Variational Framework for Structure-Preserving Electromagnetic Particle-In-Cell Methods

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Abstract

In this article we apply a discrete action principle for the Vlasov–Maxwell equations in a structure-preserving particle-field discretization framework. In this framework the finite-dimensional electromagnetic potentials and fields are represented in a discrete de Rham sequence involving general finite element spaces, and the particle-field coupling is represented by a set of projection operators that commute with the differential operators. With a minimal number of assumptions which allow for a variety of finite elements and shape functions for the particles, we show that the resulting variational scheme has a general discrete Poisson structure and thus leads to a semi-discrete Hamiltonian system. By introducing discrete interior products we derive a second type of space discretization which is momentum preserving, based on the same finite elements and shape functions. We illustrate our method by applying it to spline finite elements, and to a new spectral discretization where the particle-field coupling relies on discrete Fourier transforms.

1 Introduction

Since the early days of Particle-in-Cell (PIC) schemes, plasma physicists have devised variational algorithms based on least action principles to preserve key invariants such as the total energy and Gauss’s laws \cite{25, 26, 14}. In parallel, a Hamiltonian structure of the Vlasov–Maxwell equations has been proposed, that involves a non-canonical Poisson bracket \cite{30, 34, 28}. Although the first methods were developed for finite difference field solvers, many improvements have been made and in the last decade several schemes have been proposed that rely on the de Rham structure of the Maxwell equations \cite{4, 20} to guarantee an exact preservation of proper discrete Gauss laws for general Finite Element PIC methods on general meshes \cite{12}, later extended to variational PIC schemes in e.g. \cite{33} and \cite{15, 32}, where it was shown that variational spectral methods also preserve the total momentum of the plasma.

Following these ideas a Geometric Electromagnetic PIC (GEMPIC) method based on spline finite elements has been proposed in \cite{23}, that possess a Hamiltonian structure relying on a discrete Poisson bracket. Coupled with Hamiltonian splitting methods \cite{18, 13, 19}, this approach leads to fully discrete schemes that preserve a modified energy, discrete Gauss laws, and the Poisson structure of the semi-discrete problem, including its associated Casimir invariants \cite{23}.

In this article, we extend these constructions to a flexible and general setting that allows for arbitrary structure-preserving discretizations of the electromagnetic fields and a variety of particle-field coupling operators which in particular includes almost arbitrary smoothing shape
functions. By applying a discrete action principle we rigorously derive a variational system of discrete Vlasov–Maxwell equations, and we show that it has a non-canonical Poisson structure. This approach allows for instance to derive numerical Maxwell solvers with a strong Ampère and Gauss equation, and also extends the strong Faraday solver of [23] to more general particle-field coupling schemes. Another direct application is the design of variational spectral particle methods, where the Maxwell equations are solved in discrete Fourier spaces.

The outline of the paper is as follows. In Section 2 we first present the commuting de Rham complex that serves as the basis of our discrete derivation. This setting is now common in the structure-preserving (mimetic) discretization of Maxwell equations, and has been thoroughly studied in the Finite Element Exterior Calculus (FEEC) literature. For the Vlasov–Maxwell equations it describes how the particle-field coupling operators are connected with the differential operators involved in the discrete Maxwell equations. Then, we derive a variational particle discretization of the Vlasov–Maxwell system in a strong Ampère formulation from a discrete action principle, and analyze its main conservation properties together with its discrete Poisson structure. In Section 3, we present a variant of our method that preserves exactly the Gauss laws and the total momentum. In Section 4 a matrix form of the equations is carefully detailed, which also allows to derive a matrix form of the discrete Poisson bracket. In Section 5 we show how our analysis extends to a more general setting, and easily applies to the case of strong Faraday solvers. A detailed application to the case of structure-preserving Spline and Fourier discretizations is then presented in Section 6 with particle-field coupling operators based on geometric degrees of freedom which amount to discrete Fourier transforms in the spectral case. In Section 7 we conclude with preliminary numerical experiments that validate our approach and we compare the results obtained by various space discretizations that fit into our general framework, including different Maxwell solvers and different orders of particle smoothing.

2 Variational particle-field discretization

2.1 Maxwell equations and particle trajectories

A kinetic description of the dynamics of a plasma in an electromagnetic field \((E, B)\) models the particles of species \(s\) by a distribution function \(f_s\) in phase-space that evolves according to the Vlasov equation

\[
\partial_t f_s(t, x, v) + v \cdot \nabla_x f_s(t, x, v) + \frac{q_s}{m_s} \left( E(t, x) + v \times B(t, x) \right) \cdot \nabla_v f_s(t, x, v) = 0 \tag{1}
\]

where \(m_s\) and \(q_s\) denote the mass and charge of the particle species \(s\). The self-consistent fields evolve according to Maxwell’s equations

\[
\begin{align*}
\partial_t E(t, x) &= \text{curl} \ B(t, x) - J(t, x) \\
\partial_t B(t, x) &= - \text{curl} \ E(t, x) \\
\text{div} \ E(t, x) &= \rho(t, x) \\
\text{div} \ B(t, x) &= 0 \tag{2}
\end{align*}
\]

which are coupled to the Vlasov equation through the charge and current densities,

\[
\rho(t, x) = \sum_s q_s \int_{\mathbb{R}^3} f_s(t, x, v) \, dv, \quad J(t, x) = \sum_s q_s \int_{\mathbb{R}^3} v f_s(t, x, v) \, dv. \tag{3}
\]
We refer to e.g. [17, 4] for a detailed presentation of these equations. As the Vlasov equation is a conservative transport equation, the distribution function $f_s$ is constant over time along the characteristic trajectories for that species, which are solution to the characteristic ODEs

$$
\frac{d}{dt}X(t) = V(t), \quad \frac{d}{dt}V(t) = \frac{q_s}{m_s}(E(t, X(t)) + V(t) \times B(t, X(t))).
$$

(4)

In particle methods the distribution function is often represented by a collection of $N$ macro-particles with phase-space positions $(X_p, V_p)(t)$ and weights $w_p$, of the form

$$
f^{S}_{s,N}(t, x, v) = \sum_{p=1}^{N} w_p S(x - X_p(t))\delta(v - V_p(t)),
$$

(5)

where $S$ is a shape function that can either by the Dirac $\delta$ distribution or some smoothing kernel, depending on the particular configuration of the particle method. Starting from a collection of initial positions $(X^0_p, V^0_p)$, $p = 1, \ldots, N$, the weights are initialized so as to provide a good approximation to the initial density $f^{0}_s$, and the particle positions are evolved according to some discrete characteristic equation, in order to approximate the trajectories (4). For the solution of Maxwell’s equations, a grid-based solver is commonly used.

