Geometric Particle-in-Cell Simulations of the Vlasov–Maxwell System in Curvilinear Coordinates

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Vlasov–Maxwell equations

The non-relativistic Vlasov equation:

$$\frac{f_s}{t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s + \frac{q_s}{m_s}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_{\mathbf{v}} f_s = 0.$$

Maxwell equations:

$$\frac{\partial \mathbf{E}}{\partial t} - \operatorname{curl} \mathbf{B} = -\mathbf{J}, \qquad \frac{\partial \mathbf{B}}{\partial t} + \operatorname{curl} \mathbf{E} = 0,$$

$$\operatorname{div} \mathbf{E} = \rho, \qquad \operatorname{div} \mathbf{B} = 0.$$

Charge density: $\rho = \sum_s q_s \int f_s \mathrm{d}\mathbf{v}$.
Current density: $\mathbf{J} = \sum_s q_s \int f_s \mathbf{v} \mathrm{d}\mathbf{v}$.

Characteristic equations:

$$\frac{\mathrm{d}\mathbf{X}}{\mathrm{d}t} = \mathbf{V}, \quad \frac{\mathrm{d}\mathbf{V}}{\mathrm{d}t} = \mathbf{E} + \mathbf{V} \times \mathbf{B}.$$

Structure of the Vlasov–Maxwell system

- Energy, momentum, and charge **conservation**.
- Hamiltonian of the system:

$$\mathcal{H} = \sum_s \frac{m_s}{2} \int |\mathbf{v}|^2 \, f_s(\mathbf{x}, \mathbf{v}) \, \mathrm{d}\mathbf{x} \, \mathrm{d}\mathbf{v} + \frac{1}{2} \int \left(|\mathbf{E}(\mathbf{x})|^2 + |\mathbf{B}(\mathbf{x})|^2 \right) \mathrm{d}\mathbf{x}.$$

- Ampère's equation and Faraday's law have a unique solution by themselves (provided adequate initial and boundary conditions). The **divergence constraints** remain satisfied over time.
- Spaces of electromagnetics form a de Rham complex

$$H^1(\Omega) \xrightarrow{\text{grad}} H(\text{curl}, \Omega) \xrightarrow{\text{curl}} H(\text{div}, \Omega) \xrightarrow{\text{div}} L^2(\Omega)$$

  with $\phi \in H^1(\Omega)$, $\mathbf{E}, \mathbf{A} \in H(\text{curl}, \Omega)$, $\mathbf{B}, \mathbf{J} \in H(\text{div}, \Omega)$, and $\rho \in L^2(\Omega)$.
- Exactness: div curl $= 0$, curl grad $= 0$.

GEMPIC framework

- **Discretisation**: Conforming spline finite elements for fields (discrete deRham complex), Particle–In–Cell for distribution functions.
- **Formulation** of equations based on semi-discrete Hamiltonian and Poisson bracket.
- **Temporal discretisations**: Hamiltonian splitting and (semi)-implicit methods based on discrete gradient methods.

References: M. Kraus, K. Kormann, Ph. J. Morrison, E. Sonnendrücker: GEMPIC: geometric electromagnetic particle-in-cell methods, *J. Plasma Phys.* 83:905830401, 2017.
K. Kormann, E. Sonnendrücker: Energy-conserving time propagation for a geometric particle-in-cell Vlasov–Maxwell solver, https://arxiv.org/abs/1910.04000.

Geometry

Main limitation of the current GEMPIC framework: Limited to Cartesian coordinates.

Geometry of a fusion reactor: D-shaped torus.

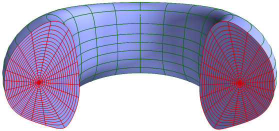


Figure: Schematic view of a tokamak mesh by Yaman Güçlü

Purpose of this talk: Add curvilinear coordinates to the description.

Curvilinear coordinates

- **Coordinate transformation** from the logical to the physical space: $F : [0,1]^3 \to \Omega, \boldsymbol{\xi} \mapsto F(\boldsymbol{\xi}) = \mathbf{x}$.
- Jacobian matrix $DF(\xi)_{ij} = \frac{\partial F(\boldsymbol{\xi})}{\partial \xi_j}$ and Jacobian determinant $J_F(\boldsymbol{\xi}) = \det(DF(\boldsymbol{\xi}))$.
- Covariant basis of the tangent space: $\mathbf{t}_i = \frac{\partial F(\boldsymbol{\xi})}{\partial \xi_i} \to DF = (\mathbf{t}_1|\mathbf{t}_2|\mathbf{t}_3)$.
- Contravariant basis of the cotangent space: Columns of the transposed inverse Jacobian: $N(\boldsymbol{\xi}) := DF^{-\top} = (\mathbf{n}^1|\mathbf{n}^2|\mathbf{n}^3)$
- Metric: $G_t := DF^\top DF, G_n := N^\top N$

Transformation of differential forms

- 0-form: $\tilde{g}(\boldsymbol{\xi}) := g(F(\boldsymbol{\xi})) = g(\mathbf{x})$;
- 1-form: $\mathbf{E}(\mathbf{x}) = N(\boldsymbol{\xi})\tilde{\mathbf{E}}(\boldsymbol{\xi})$;
  Consider the gradient of a 0-form:
  $\nabla_{\boldsymbol{\xi}}\tilde{g}(\boldsymbol{\xi}) = \nabla_{\boldsymbol{\xi}} g(F(\boldsymbol{\xi})) = DF(\boldsymbol{\xi})^T \nabla_{\mathbf{x}} g(\mathbf{x})$
  $\Rightarrow \nabla_{\mathbf{x}} g(\mathbf{x}) = N(\boldsymbol{\xi})\nabla_{\boldsymbol{\xi}}\tilde{g}(\boldsymbol{\xi})$.
- 2-form: $\mathbf{B}(\mathbf{x}) = \frac{DF(\boldsymbol{\xi})}{J_F(\boldsymbol{\xi})}\tilde{\mathbf{B}}(\boldsymbol{\xi})$;
  Rotation of a 1-form $\mathbf{E}$: $\nabla_{\mathbf{x}} \times \mathbf{E}(\mathbf{x}) = \frac{DF(\boldsymbol{\xi})}{J_F(\boldsymbol{\xi})}\nabla_{\boldsymbol{\xi}} \times \tilde{\mathbf{E}}(\boldsymbol{\xi})$.
- 3-form: $g(\mathbf{x}) = \frac{1}{J_F(\boldsymbol{\xi})}\tilde{g}(\boldsymbol{\xi})$;
  Divergence of a 2-form $\mathbf{B}$: $\nabla_{\mathbf{x}} \cdot \mathbf{B}(\mathbf{x}) = \frac{1}{J_F(\boldsymbol{\xi})}\nabla_{\boldsymbol{\xi}} \cdot \tilde{\mathbf{B}}(\boldsymbol{\xi})$.

