}_p})_{\boldsymbol{k}} \\ \frac{\mathrm{d}}{\mathrm{d}t}E_{\boldsymbol{k},\alpha\pm1} = \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{B}_{\boldsymbol{k}} = 0 \end{cases}$$

where $\boldsymbol{G}^{[\alpha]} := \hat{\boldsymbol{e}}_\alpha(\hat{\boldsymbol{e}}_\alpha \cdot \boldsymbol{G})$

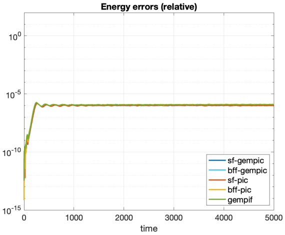
- exact solutions, explicit formulas $\rightsquigarrow$ spectral PIC with standard DFT

1. Crouseilles, Einkemmer, Faou ('15), Kraus, Kormann, Morrison, Sonnendrücker ('17)

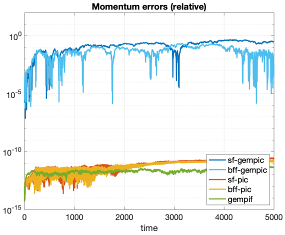
Long-time conservation of energy and momentum (Weibel instability)



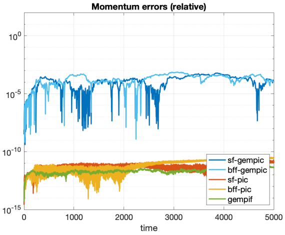
Energy errors, cubic smoothing



Energy errors, 7-degree smoothing

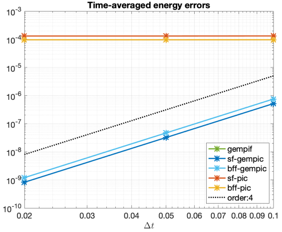


Momentum errors, cubic smoothing

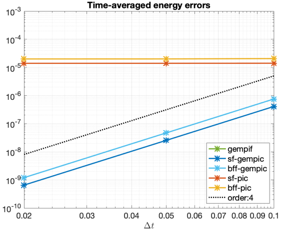


Momentum errors, 7-degree smoothing

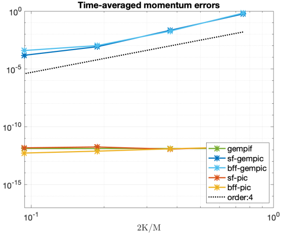
Convergence of energy and momentum errors (4-th order time splitting)



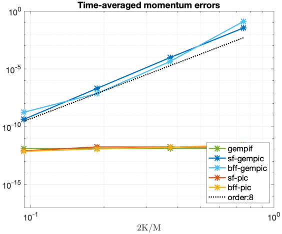
Energy errors, cubic smoothing



Energy errors, 5-degree smoothing

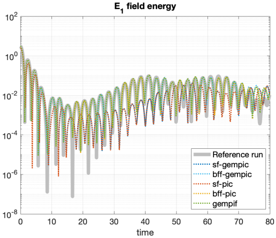


Momentum errors, cubic smoothing

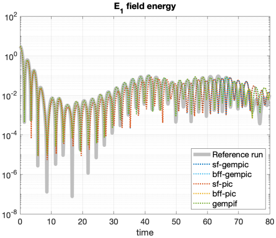


Momentum errors, 7-degree smoothing

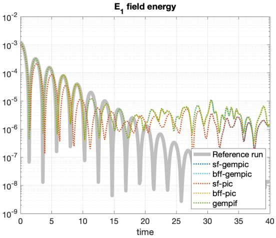
Anti-aliasing with back-filtered projection operators (Landau damping)



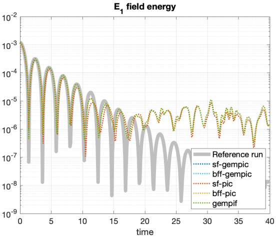
strong damping with an $M = 8$ grid



strong damping with an $M = 16$ grid

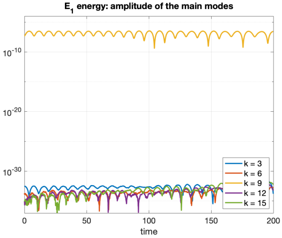


weak damping with an $M = 8$ grid

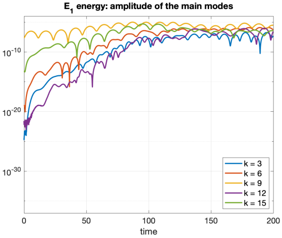


weak damping with an $M = 16$ grid

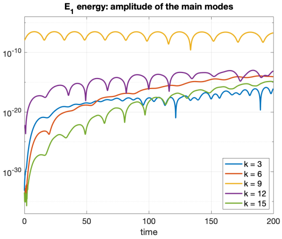
Anti-aliasing and back-filtering (FGI for a single mode oscillation)



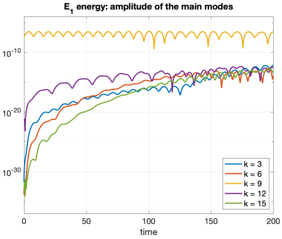
PIF ($K = 16$) : no spurious modes



GEMPIC with quadratic splines



7-degree smoothing, no back-filtering



7-degree smoothing with back-filtering

Outline

Summary

- unifying framework for Hamiltonian FEM-PIC schemes
- particle-field coupling encoded by commuting projection operators
- key physical invariants on general geometries
- application to FEEC and broken-FEEC schemes on complex domains
- application to spectral particle schemes :
  - L^2 projection operators : gridless PIF (energy+momentum preserving)
  - DFT projection operators : new spectral PIC (energy preserving)
  - std spectral PIC : momentum preserving variant
  - fast convergence to PIF with anti-aliasing (smooth particles) + back-filtering
- with J. Ameres, K. Kormann and E. Sonnendrücker :
  - Variational Framework for Structure-Preserving Electromagnetic PIC Methods (2021)
  - On Geometric Fourier Particle In Cell Methods (2021)
  - On Particle-in-Cell approximations to Particle-in-Fourier schemes (2021)
- with Y. Güçlü, S. Hadjout, F. Patrizi and F. Schnack :
  - Broken-FEEC approximations of Hodge-Laplace problems (2021)
  - A broken-FEEC framework for EM pbms on mapped multipatch domains (2022)
  - CONGA schemes for polar splines (in progress)
  - broken-FEEC for multi-patch domains with non-matching grids (PhD of F. Schnack)

▷ open problems (and positions) : large-scale codes, extension to GK models