### 2.2 Structure of Maxwell’s equations and finite element exterior calculus

As has been evidenced by several key contributions in the last decades [5, 6, 20], the Maxwell equations (2) possess a geometric structure where a central role is played by de Rham sequence

$$
H^1(\mathbb{R}^3) \xrightarrow{\text{grad}} H(\text{curl}; \mathbb{R}^3) \xrightarrow{\text{curl}} H(\text{div}; \mathbb{R}^3) \xrightarrow{\text{div}} L^2(\mathbb{R}^3).
$$

(6)

In order to derive structure-preserving schemes we will follow the framework of Finite Element Exterior Calculus (FEEC) developed in e.g. [29, 20, 1, 2, 8, 11]. A central feature of these approaches is to involve a discretization that preserves the sequence (6) at the discrete level, and that admits a sequence of projection operators $\Pi^0, \ldots, \Pi^3$ mapping infinite-dimensional function spaces into discrete ones:

$$
\begin{array}{c}
V^0 \\
\Pi^0
\end{array} \xrightarrow{\text{grad}} \begin{array}{c}
V^1 \\
\Pi^1
\end{array} \xrightarrow{\text{curl}} \begin{array}{c}
V^2 \\
\Pi^2
\end{array} \xrightarrow{\text{div}} \begin{array}{c}
V^3 \\
\Pi^3
\end{array}
$$

(7)

In our framework, it is these operators $\Pi^\ell$, together with some shape (smoothing) functions $S$, that will encode the coupling mechanism between the particles and the discrete fields. Here the top row contains the infinite-dimensional domain spaces $V^\ell$ of the operators $\Pi^\ell$, which are in general proper subsets of the natural Hilbert spaces involved in the sequence (6), and the bottom row consists of general discrete spaces such as finite-element or spectral spaces, see e.g. Section 6. A key ingredient in our variational derivation will be that the operators $\Pi^\ell$ make the diagram commuting. In practice many choices can be made for these operators and the associated finite-element spaces where the fields are discretized. Each choice will result in a different coupling mechanism between the particles and the fields, but all of them will lead to Hamiltonian systems, provided the following property holds.
Assumption 1. The operators $\Pi^\ell : V^\ell \to V^\ell_h$ are such that:

- the diagram (7) commutes, i.e., we have
  \[
  \begin{align*}
  \Pi^1 \text{grad} G &= \text{grad} \Pi^0 G & \text{for all } G \in V^0, \\
  \Pi^2 \text{curl} G &= \text{curl} \Pi^1 G & \text{for all } G \in V^1, \\
  \Pi^3 \text{div} G &= \text{div} \Pi^2 G & \text{for all } G \in V^2
  \end{align*}
  \]

- the domain spaces $V^\ell$ are translation invariant function (or distribution) spaces, in the sense that if $G \in V^0$, then $G(\cdot - x) \in V^0$ for all $x \in \mathbb{R}^3$.

Since the commuting projection operators will be applied to particle shape functions, we also need to specify when these shapes are admissible.

Definition 1 (admissible shape functions). A shape function $S$ is said to be admissible for a given sequence of operators $\Pi^\ell$ if it belongs to the domain spaces $V^0$ and $V^3$ of $\Pi^0$ and $\Pi^3$, and if for any $e \in \mathbb{R}^3$, $eS$ belongs to the domains $V^1$ and $V^2$ of $\Pi^1$ and $\Pi^2$.

Remark 1. In practice, the translation invariance assumption corresponds to defining the projection operators on domain spaces $V^\ell$ characterized by some homogeneous regularity over $\mathbb{R}^3$, which simplifies the notion of an admissible shape function $S$. In special cases where one works with localized or heterogeneous domain spaces, some additional care may need to be taken to guarantee that the projection operators can be applied on the shape functions.

2.3 Discretizing the Ampère or Faraday equations in strong form

In the article [23] the discretization ansatz was to consider fields in the spaces

\[
\begin{align*}
\hat{\phi}_h &\in V^0_h \xrightarrow{\text{grad}} \hat{E}_h, \\
\hat{A}_h &\in V^1_h \xrightarrow{\text{curl}} \hat{B}_h \in V^2_h
\end{align*}
\]

with $\hat{\phi}_h$ and $\hat{A}_h$ denoting discrete representations of the scalar and vector potentials, and this has led to an approximation of Ampère’s and Faraday’s laws in weak and strong form, respectively. Although the analysis presented here readily applies to the ansatz (11), it also covers the dual choice

\[
\begin{align*}
\hat{B}_h &\in V^1_h \xrightarrow{\text{curl}} \hat{E}_h, \\
\hat{A}_h &\in V^2_h \xrightarrow{\text{div}} \hat{\phi}_h \in V^3_h
\end{align*}
\]

which leads to a new discrete model involving a strong Ampère law and a weak Faraday law. Throughout this article we will thus focus on this new ansatz (12), and describe in Section 5 how our results apply to the ‘strong Faraday’ ansatz (11).

In both cases, the discrete equations in weak form will involve the discrete adjoints to the strong differential operators, i.e.,

\[
\begin{align*}
\text{grad}_w : V^3_h \to V^2_h, & \quad \int_\Omega (\text{grad}_w \varphi_h) \cdot F_h = - \int_\Omega \varphi_h \text{div} F_h \\
\text{curl}_w : V^2_h \to V^1_h, & \quad \int_\Omega (\text{curl}_w F_h) \cdot C_h = \int_\Omega F_h \cdot \text{curl} C_h \\
\text{div}_w : V^1_h \to V^0_h, & \quad \int_\Omega (\text{div}_w C_h) \psi_h = - \int_\Omega C_h \cdot \text{grad} \psi_h
\end{align*}
\]

for all $\varphi_h \in V^3_h$, $F_h \in V^2_h$, $C_h \in V^1_h$, and $\psi_h \in V^0_h$. These discrete operators may be seen as the discrete Riesz representatives of the differential operators in distribution’s sense.
2.4 Discrete Action principle

We now derive a general geometric electromagnetic particle method where, following the ansatz (12), the Ampère equation is discretized in a strong sense. Here the coupling mechanism is essentially encoded in the abstract operators $\Pi^t$ that are only assumed to satisfy the commuting diagram properties, see Assumption II and in the shape function $S$ that must be admissible in the sense of Definition I.

To do so we follow a discrete variational principle in the spirit of [30, 33, 22, 15], based on Low’s Lagrangian functional for the Vlasov–Maxwell equations [27],

$$ L = \sum_s \int f_s(t_0, x_0, v_0) \left( (m_s V + q_s A(t, X)) \cdot X' - \left( \frac{m_s}{2} V^2 + q_s \phi(t, X) \right) \right) \, dx_0 \, dv_0 $$

$$ + \frac{1}{2} \int_\Omega |\nabla \phi(t, x) + A'(t, x)|^2 \, dx - \frac{1}{2} \int_\Omega |\nabla A(t, x)|^2 \, dx. \quad (14) $$

Here the curves $X = X(t; x_0, v_0), X' = X'(t; x_0, v_0), V = V(t; x_0, v_0)$ depend on time and on the initial conditions, and we recall that in a variational derivation they represent independent variables of the functional, in particular the prime symbol does not stand for a derivative. We also note that a different set of characteristics is associated to each particle species, which has been left implicit here for notational simplicity.