Maxwell's equation in curvilinear coordinates

- **Faraday's law**:

$$\frac{\partial \mathbf{B}(\mathbf{x})}{\partial t} = -\nabla_{\mathbf{x}} \times \mathbf{E}(\mathbf{x}) \to \frac{DF(\boldsymbol{\xi})}{J_F}\frac{\partial \tilde{\mathbf{B}}(\boldsymbol{\xi})}{\partial t} = -\frac{DF(\boldsymbol{\xi})}{J_F}\nabla_{\boldsymbol{\xi}} \times \tilde{\mathbf{E}}(\boldsymbol{\xi}).$$

- **Gauss' law for magnetism**: $\nabla_{\mathbf{x}} \cdot \mathbf{B}(\mathbf{x}) = 0 \to \frac{1}{J_F(\boldsymbol{\xi})}\nabla_{\boldsymbol{\xi}} \cdot \tilde{\mathbf{B}}(\boldsymbol{\xi}) = 0.$
- **Ampère's law**:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega} \varphi(\mathbf{x})\cdot\mathbf{E}(\mathbf{x})\,\mathrm{d}\mathbf{x} = \int_{\Omega} \nabla_{\mathbf{x}}\times\varphi(\mathbf{x})\cdot\mathbf{B}(\mathbf{x})\,\mathrm{d}\mathbf{x} - \int_{\Omega} \varphi(\mathbf{x})\cdot\mathbf{J}(\mathbf{x})\,\mathrm{d}\mathbf{x} \text{ for all } \varphi \in H(\mathrm{curl},\Omega)$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\tilde{\Omega}} N(\boldsymbol{\xi})\tilde{\varphi}(\boldsymbol{\xi}) \cdot N(\boldsymbol{\xi})\tilde{\mathbf{E}}(\boldsymbol{\xi})|J_F(\boldsymbol{\xi})|\,\mathrm{d}\boldsymbol{\xi} = \int_{\tilde{\Omega}} DF(\boldsymbol{\xi})\nabla_{\boldsymbol{\xi}} \times \tilde{\varphi}(\boldsymbol{\xi}) \cdot DF(\boldsymbol{\xi})\tilde{\mathbf{B}}(\boldsymbol{\xi})\frac{1}{|J_F(\boldsymbol{\xi})|}\,\mathrm{d}\boldsymbol{\xi}$$

$$-\int_{\tilde{\Omega}} \tilde{N}(\boldsymbol{\xi})\tilde{\varphi}(\boldsymbol{\xi}) \cdot DF^T(\boldsymbol{\xi})\tilde{\mathbf{J}}(\boldsymbol{\xi})|J_F(\boldsymbol{\xi})|\,\mathrm{d}\boldsymbol{\xi} \text{ for all } \tilde{\varphi} \in H(\mathrm{curl},\tilde{\Omega})$$

- **Gauss' law for electricity**:

$$-\int_{\Omega} \nabla_{\mathbf{x}}\psi(\mathbf{x}) \cdot \mathbf{E}(\mathbf{x})\,\mathrm{d}\mathbf{x} = \int_{\Omega} \psi(\mathbf{x})\rho(\mathbf{x})\,\mathrm{d}\mathbf{x} \text{ for all } \psi \in H^1(\Omega)$$

$$-\int_{\tilde{\Omega}} N(\boldsymbol{\xi})\nabla_{\boldsymbol{\xi}}\tilde{\psi}(\boldsymbol{\xi})\cdot N(\boldsymbol{\xi})\tilde{\mathbf{E}}(\boldsymbol{\xi})|J_F(\boldsymbol{\xi})|\,\mathrm{d}\boldsymbol{\xi} = \int_{\tilde{\Omega}} \tilde{\psi}(\boldsymbol{\xi})\tilde{\rho}(\boldsymbol{\xi})|J_F(\boldsymbol{\xi})|\,\mathrm{d}\boldsymbol{\xi} \text{ for all } \tilde{\psi} \in H^1(\tilde{\Omega}).$$

Vlasov–Maxwell equations in curvilinear coordinates

- Vlasov equation expressed in curvlinear coordinates

$$\frac{\partial \tilde{f}(\boldsymbol{\xi}, \mathbf{v}, t)}{\partial t} + \mathbf{v} \cdot N(\boldsymbol{\xi}) \nabla_{\boldsymbol{\xi}} \tilde{f}(\boldsymbol{\xi}, \mathbf{v}, t)$$
$$+ \frac{q}{m}(N(\boldsymbol{\xi})\tilde{\mathbf{E}}(\boldsymbol{\xi}, t) + \mathbf{v} \times \frac{DF(\boldsymbol{\xi})}{J_F(\boldsymbol{\xi})}\tilde{\mathbf{B}}(\boldsymbol{\xi}, t)) \cdot \nabla_{\mathbf{v}} \tilde{f}(\boldsymbol{\xi}, \mathbf{v}, t) = 0.$$

- Reformulate as

$$\frac{\partial \tilde{f}(\boldsymbol{\xi}, \mathbf{v}, t)}{\partial t} + N^\top(\boldsymbol{\xi})\mathbf{v} \cdot \nabla_{\boldsymbol{\xi}} \tilde{f}(\boldsymbol{\xi}, \mathbf{v}, t)$$
$$+ \frac{q}{m} N(\boldsymbol{\xi}) \left(\tilde{\mathbf{E}}(\boldsymbol{\xi}, t) + (N^\top(\boldsymbol{\xi})\mathbf{v}) \times \tilde{\mathbf{B}}(\boldsymbol{\xi}, t)\right) \cdot \nabla_{\mathbf{v}} \tilde{f}(\boldsymbol{\xi}, \mathbf{v}, t) = 0.$$

- Characteristic equations

$$\frac{\mathrm{d}\boldsymbol{\xi}}{\mathrm{d}t} = N(\boldsymbol{\xi})^\top \mathbf{v}, \quad \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \frac{q}{m} N(\boldsymbol{\xi}) \left(\tilde{\mathbf{E}}(\boldsymbol{\xi}, t) + (N^\top(\boldsymbol{\xi})\mathbf{v}) \times \tilde{\mathbf{B}}(\boldsymbol{\xi}, t)\right).$$

Vlasov–Maxwell system

Curvilinear geometry

Spatial semidiscretisation

Time-discretisation

Numerical results

Conclusions

Particle-in-cell discretisation of the distribution

- Sample N_p particles with position $\mathbf{x}_p$, velocity $\mathbf{v}_p$, and weight ω_p from the distribution function.
- Define Klimotovic distribution $f_h(\mathbf{x}, \mathbf{v}, t) = \sum_{p=1}^{N_p} \omega_p \delta(\mathbf{x} - \mathbf{x}_p(t)) \delta(\mathbf{v} - \mathbf{v}_p(t))$.
- Curvilinear version of the Klimotovic distribution

$$
\begin{aligned}
\tilde{f}_h(\boldsymbol{\xi}, \mathbf{v}, t) =& f_h(F(\boldsymbol{\xi}), \mathbf{v}, t) = \sum_{p=1}^{N_p} \omega_p \delta(F(\boldsymbol{\xi}) - F(\boldsymbol{\xi}_p(t))) \delta(\mathbf{v} - \mathbf{v}_p(t)) \\
=& \sum_{p=1}^{N_p} \omega_p \frac{\delta(\boldsymbol{\xi} - \boldsymbol{\xi}_p(t))}{J_F(\boldsymbol{\xi}_p)} \delta(\mathbf{v} - \mathbf{v}_p(t)).
\end{aligned}
$$

- Curvilinear form of charge and current densities

$$
\tilde{\mathbf{J}}_h(\boldsymbol{\xi}) = DF^T(\boldsymbol{\xi}) \int q \tilde{f}_h(\boldsymbol{\xi}, \mathbf{v}, t) \mathbf{v} \, \mathrm{d}\mathbf{v} = DF^T(\boldsymbol{\xi}) \sum_p q_p \omega_p \frac{\delta(\boldsymbol{\xi} - \boldsymbol{\xi}_p(t))}{J_F(\boldsymbol{\xi}_p)} \mathbf{v}_p,
$$

$$
\tilde{\rho}_h(\boldsymbol{\xi}) = \int q \tilde{f}_h(\boldsymbol{\xi}, \mathbf{v}, t) \, \mathrm{d}\mathbf{v} = \sum_p q_p \omega_p \frac{\delta(\boldsymbol{\xi} - \boldsymbol{\xi}_p(t))}{J_F(\boldsymbol{\xi}_p)}.
$$

Curvilinear form of the characteristic equations

Now we define $\boldsymbol{\Xi} = (\boldsymbol{\xi}_1, ..., \boldsymbol{\xi}_{N_P})^T, \mathbf{V} = (\mathbf{v}_1, ..., \mathbf{v}_{N_P})^T$ to write down the equations for the characteristics of the particles as

$$\begin{aligned} \dot{\boldsymbol{\Xi}}(t) &= \mathbb{N}^T(\boldsymbol{\Xi})\mathbf{V}(t), \\ \dot{\mathbf{V}}(t) &= \mathbb{M}_q \mathbb{M}_m^{-1} \mathbb{N}(\boldsymbol{\Xi}) \left(\tilde{\mathbf{E}}(\boldsymbol{\Xi}, t) + \mathbb{N}^T(\boldsymbol{\Xi})\mathbf{V}(t) \times \tilde{\mathbf{B}}(\boldsymbol{\Xi}, t) \right), \end{aligned}$$

where the matrix $\mathbb{N}(\boldsymbol{\Xi}) \in \mathbb{R}^{3N_p \times 3N_p}$ is defined as the block-diagonal matrix with block $N(\boldsymbol{\xi}_p)$ for each particle and $\mathbb{M}_m = \mathrm{diag}(\omega_p m_p) \otimes \mathbb{I}_3, \mathbb{M}_q = \mathrm{diag}(\omega_p q_p) \otimes \mathbb{I}_3$ the mass and charge matrix for the particles.