Formally, the Vlasov–Maxwell equations can be derived as the Euler-Lagrange equations associated with this Lagrangian, as shown in [27]. Here we will carefully apply this principle at the discrete level, starting from the discrete Lagrangian functional

$$ L_h = \sum_{p=1}^N w_p \left( (m_s V_p + q_s A^S(X_p)) \cdot X'_p - \left( \frac{m_s}{2} V_P^2 + q_s \phi^S(X_p) \right) \right) $$

$$ + \frac{1}{2} \int_\Omega |\nabla w \phi_h(x) + A'_h(x)|^2 \, dx - \frac{1}{2} \int_\Omega |\nabla A_h(x)|^2 \, dx. \quad (15) $$

This Lagrangian is a function of discrete variables, $L_h = L_h(X_N, X'_N, V_N, A_h, A'_h, \phi_h)$, where $X_N(t) = (X_p(t))_{p=1,\ldots,N}, \; X'_N(t) = (X'_p(t))_{p=1,\ldots,N}, \; V_N(t) = (V_p(t))_{p=1,\ldots,N}$ in $(\mathbb{R}^3)^N$, are arbitrary collections of trajectories and $A_h(t), A'_h(t) \in V^2_h; \; \phi_h(t) \in V^3_h$ are arbitrary finite element potential fields. In [15] the dependence on $t$ is implicit, and again we recall that the prime symbol does not mean a derivative, as all these functions are independent in the variational derivation. Finally the coupling potentials are defined as

$$ \begin{cases} 
A^S(X_p) := \sum_{\alpha=1}^2 e_\alpha \int_\Omega \left( A_h \cdot \Pi^2(e_\alpha S_{X_p}) \right) \, dx, \\
\phi^S(X_p) := \int_\Omega \left( \delta_h \Pi^3(S_{X_p}) \right) \, dx 
\end{cases} \quad (16) $$

where $S_{X_p}(x) = S(x - X_p)$ denotes the shape function centered on a particle. We note that $L_h$ is formally derived from the continuous functional (14) by (i) replacing the initial density $f_s$ by its Dirac approximation in [5], i.e., $f^\delta_s N(t_0, x_0, v_0) = \sum_{p=1}^N w_p \delta(x_0 - X_0^p) \delta(v_0 - V^0_p)$, (ii) using trajectories satisfying $(X, V)(t; X_0^p, V_0^p) = (X_p, V_p)(t)$, (iii) potential fields in the discrete (finite element) spaces, (iv) weak discrete differentials [13] instead of the exact ones,
and finally (v) the coupling fields (16) defined with admissible shape (smoothing) functions in (7). In the case of several species, each density \( f_s \) is approximated by a different set of discrete particles, so that we actually have \( s = s(p) \) in (15). For this reason it will be convenient to denote in the sequel particle masses and charges by

\[
m_p := w_p m_{s(p)} \quad \text{and} \quad q_p := w_p q_{s(p)}, \quad \text{for} \quad p = 1, \ldots, N.
\]

The discrete Action functional is then defined as

\[
S_h(X_N, V_N, \phi_h, A_h) := \int_0^T L_h((X_N, \frac{d}{dt} X_N, V_N, \phi_h, A_h, \partial_t A_h)(t)) \ dt
\]

and following a discrete action principle we look for generalized trajectories that form an extremum of \( S_h \). We already point out that the resulting equations will only involve the fields

\[
E_h := -\partial_t A_h - \text{grad}_w \phi_h \in V_h^2 \quad \text{and} \quad B_h := \text{curl}_w A_h \in V_h^1,
\]

hence they will be gauge-independent. Formally, extremality conditions for \( S_h \) are associated to the Euler-Lagrange equations of the discrete Lagrangian functional (15). Thus we look for \( X_N, V_N, \phi_h, A_h \) such that the following relations hold for all \( t \in [0, T] \), with functional Gateaux derivatives evaluated at \((X_N, X_N', V_N, \phi_h, A_h, A_h') = (X_N, \frac{d}{dt} X_N, V_N, \phi_h, A_h, \partial_t A_h)\):

\[
\begin{align*}
\left\langle \frac{\delta L_h}{\delta V_N}, V_N \right\rangle &= 0, \quad \forall V_N \in \mathbb{R}^{3N} \quad (20) \\
\left\langle \frac{\delta L_h}{\delta X_N}, X_N \right\rangle &= \left\langle \frac{\partial}{\partial t} \frac{\delta L_h}{\delta X_N}, X_N \right\rangle, \quad \forall X_N \in \mathbb{R}^{3N} \quad (21) \\
\left\langle \frac{\delta L_h}{\delta \phi_h}, \phi_h \right\rangle &= 0, \quad \forall \phi_h \in V_h^3 \quad (22) \\
\left\langle \frac{\delta L_h}{\delta A_h}, A_h \right\rangle &= \left\langle \frac{\partial}{\partial t} \frac{\delta L_h}{\delta A_h}, A_h \right\rangle, \quad \forall A_h \in V_h^2. \quad (23)
\end{align*}
\]

For the variations with respect to \( V_N \), we compute

\[
\left\langle \frac{\delta L_h}{\delta V_N}, V_N \right\rangle := \frac{d}{d\epsilon} \bigg|_{\epsilon=0} \left( L_h(X_N, \frac{d}{dt} X_N, V_N + \epsilon V_N, \phi_h, A_h) \right) = \sum_p m_p \left( \frac{dX_p}{dt} - V_p \right) \cdot V_p
\]

for an arbitrary \( V_N = (V_p)_{p=1,\ldots,N} \), so that (20) gives

\[
\frac{dX_p}{dt} = V_p \quad \text{for} \quad p = 1, \ldots, N. \quad (24)
\]

Using the coupling potentials (16), we compute for the variations with respect to \( X_N \)

\[
\begin{align*}
\left\langle \frac{\delta L_h}{\delta X_N}, \dot{X}_N \right\rangle &= \sum_p \left( m_p V_p + q_p A^S(t, X_p) \right) \cdot \dot{X}_p = \sum_p m_p V_p \dot{X}_p + q_p \int_{\Omega} A_h \cdot \Pi^2(\dot{X}_p S X_p) \quad (25.1) \\
\left\langle \frac{\delta L_h}{\delta X_N}, \ddot{X}_N \right\rangle &= -\sum_p q_p \int_{\Omega} \left( A_h \cdot \Pi^2(V_p(\dot{X}_p \cdot \text{grad} S X_p)) - \phi_h \Pi^3(\dot{X}_p \cdot \text{grad} S X_p) \right) \quad (25.2)
\end{align*}
\]
for an arbitrary $\dot{X}_N = (\dot{X}_p)_{p=1,\ldots,N}$. We then write Equation (21) for a variation of a single particle 1 ≤ $p$ ≤ $N$ along the unit basis vector $e_\alpha \in \mathbb{R}^3$ for some dimension 1 ≤ $\alpha$ ≤ 3. Thus we take $\dot{X}_{p'} = \delta_{p',p} e_\alpha$, which gives

$$\frac{m_p}{q_p} \frac{dV_p}{dt} \cdot e_\alpha = \int_\Omega A_h \cdot \Pi^2(e_\alpha (V_p \cdot \text{grad} S_{X_p}) - V_p (e_\alpha \cdot \text{grad} S_{X_p})) - \int_\Omega \partial_t A_h \cdot \Pi^2(e_\alpha S_{X_p}) + \int_\Omega \phi_h \Pi^3(e_\alpha \cdot \text{grad} S_{X_p})$$

$$= \int_\Omega A_h \cdot \Pi^2 \text{curl}(e_\alpha \times V_p S_{X_p}) - \int_\Omega \partial_t A_h \cdot \Pi^2(e_\alpha S_{X_p}) + \int_\Omega \phi_h \text{div}(e_\alpha S_{X_p})$$

$$= \int_\Omega A_h \cdot \Pi^1(e_\alpha \times V_p S_{X_p}) - \int_\Omega \partial_t A_h \cdot \Pi^2(e_\alpha S_{X_p}) + \int_\Omega \phi_h \text{div}(e_\alpha S_{X_p})$$

$$= \int_\Omega \text{curl}_w A_h \cdot \Pi^1(e_\alpha \times V_p S_{X_p}) - \int_\Omega (\partial_t A_h + \text{grad}_w \phi_h) \cdot \Pi^2(e_\alpha S_{X_p})$$

$$= \int_\Omega B_h \cdot \Pi^1(e_\alpha \times V_p S_{X_p}) + \int_\Omega E_h \cdot \Pi^2(e_\alpha S_{X_p})$$

where we have used the commuting diagram property [8]–[10] of the operators $\Pi^\ell$, and the definition [10] of the fields in the last equality. Using the linearity of the projection operator we rewrite the magnetic rotation term as

$$\int_\Omega B_h \cdot \Pi^1(e_\alpha \times V_p S_{X_p}) = \sum_{\beta=1}^3 e_\alpha \int_\Omega \Phi_h(x) \cdot \Pi^1(e_\alpha S_{X_p})(x) \, dx.$$

Defining similarly the coupling electric field by

$$E^S(X_p) := \sum_{\alpha=1}^3 e_\alpha \int_\Omega E_h(x) \cdot \Pi^2(e_\alpha S_{X_p})(x) \, dx.$$

we arrive at a velocity equation of the form

$$\frac{dV_p}{dt} = \frac{q_p}{m_p} (E^S(X_p) + V_p \times B^S(X_p)).$$

Turning to the variations with respect to $A_h$, using again [16] we compute

$$\begin{cases} \frac{\delta \mathcal{L}_h}{\delta A_h}, A_h \end{cases} = \sum_p q_p \int_\Omega \Pi^2(V_p S_{X_p}) \cdot A_h - \int_\Omega (\text{curl}_w A_h) \cdot (\text{curl}_w A_h)$$

$$\begin{cases} \frac{\delta \mathcal{L}_h}{\delta A_h}, A_h \end{cases} = \int_\Omega (\partial_t A_h + \text{grad}_w \phi_h) \cdot A_h$$

so that Equation (23) gives

$$\int_\Omega \partial_t (\partial_t A_h + \text{grad}_w \phi_h) \cdot A_h + \int_\Omega (\text{curl}_w A_h) \cdot (\text{curl}_w A_h) = \sum_p q_p \int_\Omega \Pi^2(V_p S_{X_p}) \cdot A_h.$$
The latter can be rewritten only in terms of the fields (19) and the particle current defined as

\[ J_{SN}^{S}(t, x) := \sum_{s} q_s \int_{\mathbb{R}^3} v f_{s,N}^{S}(t, x, v) \, dv = \sum_{p} q_p V_p S_{X_p(t)}(x), \]

see (5) and (17), as

\[ -\int_{\Omega} \partial_t E_h \cdot \tilde{A}_h + \int_{\Omega} \text{curl } B_h \cdot \tilde{A}_h = \int_{\Omega} (\Pi^2 J_{SN}^{S}) \cdot \tilde{A}_h \tag{31} \]

where we have used again the definition of the weak operators (13). Since both \(-\partial_t E_h + \text{curl } B_h\) and \(\Pi^2 J_{SN}^{S}\) belong to \(V_h^2\), and (31) holds for all \(\tilde{A}_h \in V_h^2\), it leads to an Ampère equation in strong form,

\[ -\partial_t E_h + \text{curl } B_h = \Pi^2 J_{SN}^{S}. \tag{32} \]

In turn, a weak Faraday equation involving the discrete curl (13),

\[ \partial_t B_h + \text{curl}_w E_h = 0 \tag{33} \]

follows from the definition of the fields (19): Indeed, for all \(\tilde{B}_h \in V_h^1\) we have

\[ \int_{\Omega} \partial_t B_h \cdot \tilde{B}_h = \int_{\Omega} \partial_t A_h \cdot \text{curl } \tilde{B}_h = -\int_{\Omega} (E_h + \text{grad}_w \phi_h) \cdot \text{curl } \tilde{B}_h = -\int_{\Omega} E_h \cdot \text{curl } \tilde{B}_h \]

which amounts to (33), by using the fact that \(\int_{\Omega} \text{grad}_w \phi_h \cdot \text{curl } \tilde{B}_h = \int_{\Omega} \phi_h \text{ div curl } \tilde{B}_h = 0\). For the variations with respect to \(\phi_h\) we use once more (16) and compute

\[ \langle \frac{\delta L_h}{\delta \phi_h}, \tilde{\phi}_h \rangle = -\sum_{p} q_p \int_{\Omega} (\Pi^3 S_{X_p}) \tilde{\phi}_h + \int_{\Omega} (\partial_t A_h + \text{grad}_w \phi_h) \cdot \text{grad}_w \tilde{\phi}_h \]

for an arbitrary \(\tilde{\phi}_h \in V_h^3\), so that (22) gives

\[ \int_{\Omega} (\partial_t A_h + \text{grad}_w \phi_h) \cdot \text{grad}_w \tilde{\phi}_h = \sum_{p} q_p \int_{\Omega} (\Pi^3 S_{X_p}) \tilde{\phi}_h. \tag{34} \]

Using the field \(E_h\) defined in (19) and noting that (34) must hold for all \(\tilde{\phi}_h \in V_h^3\), we arrive at a Gauss law in strong form,

\[ \text{div } E_h = \Pi^3 \rho_{SN}^{S} \quad \text{with} \quad \rho_{SN}^{S}(t, x) := \sum_{s} q_s \int_{\mathbb{R}^3} f_{s,N}^{S}(t, x, v) \, dv = \sum_{p=1}^{N} q_p S_{X_p(t)}(x), \tag{35} \]

see again (5), (17). Finally a discrete magnetic Gauss law, this time in weak form, follows again from the definition (19) of \(B_h = \text{curl}_w A_h\), writing that

\[ \int_{\Omega} (\text{div}_w B_h) \psi_h = -\int_{\Omega} B_h \cdot \text{grad } \psi_h = -\int_{\Omega} A_h \cdot \text{curl } \psi_h = 0 \quad \forall \psi_h \in V_h^0. \tag{36} \]
2.5 The variational equations