Structure preserving finite elements

- Spaces of electromagnetics form a de Rham complex

  with $\phi \in H^1(\Omega)$, $\mathbf{E}, \mathbf{A} \in H(\mathrm{curl}, \Omega)$, $\mathbf{B}, \mathbf{J} \in H(\mathrm{div}, \Omega)$, $\rho \in L_2(\Omega)$.
- Exactness: div curl $= 0$, curl grad $= 0$.
- **Finite Element Exterior Calculus** (FEEC): Mathematical theory for finite element discretisation that mimic de Rham structure.[1]

$$
\begin{tikzcd}
H^1(\Omega) \arrow[r, "\mathrm{grad}"] \arrow[d, "\Pi_0"'] & H(\mathrm{curl}, \Omega) \arrow[r, "\mathrm{curl}"] \arrow[d, "\Pi_1"'] & H(\mathrm{div}, \Omega) \arrow[r, "\mathrm{div}"] \arrow[d, "\Pi_2"'] & L^2(\Omega) \arrow[d, "\Pi_3"'] \\
V_0 \arrow[r, "\mathrm{grad}"] & V_1 \arrow[r, "\mathrm{curl}"] & V_2 \arrow[r, "\mathrm{div}"] & V_3
\end{tikzcd}
$$

[1] Arnold, Falk, Winther, Acta Numerica, 2006.

Discrete deRham sequence

The de Rham structure can also be expressed on the level of matrices and vectors. For some $\xi \in \tilde{\Omega}$ we collect the value of each basis function in a row vector as $\tilde{\Lambda}^0(\boldsymbol{\xi}) \in \mathbb{R}^{1\times N}$, $\tilde{\boldsymbol{\Lambda}}^1(\boldsymbol{\xi}) \in \mathbb{R}^{3\times 3N}$, $\tilde{\boldsymbol{\Lambda}}^2(\boldsymbol{\xi}) \in \mathbb{R}^{3\times 3N}$, $\tilde{\Lambda}^3(\boldsymbol{\xi}) \in \mathbb{R}^{1\times N}$. Then the following relation holds between the basis functions

$$\nabla_{\boldsymbol{\xi}} \tilde{\Lambda}^0(\boldsymbol{\xi}) = \tilde{\boldsymbol{\Lambda}}^1(\boldsymbol{\xi})\mathsf{G}$$

$$\nabla_{\boldsymbol{\xi}} \times \tilde{\boldsymbol{\Lambda}}^1(\boldsymbol{\xi}) = \tilde{\boldsymbol{\Lambda}}^2(\boldsymbol{\xi})\mathsf{C}$$

$$\nabla_{\boldsymbol{\xi}} \cdot \tilde{\boldsymbol{\Lambda}}^2(\boldsymbol{\xi}) = \tilde{\Lambda}^3(\boldsymbol{\xi})\mathsf{D}$$

for some matrix $\mathsf{G} \in \mathbb{R}^{N\times 3N}$ denoting the discrete gradient matrix, $\mathsf{C} \in \mathbb{R}^{3N\times 3N}$ denoting the discrete curl matrix and $\mathsf{D} = \mathsf{G}^\top$ denoting the discrete divergence, all independent of $\boldsymbol{\xi}$. These matrices need to satisfy

$$\mathsf{DC} = \mathsf{G}^\top\mathsf{C} = 0 \text{ and } \mathsf{CG} = 0$$

to mimic the exactness properties $\operatorname{div}\operatorname{curl} = 0$ and $\operatorname{curl}\operatorname{grad} = 0$.

Spline de Rham complex[a]

[a] Buffa, Rivas, Sangalli, Vásquez, SIAM J. Numer. Anal., 2011

On Cartesian meshes (i.e. on our logical mesh) a de Rham sequence can be constructed based on a tensor product of splines:

- 0-form basis: $V_0 = \mathrm{span}\{\mathcal{S}^p(x_1)\mathcal{S}^p(x_2)\mathcal{S}^p(x_3)\}$
- 1-form basis:

$$V_1 = \mathrm{span}\left\{ \begin{pmatrix} \mathcal{S}^{p-1}\mathcal{S}^p\mathcal{S}^p \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \mathcal{S}^p\mathcal{S}^{p-1}\mathcal{S}^p \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \mathcal{S}^p\mathcal{S}^p\mathcal{S}^{p-1} \end{pmatrix} \right\}$$

- 2-form basis:

$$V_2 = \mathrm{span}\left\{ \begin{pmatrix} \mathcal{S}^p\mathcal{S}^{p-1}\mathcal{S}^{p-1} \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \mathcal{S}^{p-1}\mathcal{S}^p\mathcal{S}^{p-1} \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \mathcal{S}^{p-1}\mathcal{S}^{p-1}\mathcal{S}^p \end{pmatrix} \right\}$$

- 3-form basis: $V_3 = \mathrm{span}\{\mathcal{S}^{p-1}(x_1)\mathcal{S}^{p-1}(x_2)\mathcal{S}^{p-1}(x_3)\}$

Essential for the construction of the matrices G and C is the following relation between splines of degree p an $p-1$:

$$\frac{\mathrm{d}}{\mathrm{d}x}\mathcal{S}_i^p(x) = \frac{p}{x_{i+p}-x_i}\mathcal{S}_i^{p-1}(x) - \frac{p}{x_{i+1+p}-x_{i+1}}\mathcal{S}_{i+1}^{p-1}(x).$$

Discrete de Rham sequence in physical space

From the de Rham sequence on the logical mesh, a de Rham sequence can be constructed on the physical domain by

$$\Lambda^0(\mathbf{x}) = \tilde{\Lambda}^0(\mathbf{x}), \quad \mathbf{\Lambda}^1(\mathbf{x}) = N(\boldsymbol{\xi})\tilde{\mathbf{\Lambda}}^1(\boldsymbol{\xi})$$

$$\mathbf{\Lambda}^2(\mathbf{x}) = \frac{DF(\boldsymbol{\xi})}{J_F(\boldsymbol{\xi})}\tilde{\mathbf{\Lambda}}^2(\boldsymbol{\xi}), \quad \Lambda^3(\mathbf{x}) = \frac{1}{J_F(\boldsymbol{\xi})}\tilde{\Lambda}^3(\boldsymbol{\xi}).$$

Indeed it holds that

$$\nabla_{\mathbf{x}}\Lambda^0(\mathbf{x}) = N(\boldsymbol{\xi})\nabla_{\boldsymbol{\xi}}\tilde{\Lambda}^0(\boldsymbol{\xi}) = N(\boldsymbol{\xi})\tilde{\mathbf{\Lambda}}^1(\boldsymbol{\xi})\mathsf{G} = \mathbf{\Lambda}^1(\mathbf{x})\mathsf{G}$$

$$\nabla_{\mathbf{x}} \times \mathbf{\Lambda}^1(\mathbf{x}) = \frac{DF(\boldsymbol{\xi})}{J_F(\boldsymbol{\xi})}\nabla_{\boldsymbol{\xi}} \times \tilde{\mathbf{\Lambda}}^1(\boldsymbol{\xi}) = \frac{DF(\boldsymbol{\xi})}{J_F(\boldsymbol{\xi})}\tilde{\mathbf{\Lambda}}^1(\boldsymbol{\xi})\mathsf{C} = \mathbf{\Lambda}^2(\mathbf{x})\mathsf{C}$$

$$\nabla_{\mathbf{x}} \cdot \mathbf{\Lambda}^2(\mathbf{x}) = \frac{1}{J_F(\boldsymbol{\xi})}\nabla_{\boldsymbol{\xi}} \cdot \tilde{\mathbf{\Lambda}}^2(\boldsymbol{\xi}) = \frac{1}{J_F(\boldsymbol{\xi})}\tilde{\mathbf{\Lambda}}^2(\boldsymbol{\xi})\mathsf{D} = \Lambda^3(\mathbf{x})\mathsf{D}$$

for the same matrices G and C as on the logical mesh.