Gathering the findings of the variational derivation just detailed, we obtain a system of semi-discrete equations where the fields $E_h = E_h(t) \in V^2_h$ and $B_h = B_h(t) \in V^1_h$ are governed by the discrete Ampère and Faraday equations

$$\begin{cases}
    -\partial_t E_h + \text{curl} B_h = \Pi^2 J_N^S \\
    \partial_t B_h + \text{curl}_w E_h = 0
\end{cases} \quad \text{with} \quad \Pi^2 J_N^S = \sum_{p=1}^{N} q_p \Pi^2 (V_p^S X_p) \quad (37)$$

with a weak curl$_w : V^2_h \rightarrow V^1_h$ defined by (13), and particles follow the trajectory equations

$$\begin{cases}
    \frac{dX_p}{dt} = V_p \\
    \frac{dV_p}{dt} = \frac{q_p}{m_p} (E^S(X_p) + V_p \times B^S(X_p))
\end{cases} \quad \text{for } p = 1, \ldots, N \quad (38)$$

with coupling fields defined by (27)–(28), namely

$$E^S(X_p) = 3 \sum_{\alpha=1}^{3} e_{\alpha} \int_{\Omega} E_h \cdot \Pi^2 (e_{\alpha} S X_p), \quad B^S(X_p) = 3 \sum_{\alpha=1}^{3} e_{\alpha} \int_{\Omega} B_h \cdot \Pi^1 (e_{\alpha} S X_p) \quad (39)$$

where $(e_1, e_2, e_3)$ is an orthonormal basis of $\mathbb{R}^3$. These evolution equations are completed with two discrete Gauss laws,

$$\begin{cases}
    \text{div} E_h = \Pi^3 \rho_N^S \\
    \text{div}_w B_h = 0
\end{cases} \quad (40)$$

with $\rho_N^S = \sum_{p=1}^{N} q_p S X_p$ and the weak divergence operator div$_w : V^1_h \rightarrow V^0_h$ defined by (13). We note that here the first Gauss law has been derived from the variational principle (considering variations in the electric potential), whereas the second one follows from the definition of the magnetic field.

2.6 Derivation of a discrete Hamiltonian and an associated Poisson bracket

In this section we describe how the above variational equations can be associated with a discrete Poisson bracket.

Following Hamilton’s method [18, Sec. VI.1.2], we observe that our discrete Lagrangian has two nonzero conjugate momenta given by (25) and (30), which we may identify with their Riesz representant in the proper spaces. Assuming that the discrete solution satisfies the variational equations (37)–(40), we have

$$P_{X_N} := \frac{\delta L_h}{\delta X_N} \equiv (m_p V_p + q_p A^S(t, X_p))_{p=1, \ldots, N} \quad \text{and} \quad P_{A_h} := \frac{\delta L_h}{\delta A_h} \equiv -E_h$$

which allows to define a discrete Hamiltonian $\mathcal{H}_h = \mathcal{H}_h(X_N, V_N, A_h, \phi_h)$ as

$$\mathcal{H}_h := \langle P_{X_N}, V_N \rangle + \langle P_{A_h}, \partial_t A_h \rangle - \mathcal{L}_h$$

$$= \sum_{p=1}^{N} (m_p V_p + q_p A^S(t, X_p)) \cdot V_p - \int_{\Omega} E_h \cdot \partial_t A_h - \mathcal{L}_h.$$

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Using the form of the coupling potential (16) and the variational Gauss law (40) we have
\[
\sum_p q_p \phi^S(X_p) = \int_{\Omega} \phi_h \sum_p q_p \Pi^3(S X_p) = \int_{\Omega} \phi_h \rho^{S}_N = \int_{\Omega} \phi_h \text{div} E_h = - \int_{\Omega} E_h \cdot \text{grad}_w \phi_h,
\]
so that the resulting Hamiltonian can be reformulated as a function of the fields (19), namely
\[
\mathcal{H}_h(X_N, V_N, E_h, B_h) = \sum_{p=1}^{N} \frac{m_p}{2} V_p^2 + \frac{1}{2} \int_{\Omega} |E_h|^2 \text{d}x + \frac{1}{2} \int_{\Omega} |B_h|^2 \text{d}x.
\]
(41)

By construction this Hamiltonian is preserved by any solution satisfying the Euler-Lagrange equations (20)–(23). Following [3, Sec. 40-A], a discrete Poisson bracket
\[
\{ F_h, G_h \} = \{ F_h, \mathcal{H}_h \}
\]
holds for an arbitrary functional $F_h$ of the discrete solution. To identify this bracket we may simply consider linear functionals of the form defined by
\[
F_h = F_{X_N, V_N, E_h, B_h} : (X_N, V_N, E_h, B_h) \rightarrow \sum_{p=1}^{N} X_p \cdot \dot{X}_p + V_p \cdot \dot{V}_p + \int_{\Omega} E_h \cdot \dot{E}_h + \int_{\Omega} B_h \cdot \dot{B}_h,
\]
and $G_h = \mathcal{H}_h$. Since the Poisson bracket should be a bilinear antisymmetric expression of the derivatives of its respective functionals, which read (upon identification with their proper discrete Riesz representant)
\[
\frac{\delta F_h}{\delta X_p} = \dot{X}_p, \quad \frac{\delta F_h}{\delta V_p} = \dot{V}_p, \quad \frac{\delta F_h}{\delta E_h} = \dot{E}_h, \quad \frac{\delta F_h}{\delta B_h} = \dot{B}_h
\]
and (for $G_h = \mathcal{H}_h$),
\[
\frac{\delta G_h}{\delta X_p} = 0, \quad \frac{\delta G_h}{\delta V_p} = m_p V_p, \quad \frac{\delta G_h}{\delta E_h} = E_h, \quad \frac{\delta G_h}{\delta B_h} = B_h,
\]
and observing by linearity of $F$ that (12) just amounts to the evolution equations (37)–(39) written in weak forms, with $X_N, V_N, E_h, B_h$ as test fields, we verify that (12) holds with the following discrete bracket
\[
\{ F_h, G_h \} = \sum_{p=1}^{N} \left[ \frac{1}{m_p} \left( \frac{\delta F_h}{\delta X_p} \cdot \frac{\delta G_h}{\delta V_p} - \frac{\delta F_h}{\delta V_p} \cdot \frac{\delta G_h}{\delta X_p} \right) + \frac{q_p}{m_p^2} B^S(X_p) \cdot \left( \frac{\delta F_h}{\delta V_p} \times \frac{\delta G_h}{\delta V_p} \right) \right]
+ \int_{\Omega} \left( \Pi^2 \left( S X_p \frac{\delta F_h}{\delta V_p} \right) \cdot \frac{\delta G_h}{\delta E_h} - \frac{\delta F_h}{\delta E_h} \cdot \Pi^2 \left( S X_p \frac{\delta G_h}{\delta V_p} \right) \right) \text{d}x
+ \int_{\Omega} \left( \frac{\delta F_h}{\delta E_h} \cdot \text{curl} \frac{\delta G_h}{\delta B_h} - \text{curl} \frac{\delta F_h}{\delta B_h} \cdot \frac{\delta G_h}{\delta E_h} \right) \text{d}x
\]
(43)
where we remind that the coupling magnetic field $B^S(X_p)$ is defined in (39) and involves the projection operator $\Pi^1$. We observe that this field plays the role of a parameter of the bracket, as do the shape functions centered on the particle positions, $S X_p$. A different role is played by the electric coupling terms, which enter the bracket through the product of $V \cdot E$ derivatives.
Below we will verify that this bracket is a (non-canonical) Poisson bracket in the sense of [18, Def. VII.2.4], in particular it satisfies the Jacobi identity. We note that other brackets involving different coupling fields $B^S$ would still be antisymmetric, and hence also energy-preserving. As the different projection operators are connected by the commuting diagram properties which have been used in several steps of the least action principle derivation, such brackets would probably not be variational, but they could maybe still satisfy the Jacobi identity.

2.7 Semi-discrete conservation properties of the variational system

One major property of the above derivation is that the resulting semi-discrete system has a Poisson structure, under the very general assumption that the diagram (7) is commuting.

**Theorem 1.** If the operators $\Pi^\ell$ satisfy Assumption 7 and if the shape function $S$ is admissible in the sense of Definition 7, then the discrete bracket (43) is a (non-canonical) Poisson bracket and the semi-discrete equations (37)–(39) are a Poisson system in the sense of [18, Def. VII.2.4].

This result, whose proof will be given in Section 4.3, implies in particular that the evolution equations (37)–(39) preserve all the functionals $F_h$ such that

$$\{F_h, H_h\} = 0,$$

which includes the Hamiltonian itself, $F_h = H_h$, but also all the Casimirs of the bracket (43) which are the functionals $C_h$ such that $\{C_h, G_h\} = 0$ for all $G_h$, and new Casimirs may be derived using the Jacobi identity, see e.g. [18]. An important example is provided by the functionals

$$C_h : (X_N, V_N, E_h, B_h) \mapsto \int_\Omega \tilde{\phi}_h \left( \text{div} E_h - \Pi^3 \left( \sum_{p=1}^N q_p S X_p \right) \right)$$

(44)

associated to an arbitrary $\tilde{\phi}_h \in V^3_h$. The fact that they are Casimirs will be verified just below, and it implies that the discrete Gauss law $\text{div} E_h = \Pi^3 \rho^S_N$ is preserved by our equations.

**Theorem 2.** Under the conditions of Theorem 1, the evolution equations (37)–(39) preserve the discrete Hamiltonian (41) as well as the variational Gauss laws (40).

**Remark 2** (weak Gauss law). Similarly as for the GEMPIC method [23], the magnetic Gauss law plays the role of a pseudo-Casimir, in the sense that its conservation is actually needed to establish that the evolution system has a discrete Hamiltonian structure. With a strong-Ampère ansatz (12), we observe that this divergence-free constraint is only preserved in a weak sense, see (36). Although this may seem very weak, we will see below that it is the natural discrete invariant that provides a Poisson structure for the resulting Hamiltonian system.

**Proof.** The preservation of the magnetic Gauss law readily follows from the weak Faraday equation in (37), indeed we have

$$-\frac{d}{dt} \int_\Omega B_h \cdot \text{grad} \varphi_h = \int_\Omega \text{curl}_\omega E_h \cdot \text{grad} \varphi_h = \int_\Omega E_h \cdot \text{curl} \text{grad} \varphi_h = 0$$
for all \( \varphi_h \in V_h^0 \), using again the definition (13) of the weak curl operator. Turning to the electric Gauss law, we use \( \frac{d}{dt} X_p(t) = V_p \) to compute for an arbitrary smooth function \( \psi \)

\[
\frac{d}{dt} \int_{\Omega} \rho^S_N(t, x) \psi(x) \, dx = \sum_{p=1}^{N} q_p \int_{\Omega} S(\tilde{x}) V_p \cdot \text{grad} \, \psi(\tilde{x} + X_p) \, d\tilde{x} = \int_{\Omega} J^S_N(t, x) \cdot \text{grad} \, \psi(x) \, dx
\]

which shows that the continuity equation

\[
\partial_t \rho^S_N + \text{div} \, J^S_N = 0 \tag{45}
\]

always holds in distribution’s sense, independently of the discrete particle trajectories. Taking next the divergence of the discrete Ampère equation in (37), the commuting diagram property (10) (which holds thanks to the admissibility of \( S \)) allows us to write

\[
\partial_t \text{div} \, E_h = - \text{div} \, \Pi^2 J^S_N = - \Pi^3 \text{div} \, J^S_N = \partial_t \Pi^3 \rho^S_N
\]

where the last equality follows from (15) and from the time-invariance of the operator \( \Pi^3 \). Integrating over time this shows that the electric Gauss law is indeed preserved. Another argument consists of verifying that any functional of the form (42) is indeed a Casimir. To do so we compute that the (Riesz representants of the) functional derivatives of \( C_h \) read

\[
\frac{\delta C_h}{\delta X_p} = q_p \sum_{\alpha=1}^{3} \left( \int_{\Omega} \tilde{\varphi}_h \Pi^3 (e_\alpha \cdot \text{grad} \, S X_p) \right) e_\alpha = q_p \sum_{\alpha=1}^{3} \left( \int_{\Omega} \tilde{\varphi}_h \Pi^3 \text{div} (e_\alpha S X_p) \right) \frac{\delta G_h}{\delta V_p}
\]

and

\[
\frac{\delta C_h}{\delta E_h} = - \text{grad}_{\text{w}} \tilde{\varphi}_h.
\]

As for the derivatives \( \frac{\delta C_h}{\delta V_p} \) and \( \frac{\delta C_h}{\delta B_h} \), they vanish. For the discrete bracket (43) we thus find

\[
\{ C_h, G_h \} = \sum_{p=1}^{N} \frac{q_p}{m_p} \int_{\Omega} \left( \tilde{\varphi}_h \Pi^3 \text{div} \left( \frac{\delta G_h}{\delta V_p} S X_p \right) + \text{grad}_w \tilde{\varphi}_h \cdot \Pi^2 \left( S X_p \frac{\delta G_h}{\delta V_p} \right) \right) \, dx
\]

\[
- \int_{\Omega} \text{grad}_{\text{w}} \tilde{\varphi}_h \cdot \text{curl} \left( \frac{\delta G_h}{\delta B_h} \right) \, dx.
\]

Here the first term vanishes for arbitrary vectors \( \frac{\delta G_h}{\delta V_p} \in \mathbb{R}^3 \), by using the commuting diagram property and the definition of the weak gradient operator. As for the second term, a discrete integration by parts yields \( \int_{\Omega} \text{grad}_{\text{w}} \tilde{\varphi}_h \cdot \text{curl} \left( \frac{\delta G_h}{\delta B_h} \right) \, dx = - \int_{\Omega} \tilde{\varphi}_h \text{div} \text{curl} \left( \frac{\delta G_h}{\delta B_h} \right) \, dx = 0 \), which establishes that \( \{ C_h, G_h \} = 0 \) for any \( G_h \). Equation (42) applied to \( F_h = C_h \) then shows that the quantity \( \text{div} \, E_h - \Pi^3 \rho^S_N \) is an invariant of the evolution system. Finally to verify the energy conservation, we may simply observe that the bracket (43) is antisymmetric, so that \( F_h = H_h \) is an obvious invariant of (42). A more pedestrian argument is to first compute using (37)

\[
\frac{d}{dt} \left( \frac{1}{2} \int_{\Omega} |E_h|^2 + |B_h|^2 \right) = \int_{\Omega} E_h \cdot (\text{curl} \, B_h - \Pi^2 J^S_N) - B_h \cdot \text{curl}_w \, E_h = - \int_{\Omega} E_h \cdot \Pi^2 J^S_N
\]

where we have used the adjoint definition of \( \text{curl}_w \), and then, using the trajectory equations (38)–(39),

\[
\frac{d}{dt} \left( \sum_{p=1}^{N} \frac{m_p}{2} |V_p|^2 \right) = \sum_{p=1}^{N} q_p V_p \cdot (E^S(X_p) + V_p \times B^S(X_p)) = \sum_{p=1}^{N} q_p \int_{\Omega} E_h \cdot \Pi^2 (V_p S X_p) = \int_{\Omega} E_h \cdot \Pi^2 J^S_N
\]

which shows that the discrete energy (41) is indeed constant over time.