Field discretisation in curvilinear coordinates

- Ansatz: $\tilde{\mathbf{E}}_h(\xi,t) = \tilde{\boldsymbol{\Lambda}}^1(\xi)\tilde{\mathbf{e}}(t)$ and $\tilde{\mathbf{B}}_h(\xi,t) = \tilde{\boldsymbol{\Lambda}}^2(\xi)\tilde{\mathbf{b}}(t)$
- Faraday's law:

$$\frac{\partial \tilde{\mathbf{B}}_h(\boldsymbol{\xi})}{\partial t} = \tilde{\boldsymbol{\Lambda}}^2(\boldsymbol{\xi})\frac{\mathrm{d}\tilde{\mathbf{b}}}{\mathrm{d}t} = \nabla_{\boldsymbol{\xi}} \times \tilde{\mathbf{E}}_h(\boldsymbol{\xi}) = \nabla_{\boldsymbol{\xi}} \times \tilde{\boldsymbol{\Lambda}}^1(\boldsymbol{\xi})\tilde{\mathbf{e}} = \tilde{\boldsymbol{\Lambda}}^2(\boldsymbol{\xi})\mathbb{C}\tilde{\mathbf{e}} \Rightarrow \frac{\mathrm{d}\tilde{\mathbf{b}}}{\mathrm{d}t} = \mathbb{C}\tilde{\mathbf{e}}$$

- Ampère's law with test functions $\tilde{\boldsymbol{\Lambda}}^1$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\tilde{\Omega}} \tilde{\boldsymbol{\Lambda}}^1(\boldsymbol{\xi})^\top G_n(\boldsymbol{\xi})\tilde{\boldsymbol{\Lambda}}^1(\boldsymbol{\xi})\tilde{\mathbf{e}}|J_F(\boldsymbol{\xi})|\,\mathrm{d}\boldsymbol{\xi} = \int_{\tilde{\Omega}} \left(\tilde{\boldsymbol{\Lambda}}^2(\boldsymbol{\xi})\mathbb{C}\right)^\top G_t(\boldsymbol{\xi})\tilde{\boldsymbol{\Lambda}}^2(\boldsymbol{\xi})\tilde{\mathbf{b}}\frac{1}{|J_F(\boldsymbol{\xi})|}\,\mathrm{d}\boldsymbol{\xi}$$
$$- \int_{\tilde{\Omega}} \tilde{\boldsymbol{\Lambda}}^1(\boldsymbol{\xi})^\top N(\boldsymbol{\xi})^\top N(\boldsymbol{\xi})\tilde{\mathbf{J}}(\boldsymbol{\xi})|J_F(\boldsymbol{\xi})|\,\mathrm{d}\boldsymbol{\xi}$$

We define the mass matrices $\tilde{\mathbb{M}}_1 = \int_{\tilde{\Omega}} \tilde{\boldsymbol{\Lambda}}^1(\boldsymbol{\xi})^\top G_n(\boldsymbol{\xi})\tilde{\boldsymbol{\Lambda}}^1(\boldsymbol{\xi})|J_F(\boldsymbol{\xi})|\,\mathrm{d}\boldsymbol{\xi}$ and $\tilde{\mathbb{M}}_2 = \int_{\tilde{\Omega}} \tilde{\boldsymbol{\Lambda}}^2(\boldsymbol{\xi})^\top G_t(\boldsymbol{\xi})\tilde{\boldsymbol{\Lambda}}^2(\boldsymbol{\xi})\frac{1}{|J_F(\boldsymbol{\xi})|}\,\mathrm{d}\boldsymbol{\xi}$ to find:

$$\tilde{\mathbb{M}}_1\frac{\mathrm{d}\tilde{\mathbf{e}}}{\mathrm{d}t} = \mathbb{C}^\top\tilde{\mathbb{M}}_2\tilde{\mathbf{b}} - \tilde{\mathbb{\Lambda}}^1(\boldsymbol{\Xi})^\top\mathbb{M}_q\mathbb{N}(\boldsymbol{\Xi})^T\mathbf{V}.$$

Divergence constraints in curvilinear coordinates

- Gauss' law for electricity with test functions $\tilde{\Lambda}^0$:

$$\int_{\tilde{\Omega}} \left(N(\boldsymbol{\xi}) \nabla_{\boldsymbol{\xi}} \tilde{\Lambda}^0(\boldsymbol{\xi}) \right)^\top N(\boldsymbol{\xi}) \tilde{\boldsymbol{\Lambda}}^1(\boldsymbol{\xi}) \tilde{\mathbf{e}} |J_F(\boldsymbol{\xi})| \, \mathrm{d}\boldsymbol{\xi} =$$
$$\mathrm{G}^T \int_{\tilde{\Omega}} \tilde{\boldsymbol{\Lambda}}^1(\boldsymbol{\xi})^\top N(\boldsymbol{\xi})^\top N(\boldsymbol{\xi}) \tilde{\boldsymbol{\Lambda}}^1(\boldsymbol{\xi}) |J_F(\boldsymbol{\xi})| \, \mathrm{d}\boldsymbol{\xi} \tilde{\mathbf{e}} =$$
$$\int_{\tilde{\Omega}} \tilde{\Lambda}^0(\boldsymbol{\xi})^\top \tilde{\rho}(\boldsymbol{\xi}) |J_F(\boldsymbol{\xi})| \, \mathrm{d}\boldsymbol{\xi} = \sum_p q_p w_p \tilde{\Lambda}^0(\boldsymbol{\xi}_p)^\top.$$

  With the definition of the mass matrix and the current density, we get:

$$-\mathrm{G}^T \tilde{\mathrm{M}}_1 \tilde{\mathbf{e}} = \mathbb{M}_q \tilde{\mathbb{\Lambda}}^0(\boldsymbol{\Xi})^\top \mathbb{1}_{N_p}$$

- Gauss' law for magnetism:

$$\nabla_{\boldsymbol{\xi}} \cdot \tilde{\boldsymbol{\Lambda}}^2(\boldsymbol{\xi}) \tilde{\mathbf{b}} = \tilde{\Lambda}^3(\boldsymbol{\xi}) \mathrm{D} \tilde{\mathbf{b}} = 0$$
$$\Rightarrow \mathrm{D}\tilde{\mathbf{b}} = 0.$$

Semi-discrete equations

- Dynamical variables: $\mathbf{u} = (\boldsymbol{\Xi}, \mathbf{V}, \tilde{\mathbf{e}}, \tilde{\mathbf{b}})^\top$.
- Discrete Hamiltonian:

$$\tilde{\mathcal{H}}_h = \frac{1}{2}\,\mathbf{V}^\top \mathbb{M}_p \mathbf{V} + \frac{1}{2}\,\tilde{\mathbf{e}}^\top \tilde{\mathbb{M}}_1 \tilde{\mathbf{e}} + \frac{1}{2}\,\tilde{\mathbf{b}}^\top \tilde{\mathbb{M}}_2 \tilde{\mathbf{b}}.$$

- Semi-discrete equations of motion

$$\begin{aligned}
\dot{\boldsymbol{\Xi}} &= \mathbb{N}(\boldsymbol{\Xi})^\top \mathbf{V}, \\
\dot{\mathbf{V}} &= \mathbb{M}_p^{-1}\mathbb{M}_q \mathbb{N}(\boldsymbol{\Xi}) \left(\tilde{\mathbb{\Lambda}}^1(\boldsymbol{\Xi})\tilde{\mathbf{e}} + \tilde{\mathbb{B}}(\boldsymbol{\Xi}, \tilde{\mathbf{b}})\mathbb{N}(\boldsymbol{\Xi})^\top \mathbf{V} \right), \\
\dot{\tilde{\mathbf{e}}} &= \tilde{\mathbb{M}}_1^{-1} \left(\mathbb{C}^\top \tilde{\mathbb{M}}_2 \tilde{\mathbf{b}}(t) - \tilde{\mathbb{\Lambda}}^1(\boldsymbol{\Xi})^\top \mathbb{M}_q \mathbf{V} \right), \\
\dot{\tilde{\mathbf{b}}} &= -\mathbb{C}\tilde{\mathbf{e}}(t).
\end{aligned}$$

$\tilde{\mathbb{B}} \in \mathbb{R}^{3N_p \times 3N_p}$ block diagonal matrix with blocks

$$\hat{\tilde{B}}_h = \sum_{i=1}^N \begin{pmatrix} 0 & \tilde{b}_{i,3}(t)\tilde{\Lambda}_i^{2,3}(\boldsymbol{\xi}_p) & -\tilde{b}_{i,2}(t)\tilde{\Lambda}_i^{2,2}(\boldsymbol{\xi}_p) \\ -\tilde{b}_{i,3}(t)\tilde{\Lambda}_i^{2,3}(\boldsymbol{\xi}_p) & 0 & \tilde{b}_{i,1}(t)\tilde{\Lambda}_i^{2,1}(\boldsymbol{\xi}_p) \\ \tilde{b}_{i,2}(t)\tilde{\Lambda}_i^{2,2}(\boldsymbol{\xi}_p) & -\tilde{b}_{i,1}(t)\tilde{\Lambda}_i^{2,1}(\boldsymbol{\xi}_p) & 0 \end{pmatrix} .,$$

Discrete Gauss' laws

- Magnetism: Multiply Faraday's law by D to find

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{D}\tilde{\mathbf{b}} = -\mathrm{D}\mathrm{C}\tilde{\mathbf{e}} = 0.$$

- Electricity: Multiply Ampère's law with $\mathrm{G}^\top$ to find

$$\mathrm{G}^\top \tilde{\mathrm{M}}_1 \frac{\mathrm{d}\tilde{\mathbf{e}}}{\mathrm{d}t} = \mathrm{G}^\top \mathrm{C}^\top \tilde{\mathrm{M}}_2 \tilde{\mathbf{b}}(t) - \mathrm{G}^\top \tilde{\mathbb{\Lambda}}^1(\mathbf{\Xi})^\top \mathbb{M}_q \mathbb{N}^\top \mathbf{V}$$

$$= -\,\mathrm{grad}\,\tilde{\mathbb{\Lambda}}^0(\mathbf{\Xi})^\top \mathbb{M}_q \dot{\mathbf{\Xi}} = -\frac{\mathrm{d}\tilde{\mathbb{\Lambda}}^0(\mathbf{\Xi})^\top}{\mathrm{d}t}\mathbb{M}_q \mathbb{1}_{N_p}$$

Semi-discrete Poisson system

- Semi-discrete equations of motion expressed with Poisson matrix:

$$\dot{\mathbf{u}} = \mathcal{J}(\mathbf{u})\, \mathrm{D}_{\mathbf{u}} \tilde{\mathcal{H}}_h(\mathbf{u}).$$

- Poisson matrix:

$$\mathcal{J}(\mathbf{u}) = \begin{pmatrix} 0 & \mathbb{N}^\top \mathbb{M}_p^{-1} & 0 & 0 \\ -\mathbb{M}_p^{-1}\mathbb{N} & \mathbb{M}_p^{-1}\mathbb{M}_q \mathbb{N}\tilde{\mathbb{B}}\mathbb{N}^\top \mathbb{M}_p^{-1} & \mathbb{M}_p^{-1}\mathbb{M}_q \mathbb{N}\tilde{\mathbb{\Lambda}}^1 \tilde{\mathsf{M}}_1^{-1} & 0 \\ 0 & -\tilde{\mathsf{M}}_1^{-1}(\tilde{\mathbb{\Lambda}}^1)^\top \mathbb{N}^\top \mathbb{M}_q \mathbb{M}_p^{-1} & 0 & \tilde{\mathsf{M}}_1^{-1}\mathsf{C}^\top \\ 0 & 0 & -\mathsf{C}\tilde{\mathsf{M}}_1^{-1} & 0 \end{pmatrix}.$$

- Antisymmetric matrix, satisfies Leibniz's rule and the Jacobi identity

Hamiltonian splitting

- Split Hamiltonian in three parts:

$$\tilde{\mathcal{H}}_h = \tilde{\mathcal{H}}_p + \tilde{\mathcal{H}}_E + \tilde{\mathcal{H}}_B$$

with $\tilde{\mathcal{H}}_p = \frac{1}{2}\mathbf{V}^T \mathbb{M}_p \mathbf{V},\ \tilde{\mathcal{H}}_E = \frac{1}{2}\tilde{\mathbf{e}}^T \tilde{\mathsf{M}}_1 \tilde{\mathbf{e}},\ \tilde{\mathcal{H}}_B = \frac{1}{2}\tilde{\mathbf{b}}^T \tilde{\mathsf{M}}_2 \tilde{\mathbf{b}}$.

- Leads to the three subsystems:

$$\dot{\mathbf{u}} = \{\mathbf{u}, \tilde{\mathcal{H}}_p\},\ \dot{\mathbf{u}} = \{\mathbf{u}, \tilde{\mathcal{H}}_E\},\ \dot{\mathbf{u}} = \{\mathbf{u}, \tilde{\mathcal{H}}_B\}.$$

1. $\tilde{\mathcal{H}}_p$ system: $\dot{\mathbf{\Xi}} = \mathbb{N}^\top(\mathbf{\Xi})\mathbf{V}$, $\dot{\mathbf{V}} = \mathbb{M}_p^{-1}\mathbb{M}_q\mathbb{N}(\mathbf{\Xi})\tilde{\mathbb{B}}(\mathbf{\Xi}, \tilde{\mathbf{b}})\mathbb{N}^\top(\mathbf{\Xi})\mathbf{V}$, $\tilde{\mathsf{M}}_1\dot{\tilde{\mathbf{e}}} = -\tilde{\mathbb{\Lambda}}^1(\mathbf{\Xi})^\top\mathbb{N}^\top(\mathbf{\Xi})\mathbb{M}_q\mathbf{V}$,
2. $\tilde{\mathcal{H}}_E$ system: $\dot{\mathbf{V}} = \mathbb{M}_p^{-1}\mathbb{M}_q\mathbb{N}(\xi)\tilde{\mathbb{\Lambda}}^1(\mathbf{\Xi})\tilde{\mathbf{e}}$, $\dot{\tilde{\mathbf{b}}} = -\mathsf{C}\tilde{\mathbf{e}}$,
3. $\tilde{\mathcal{H}}_B$ system: $\tilde{\mathsf{M}}_1\dot{\tilde{\mathbf{e}}} = \mathsf{C}^\top\tilde{\mathsf{M}}_2\tilde{\mathbf{b}}$.