\( \square \)
3 Generic Gauss and momentum preserving schemes

Similarly as for the method in [23], the semi-discrete scheme derived above is in general not momentum-preserving. However it is possible to describe a general variant that preserves both the Gauss laws and a discrete momentum. This modified scheme comes at the price of losing the discrete Hamiltonian (Poisson) structure and the conservation of energy, but it may be preferred for problems where momentum preservation is critical.

3.1 Particle-field coupling with discrete interior products

Our momentum-preserving schemes rely on discrete interior products of the form

\[ I^\ell_{e_\alpha} = A_{h,\alpha} i^\ell_{e_\alpha} : V^\ell_{h+1} \to V^\ell_h \]

which involve the continuous interior products \( i^\ell_{e_\alpha} : V^{\ell+1} \to V^\ell \) associated with a canonical unit vector \( e_\alpha, \alpha \in [1,3] \), namely

\[ i^0_{e_\alpha} C := C \cdot e_\alpha, \quad i^1_{e_\alpha} F := F \times e_\alpha, \quad i^2_{e_\alpha} g := g e_\alpha, \]

and where \( A_{h,\alpha} \) is a linear approximation operator, such that the operators \( I^\ell_{e_\alpha} \) map every discrete space to its predecessor in the sequence, as stated in (46).

As a key property, denoting by \( d^0 = \text{grad}, d^1 = \text{curl} \) and \( d^2 = \text{div} \), we require that the associated discrete Lie derivatives, defined as

\[ I^\ell_{h, e_\alpha} := d^{\ell-1} I^\ell_{h, e_\alpha} + I^\ell_{h, e_\alpha} d^\ell : V^\ell_h \to V^\ell_h \]

are antisymmetric, in the sense that \( \int \Omega G \cdot I^\ell_{h, e_\alpha} G = 0 \) for all \( G \in V^\ell_h, \ell \in \{1,2\} \) and \( 1 \leq \alpha \leq 3 \). Specifically, the momentum preserving properties will rely on the following relations

\[ \int \Omega C_h \cdot \text{grad} I^0_{e_\alpha} C_h = - \int \Omega C_h \cdot I^1_{e_\alpha} \text{curl} C_h \quad \forall C_h \in V^1_h \]

and

\[ \int \Omega F_h \cdot \text{curl} I^1_{e_\alpha} F_h = - \int \Omega F_h \cdot I^2_{e_\alpha} \text{div} F_h \quad \forall F_h \in V^2_h. \]

3.2 Gauss and momentum-preserving schemes

Using the discrete interior products described above, we obtain the following result.

**Theorem 3.** The scheme obtained by coupling the discrete Maxwell equations (37)–(38) with the modified particle equations

\[
\begin{aligned}
\frac{dX_p}{dt} &= V_p \\
\frac{dV_p}{dt} &= \frac{q_p}{m_p} \left( E^S(X_p) + R^S(B_h, X_p, V_p) \right)
\end{aligned}
\]

for \( p = 1, \ldots, N \)

with coupling fields defined as

\[
\begin{aligned}
E^S(X_p) &= \sum_{\alpha=1}^{3} e_\alpha \int \Omega E_h(x) \cdot (I^3_{e_\alpha} \Pi^2 S_X)(x) \, dx \\
R^S(B_h, X_p, V_p) &= - \sum_{\alpha=1}^{3} e_\alpha \int \Omega B_h(x) \cdot (I^1_{e_\alpha} \Pi^2 (V_p S_X))(x) \, dx,
\end{aligned}
\]

for \( \alpha \in [1,3] \).
preserves the discrete Gauss laws \((40)\), as well as the discrete momentum

\[
P_h(t) = \sum_{p=1}^{N} m_p V_p(t) - \sum_{\alpha=1}^{3} e_\alpha \int_{\Omega} (I_{e_\alpha}^1 E_h(t, x)) \cdot B_h(t, x) \, dx.
\]  

\(\text{(52)}\)

Remark 3. Given the form \((46)-(47)\) of \(I_{e_\alpha}^1\) and the linearity of \(\mathcal{A}_{h,\alpha}\), we have

\[
\int_{\Omega} (I_{e_\alpha}^1 E_h) \cdot B_h = \int_{\Omega} ((\mathcal{A}_{h,\alpha} E_h) \times e_\alpha) \cdot B_h = \int_{\Omega} (B_h \times (\mathcal{A}_{h,\alpha} E_h)) \cdot e_\alpha
\]

which makes clear how \((52)\) approximates the exact momentum along \(e_\alpha\). Similarly, we have

\[
\mathcal{R}^e(B_h, X_p, V_p) \cdot e_\alpha = \int_{\Omega} ((\mathcal{A}_{h,\alpha} \Pi^2(V_p S X_p)) \times B_h) \cdot e_\alpha
\]

\(\text{(53)}\)

which shows that the discrete magnetic force involved in \((50)\) is indeed an approximation of the “natural” term \(V_p \times B_h(X_p)\). However it is not possible in general to write \(\mathcal{R}^e(B_h, X_p, V_p)\) as a product of the form \(V_p \times B^S(X_p)\) for some field \(B^S\), because the approximation operators \(\mathcal{A}_{h,\alpha}\) involved in the trajectory equation depend a priori on the component \(\alpha\) of the latter.

\textbf{Proof.} We first observe that the arguments used in the proof of Theorem \(2\) for the conservation of the discrete Gauss laws did not rely on the particle trajectory equation, hence they are still valid for the modified scheme. Turning to the discrete momentum, we compute using \((50)\)

\[
\frac{d}{dt} \sum_{p=1}^{N} m_p V_p \cdot e_\alpha = \sum_{p=1}^{N} q_p \int_{\Omega} (E_h \cdot (I_{e_\alpha}^1 \Pi^2 S X_p) - B_h \cdot (I_{e_\alpha}^1 \Pi^2(V_p S X_p)))
\]

\[
= \int_{\Omega} E_h \cdot (I_{e_\alpha}^2 \Pi^3 \rho^S N) - \int_{\Omega} B_h \cdot (I_{e_\alpha}^1 \Pi^2 J^S N).
\]