Discretisation of $\tilde{\mathcal{H}}_E$ and $\tilde{\mathcal{H}}_B$

The systems $\tilde{\mathcal{H}}_E$ and $\tilde{\mathcal{H}}_B$ can be solved explicitly:

- $\tilde{\mathcal{H}}_E$ system:

$$\mathbf{V}^{n+1} = \mathbf{V}^n + \Delta t \mathbb{M}_p^{-1} \mathbb{M}_q \mathbb{N}(\mathbf{\Xi}^n) \tilde{\mathbb{\Lambda}}^1(\mathbf{\Xi}^n) \tilde{\mathbf{e}}^n,$$
$$\tilde{\mathbf{b}}^{n+1} = \tilde{\mathbf{b}}^n - \Delta t \mathsf{C} \tilde{\mathbf{e}}^n.$$

- $\tilde{\mathcal{H}}_B$ system:

$$\tilde{\mathsf{M}}_1 \tilde{\mathbf{e}}^{n+1} = \tilde{\mathsf{M}}_1 \tilde{\mathbf{e}}^n + \Delta t \mathsf{C}^\top \tilde{\mathsf{M}}_2 \tilde{\mathbf{b}}^n.$$

Discretisation of $\tilde{\mathcal{H}}_p$

- Particle equations solved with the Crank Nicholson method

$$
\begin{aligned}
\mathbf{\Xi}^{n+1} &= \mathbf{\Xi}^n + \Delta t \frac{\mathbb{N}^\top(\mathbf{\Xi}^n)\mathbf{V}^n + \mathbb{N}^\top(\mathbf{\Xi}^{n+1})\mathbf{V}^{n+1}}{2}, \\
\mathbf{V}^{n+1} &= \mathbf{V}^n + \Delta t \mathbb{M}_m^{-1}\mathbb{M}_q \frac{\mathbb{N}(\mathbf{\Xi}^n)\tilde{\mathbb{B}}(\mathbf{\Xi}^n, \tilde{\mathbf{b}}^n)\mathbb{N}^\top(\mathbf{\Xi}^n)\mathbf{V}^n + \mathbb{N}(\mathbf{\Xi}^{n+1})\tilde{\mathbb{B}}(\mathbf{\Xi}^{n+1}, \tilde{\mathbf{b}}^n)\mathbb{N}^\top(\mathbf{\Xi}^{n+1})\mathbf{V}^{n+1}}{2}.
\end{aligned}
$$

- Current computed with veloctiy update of the particle push

$$
\tilde{\mathbf{e}}^{n+1} = \tilde{\mathbf{e}}^n - \tilde{\mathbb{M}}_1^{-1} \int_{t^n}^{t^{n+1}} \tilde{\mathbb{\Lambda}}^1(\mathbf{\Xi}(\tau))^\top \,\mathrm{d}\tau \mathbb{M}_q \frac{\mathbb{N}^\top(\mathbf{\Xi}^n)\mathbf{V}^n + \mathbb{N}^\top(\mathbf{\Xi}^{n+1})\mathbf{V}^{n+1}}{2}.
$$

- Gauss' law is conserved

Average-vector-field scheme

- Average-vector-field method:[2] Implicit energy conserving time discretisation for conservative PDEs semi-discretised in skew-gradient form $\dot{\mathbf{u}} = S(\mathbf{u}) D_{\mathbf{u}} \hat{\mathcal{H}}(\mathbf{u})$ with $S(\mathbf{u})^T = -S(\mathbf{u})$.
- Time stepping ($g(\mathbf{u}) = S(\mathbf{u}) D_{\mathbf{u}} \hat{\mathcal{H}}(\mathbf{u})$)

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = \int_0^1 g((1-\xi)\mathbf{u}^n + \xi \mathbf{u}^{n+1})\, \mathrm{d}\xi.$$

- Since the Poisson matrix is antisymmetric, we can apply this method to our semi-discrete equations.
- To avoid a nonlinear implicit system, apply AVF method to antisymmetric splitting of the Poisson matrix.

[2] Celledoni et al., J. Comput. Phys. 231, 2012.

Antisymmetric splitting of the Poisson matrix

$$\begin{pmatrix} 0 & \mathbb{N}^\top \mathbb{M}_p^{-1} & 0 & 0 \\ -\mathbb{M}_p^{-1}\mathbb{N} & \mathbb{M}_p^{-1}\mathbb{M}_q\mathbb{N}\tilde{\mathbb{B}}\mathbb{N}^\top \mathbb{M}_p^{-1} & \mathbb{M}_p^{-1}\mathbb{M}_q\mathbb{N}\tilde{\mathbb{\Lambda}}^1\tilde{\mathbb{M}}_1^{-1} & 0 \\ 0 & -\tilde{\mathbb{M}}_1^{-1}(\tilde{\mathbb{\Lambda}}^1)^\top\mathbb{N}^\top\mathbb{M}_q\mathbb{M}_p^{-1} & 0 & \tilde{\mathbb{M}}_1^{-1}\mathbb{C}^\top \\ 0 & 0 & -\mathbb{C}\tilde{\mathbb{M}}_1^{-1} & 0 \end{pmatrix}.$$

1. $\dot{\mathbf{\Xi}} = \mathbb{N}^\top \mathbf{V}$.
2. $\dot{\mathbf{V}} = \mathbb{M}_p^{-1}\mathbb{M}_q\mathbb{N}\tilde{\mathbb{B}}\mathbb{N}^\top\mathbf{V}$.
3. $\dot{\mathbf{V}} = \mathbb{M}_p^{-1}\mathbb{M}_q\mathbb{N}\tilde{\mathbb{\Lambda}}^1\tilde{\mathbf{e}}$, $\dot{\tilde{\mathbf{e}}} = -\tilde{\mathbb{M}}_1^{-1}(\tilde{\mathbb{\Lambda}}^1)^\top\mathbb{N}^\top\mathbb{M}_q\mathbf{V}$.
4. $\dot{\tilde{\mathbf{e}}} = \tilde{\mathbb{M}}_1^{-1}\mathbb{C}^\top\tilde{\mathbb{M}}_2\tilde{\mathbf{b}}$, $\dot{\tilde{\mathbf{b}}} = -\mathbb{C}\tilde{\mathbf{e}}$.

Application of the average-vector-field method yields linear-implicit equations for system 2-4. Use Crank–Nicolson with Picard iteration for the system 1.

Result: linear-implicit in field coefficients and implicit for single particles only, conserves energy but not Gauss' law for electricity.

Systems 1 and 2

- System 1 for particle p: $\dot{\boldsymbol{\xi}}_p = N(\boldsymbol{\xi}_p)^\top \mathbf{v}_p$.
  - Approximation by Crank–Nicolson method:
    $\boldsymbol{\xi}_p^{n+1} = \boldsymbol{\xi}_p^n + \frac{\Delta t}{2} \left(N(\boldsymbol{\xi}_p^n)^\top + N(\boldsymbol{\xi}_p^{n+1})^\top \right) \mathbf{v}_p$
- System 2 for particle p: $\dot{v}_p(t) = \frac{q_p}{m_p} N(\boldsymbol{\xi}_p) \hat{\hat{B}}_h(\boldsymbol{\xi}_p), N(\boldsymbol{\xi}_p)^\top \mathbf{v}_p(t)$
  - average-vector-field approximation
    $\left(\mathbb{I}_3 - \frac{\Delta t}{2} \frac{q}{m} N(\boldsymbol{\xi}_p) \hat{\hat{B}}_h(\boldsymbol{\xi}_p) N(\boldsymbol{\xi}_p)^\top \right) \mathbf{v}_p^{n+1} =$
    $\left(\mathbb{I}_3 + \frac{\Delta t}{2} \frac{q}{m} N(\boldsymbol{\xi}_p) \hat{\hat{B}}_h(\boldsymbol{\xi}_p) N(\boldsymbol{\xi}_p)^\top \right) \mathbf{v}_p^n$

Average-vector field for system 4

- Equations: $\dot{\tilde{\mathbf{e}}} = \tilde{\mathsf{M}}_1^{-1}\mathsf{C}^\top\tilde{\mathsf{M}}_2\tilde{\mathbf{b}}$, $\dot{\tilde{\mathbf{b}}} = -\mathsf{C}\tilde{\mathbf{e}}$
- Average-vector-field approximation:

$$\begin{pmatrix} \tilde{\mathsf{M}}_1 & -\frac{\Delta t}{2}\mathsf{C}^T\tilde{\mathsf{M}}_2 \\ \frac{\Delta t}{2}\mathsf{C} & \mathbb{I} \end{pmatrix}\begin{pmatrix} \tilde{\mathbf{e}}^{n+1} \\ \tilde{\mathbf{b}}^{n+1} \end{pmatrix} = \begin{pmatrix} \tilde{\mathsf{M}}_1 & \frac{\Delta t}{2}\mathsf{C}^T\tilde{\mathsf{M}}_2 \\ -\frac{\Delta t}{2}\tilde{\mathsf{M}}_2\mathsf{C} & \tilde{\mathsf{M}}_2 \end{pmatrix}\begin{pmatrix} \tilde{\mathbf{e}}^{n} \\ \tilde{\mathbf{b}}^{n} \end{pmatrix}$$

- Decoupled equation with Schur complement $S = \tilde{\mathsf{M}}_1 + \frac{\Delta t^2}{4}\mathsf{C}^\top\tilde{\mathsf{M}}_2\mathsf{C}$:

$$\tilde{\mathbf{e}}^{n+1} = S^{-1}\left((\tilde{\mathsf{M}}_1 - \frac{\Delta t^2}{4}\mathsf{C}^T\tilde{\mathsf{M}}_2\mathsf{C})\tilde{\mathbf{e}}^n + \Delta t\mathsf{C}^T\tilde{\mathsf{M}}_2\tilde{\mathbf{b}}^n\right),$$

$$\tilde{\mathbf{b}}^{n+1} = \tilde{\mathbf{b}}^n - \frac{\Delta t}{2}\mathsf{C}(\tilde{\mathbf{e}}^n + \tilde{\mathbf{e}}^{n+1}).$$

Average-vector field for system 3

- Equations: $\dot{\mathbf{V}} = \mathbb{M}_p^{-1}\mathbb{M}_q\mathbb{N}\tilde{\mathbb{\Lambda}}^1\tilde{\mathbf{e}}$, $\dot{\tilde{\mathbf{e}}} = -\tilde{\mathbb{M}}_1^{-1}(\tilde{\mathbb{\Lambda}}^1)^\top\mathbb{N}^\top\mathbb{M}_q\mathbf{V}$
- Average-vector field approximation:

$$\begin{pmatrix} \mathbb{I} & -\frac{\Delta t}{2}\mathbb{M}_p^{-1}\mathbb{M}_q\mathbb{N}\tilde{\mathbb{\Lambda}}^1 \\ \frac{\Delta t}{2}(\tilde{\mathbb{\Lambda}}^1)^\top\mathbb{N}^\top\mathbb{M}_q & \tilde{\mathbb{M}}_1 \end{pmatrix} \begin{pmatrix} \mathbf{V}^{n+1} \\ \tilde{\mathbf{e}}^{n+1} \end{pmatrix} = \begin{pmatrix} \mathbb{I} & \frac{\Delta t}{2}\mathbb{M}_p^{-1}\mathbb{M}_q\mathbb{N}\tilde{\mathbb{\Lambda}}^1 \\ -\frac{\Delta t}{2}(\tilde{\mathbb{\Lambda}}^1)^T\mathbb{N}^T\mathbb{M}_q & \tilde{\mathbb{M}}_1 \end{pmatrix} \begin{pmatrix} \mathbf{V}^{n} \\ \tilde{\mathbf{e}}^{n} \end{pmatrix}.$$

- Decoupled equation with Schur complement $S = \tilde{\mathbb{M}}_1 + \frac{\Delta t^2}{4}\mathbb{M}_q^2\mathbb{M}_p^{-1}(\tilde{\mathbb{\Lambda}}^1)^T\mathbb{N}^T\mathbb{N}\tilde{\mathbb{\Lambda}}^1$:

$$\tilde{\mathbf{e}}^{n+1} = S^{-1}\left((\tilde{\mathbb{M}}_1 - \frac{\Delta t^2}{4}\frac{q^2}{m}(\tilde{\mathbb{\Lambda}}^1)^T\mathbb{N}^T\mathbb{N}\tilde{\mathbb{\Lambda}}^1)\tilde{\mathbf{e}}^n - \Delta t(\tilde{\mathbb{\Lambda}}^1)^T\mathbb{N}^T\mathbb{M}_q\mathbf{V}^n\right),$$

$$\mathbf{V}^{n+1} = \mathbf{V}^n + \frac{\Delta t}{2}\mathbb{M}_p^{-1}\mathbb{M}_q\mathbb{N}\tilde{\mathbb{\Lambda}}^1(\tilde{\mathbf{e}}^n + \tilde{\mathbf{e}}^{n+1}),$$

Discrete gradient scheme

- Solve systems 1 and 4 from the antisymmetric splitting together in order to conserve Gauss' law

$$
\begin{aligned}
&\text{system 1:} && \dot{\mathbf{V}} = \mathbb{M}_p^{-1}\mathbb{M}_q\mathbb{N}(\boldsymbol{\Xi})\tilde{\mathbb{B}}(\boldsymbol{\Xi},\tilde{\mathbf{b}})\mathbb{N}^\top(\boldsymbol{\Xi})\mathbf{V},\\
&\text{system 2:} && \dot{\tilde{\mathbf{b}}} = -\mathsf{C}\tilde{\mathbf{e}},\ \ \tilde{\mathsf{M}}_1\dot{\tilde{\mathbf{e}}} = \mathsf{C}^\top\tilde{\mathsf{M}}_2\tilde{\mathbf{b}},\\
&\text{system 3:} && \dot{\boldsymbol{\Xi}} = \mathbb{N}^\top(\boldsymbol{\Xi})\mathbf{V}, \dot{\mathbf{V}} = \mathbb{M}_p^{-1}\mathbb{M}_q\mathbb{N}(\boldsymbol{\Xi})\tilde{\mathbb{\Lambda}}^1(\boldsymbol{\Xi})\tilde{\mathbf{e}},\\
& && \tilde{\mathsf{M}}_1\dot{\tilde{\mathbf{e}}} = -\tilde{\mathbb{\Lambda}}^1(\boldsymbol{\Xi})^\top\mathbb{N}^\top(\boldsymbol{\Xi})\mathbb{M}_q\mathbf{V}.
\end{aligned}
$$

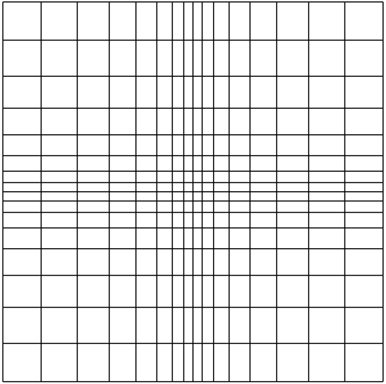
- Systems 1 and 2 are solved with the AVF scheme

Discretisation of system 3

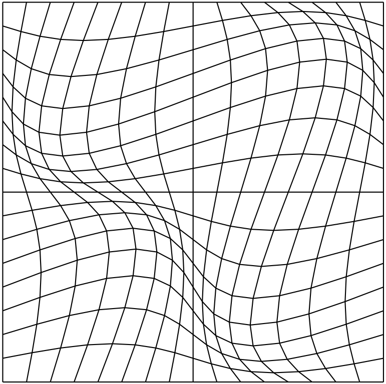
- Fixpoint iteration for the electric field
- Current is computed with the velocity update in the particle push
- Total energy and Gauss' law are conserved in this system

$$
\begin{aligned}
\frac{\boldsymbol{\Xi}^{n+1} - \boldsymbol{\Xi}^{n}}{\Delta t} &= \frac{\mathbb{N}^\top(\boldsymbol{\Xi}^{n+1}) + \mathbb{N}^\top(\boldsymbol{\Xi}^{n})}{2} \frac{\mathbf{V}^{n+1} + \mathbf{V}^{n}}{2}, \\
\frac{\mathbf{V}^{n+1} - \mathbf{V}^{n}}{\Delta t} &= \mathbb{M}_p^{-1} \mathbb{M}_q \frac{\mathbb{N}(\boldsymbol{\Xi}^{n+1}) + \mathbb{N}(\boldsymbol{\Xi}^{n})}{2} \frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} \tilde{\mathbb{\Lambda}}^1(\boldsymbol{\Xi}(\tau))\, \mathrm{d}\tau \frac{\tilde{\mathbf{e}}^{n+1} + \tilde{\mathbf{e}}^{n}}{2}, \\
\frac{\tilde{\mathbb{M}}_1 \tilde{\mathbf{e}}^{n+1} - \tilde{\mathbb{M}}_1 \tilde{\mathbf{e}}^{n}}{\Delta t} &= -\frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} \tilde{\mathbb{\Lambda}}^1(\boldsymbol{\Xi}(\tau))^\top \, \mathrm{d}\tau \frac{\mathbb{N}^\top(\boldsymbol{\Xi}^{n+1}) + \mathbb{N}^\top(\boldsymbol{\Xi}^{n})}{2} \mathbb{M}_q \frac{\mathbf{V}^{n+1} + \mathbf{V}^{n}}{2},
\end{aligned}
$$

Coordinate transformations



Orthogonal transformation



Colella transformation

$$\mathbf{x} = \begin{pmatrix} L\left(\xi_1 + \alpha \sin(2\pi\xi_1)\right) \\ L\left(\xi_2 + \alpha \sin(2\pi\xi_2)\right) \\ L\xi_3 \end{pmatrix} \qquad \mathbf{x} = \begin{pmatrix} L\left(\xi_1 + \alpha \sin(2\pi\xi_1)\sin(2\pi\xi_2)\right) \\ L\left(\xi_2 + \alpha \sin(2\pi\xi_1)\sin(2\pi\xi_2)\right) \\ L\xi_3 \end{pmatrix}.$$

Scaling of the domain: $\mathbf{x} = L\boldsymbol{\xi}$. (Uniform grid as reference)

Test case 2: Weibel instability

Electron distribution (neutralizing ion background):

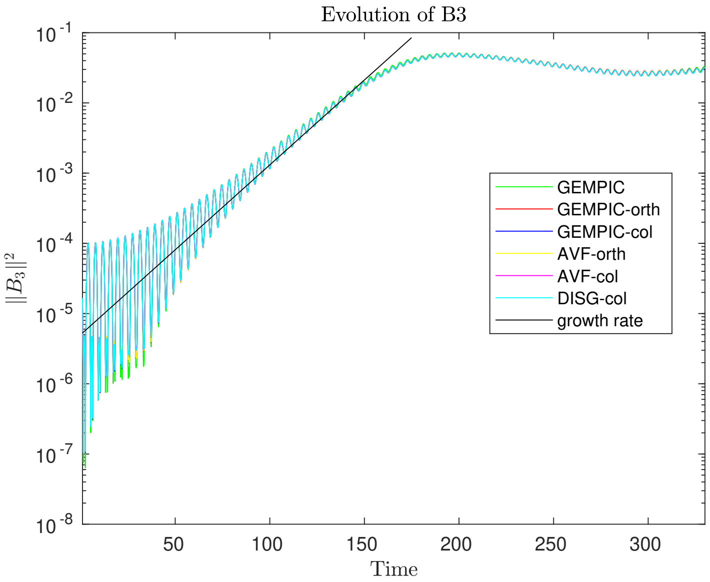
$$f(x, \mathbf{v}, t = 0) = \frac{1}{(2\pi)^{\frac{3}{2}} \sigma_1 \sigma_2^2} \exp\left(-\frac{1}{2} \left(\frac{v_1^2}{\sigma_1^2} + \frac{v_2^2 + v_3^2}{\sigma_2^2} \right) \right),$$

$$B_3(x_1, x_2, t = 0) = \beta \cos(k x_1).$$

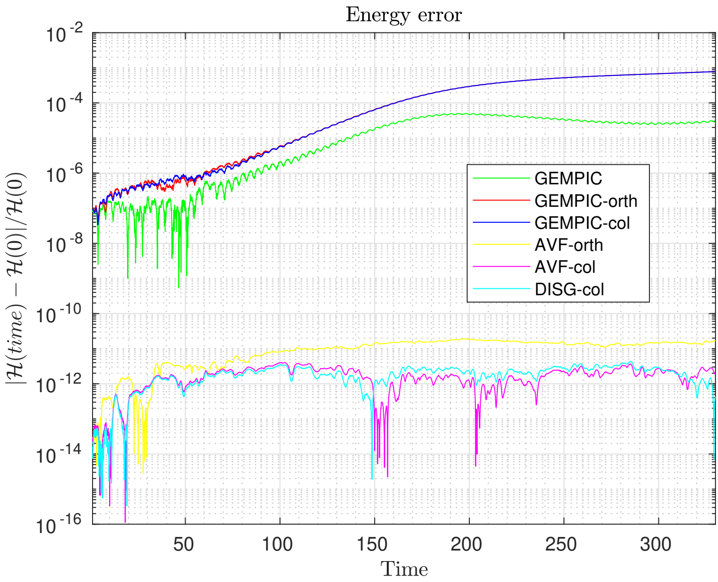
and $\mathbf{E}(x, t = 0)$ is computed from Poisson's equation.

Parameters: $\sigma_1 = 0.02/\sqrt{2}$, $\sigma_2 = \sqrt{12}\sigma_1$, $k = 1.25$, and $\beta = -10^{-3}$.
Numerical resolution: $N_p = 400,000$, $N_x = [16, 8, 2]$, spline degree $[3, 2, 1]$, tolerance for linear solvers 10^{-13}

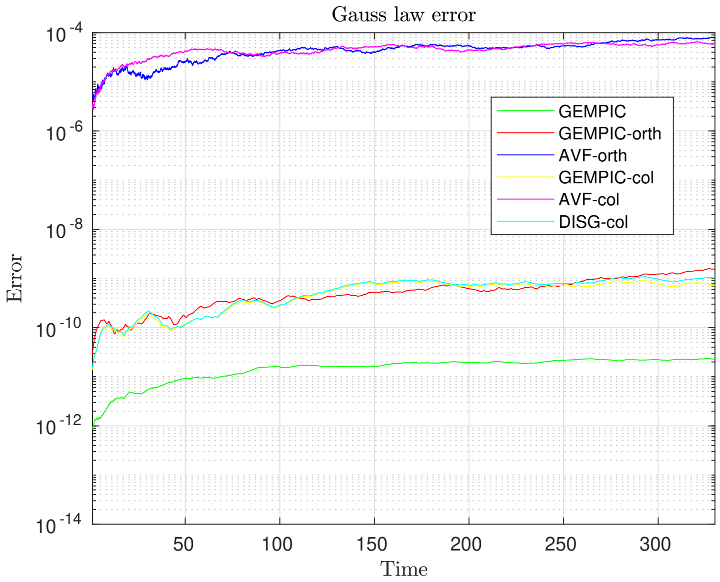
Weibel instability: Magnetic energy



Weibel instability: Energy error



Weibel instability: Energy in Gauss' law



Summary and Outlook

Summary

- GEMPIC framework based on discrete Poisson bracket and FEEC.
- Curvilinear version derived and tested on periodic grids.
- Different time propagators that conserve charge, total energy or both

Outlook

- Add nonzero boundary conditions.
- Simulate a D-shaped torus.
- Improve sampling strategy and preconditioning of linear solvers.
- Search for curvilinear testcases.

Reference: B. Perse, K. Kormann, E. Sonnendrücker: Geometric particle-in-cell simulations of the Vlasov–Maxwell system in curvilinear coordinates, manuscript in preparation.