Using next \((37)\) we write

\[
\frac{d}{dt} \int_{\Omega} I_{e_\alpha}^1 E_h \cdot B_h = -\int_{\Omega} \text{curl} I_{e_\alpha}^1 E_h \cdot \text{curl} E_h + \int_{\Omega} (I_{e_\alpha}^1 (\text{curl} B_h - \Pi^2 J^S_N)) \cdot B_h
\]

\[
= -\int_{\Omega} \text{curl} I_{e_\alpha}^1 E_h \cdot E_h + \int_{\Omega} (I_{e_\alpha}^1 \text{curl} B_h) \cdot B_h - \int_{\Omega} (I_{e_\alpha}^1 \Pi^2 J^S_N) \cdot B_h
\]

\[
= \int_{\Omega} (I_{e_\alpha}^2 \text{div} E_h) \cdot E_h - \int_{\Omega} (\text{grad} I_{e_\alpha}^0 B_h) \cdot B_h - \int_{\Omega} (I_{e_\alpha}^1 \Pi^2 J^S_N) \cdot B_h
\]

\[
= \int_{\Omega} (I_{e_\alpha}^2 \Pi^3 \rho^S N) \cdot E_h - \int_{\Omega} (I_{e_\alpha}^1 \Pi^2 J^S_N) \cdot B_h = \frac{d}{dt} \sum_{p=1}^{N} m_p V_p \cdot e_\alpha
\]

where we have used the definition of the weak curl operator in the second equality, the relations \((48)-(49)\) in the third one and the preservation of the discrete (weak and strong) Gauss laws in the last one. \(\square\)
3.3 Interior products based on directional averaging on tensor-product spaces

In this section we show that a simple construction based on directional averaging allows to design momentum-preserving schemes when the compatible sequence

$$V^0_h \xrightarrow{\text{grad}} V^1_h \xrightarrow{\text{curl}} V^2_h \xrightarrow{\text{div}} V^3_h$$

involves tensor-product spaces of the form

$$V^0_h = \mathbb{U}_h^1 \otimes \mathbb{U}_h^2 \otimes \mathbb{U}_h^3 := \text{Span} \left( \{ x \mapsto \Lambda_{k_1}^{0,1}(x_1) \Lambda_{k_2}^{0,2}(x_2) \Lambda_{k_3}^{0,3}(x_3) : (k_1, k_2, k_3) \in \prod_{\alpha=1}^{3} [1, N^\alpha_0] \} \right)$$

(47)

and

$$V^1_h = \left( \mathbb{U}_h^1 \otimes \mathbb{U}_h^2 \otimes \mathbb{U}_h^3 \right), \quad V^2_h = \left( \mathbb{U}_h^1 \otimes \mathbb{V}_h^2 \otimes \mathbb{V}_h^3 \right), \quad V^3_h = \mathbb{U}_h^1 \otimes \mathbb{V}_h^2 \otimes \mathbb{V}_h^3,$$  

(55)

where the univariate spaces $\mathbb{U}_h^\alpha$, $\mathbb{V}_h^\alpha$, form an exact sequence along each dimension $\alpha \in [1, 3]$,

$$\mathbb{R} \rightarrow \mathbb{U}_h^\alpha = \text{Span} \left( \{ \Lambda_k^{0,\alpha} : k \in [1, N^\alpha_0] \} \right) \rightarrow \mathbb{V}_h^\alpha = \text{Span} \left( \{ \Lambda_k^{1,\alpha} : k \in [1, N^\alpha_0] \} \right) \rightarrow \{0\}.$$  

(56)

**Lemma 1.** Assume that the univariate sequences (56) are exact, with spaces $\mathbb{U}_h^\alpha$ invariant over translations of $\pm h_\alpha$, $1 \leq \alpha \leq 3$. Then the discrete interior products $I_{e_{\alpha}}^\ell = \mathcal{A}_{h,\alpha} \circ I_{e_{\alpha}}^\ell$, defined by composing the exact interior products (47) with the directional averaging operator,

$$(\mathcal{A}_{h,1} G)(x) := \frac{1}{2h_1} \int_{x_1-h_1}^{x_1+h_1} G(y_1, x_2, x_3) dy_1$$

(57)

and similarly for $\alpha = 2, 3$, map $V^\ell_h$ to $V_1^\ell$. Furthermore, they satisfy the relations (48)–(49).

**Proof.** Let us show that $I^0_{e_{\alpha}}$ maps $V^1_h$ to $V^0_h$. For a generic basis function in $V^1_h$, of the form

$$\Lambda_{\alpha,k}(x) = e_{\alpha} \Lambda_{k_\alpha}^{\alpha,1}(x_\alpha) \prod_{\beta \neq \alpha} \Lambda_{k_\beta}^{0,\beta}(x_\beta),$$

we observe that $(I^0_{e_{\alpha}} \Lambda_{\alpha,k}^{1,\alpha})(x) = \delta_{\alpha, \alpha'} \Lambda_{k_\alpha}^{\alpha',1}(x_\alpha) \prod_{\beta \neq \alpha} \Lambda_{k_\beta}^{0,\beta}(x_\beta)$ using (47) and the tensor-product structure (54)–(56). The exact sequence property (56) then allows us to write $\Lambda_{k_\alpha}^{1,\alpha} = \partial_\alpha \Gamma^0_{k_\alpha}$ for some $\Gamma^0_{k_\alpha} \in \mathbb{U}_h^\alpha$, which yields

$$(I^0_{e_{\alpha}} \Lambda_{\alpha,k}^{1,\alpha})(x) = (\mathcal{A}_{h,\alpha} \Lambda_{k_\alpha}^{1,\alpha})(x_\alpha) \prod_{\beta \neq \alpha} \Lambda_{k_\beta}^{0,\beta}(x_\beta) = \frac{1}{2h_\alpha} \left[ \Gamma_{k_\alpha}^{0,\alpha} \right]_{x_\alpha-h_\alpha}^{x_\alpha+h_\alpha} \prod_{\beta \neq \alpha} \Lambda_{k_\beta}^{0,\beta}(x_\beta)$$

which belongs to $V^0_h$, according to (54) and the discrete translation invariance. The argument for the other spaces is similar. Turning to (48)–(49) we next observe that the directional averaging operators are of the form $\mathcal{A}_{h,\alpha} G = \mu_\alpha \ast G$ with a symmetric measure $\mu_\alpha(-x) = \mu_\alpha(x)$. Thus,

$$\int_{\Omega} G(\mu_\alpha \ast \partial_\beta G) = \int_{\Omega} (\mu_\alpha \ast G) \partial_\beta G = - \int_{\Omega} (\partial_\beta (\mu_\alpha \ast G)) G = - \int_{\Omega} (\mu_\alpha \ast \partial_\beta G) G = 0$$

(58)
for all $\alpha$, $\beta$, and any function $G$. This allows to write a proof that is formally the same as for the continuous interior product (47). Thus, using that $(\text{curl} C) \times e_\alpha = \partial_\alpha C - \text{grad} C_\alpha$ we have

$$\int_\Omega C \cdot \text{grad} I^0_{e_\alpha} C = \int_\Omega C \cdot (\mu_\alpha \ast \text{grad} C_\alpha) = \int_\Omega C \cdot (\mu_\alpha \ast (\partial_\alpha C - (\text{curl} C) \times e_\alpha)) = - \int_\Omega C \cdot I^1_{e_\alpha} \text{curl} C$$

which proves (48). The relation (49) follows by a similar argument. □

4 The semi-discrete Hamiltonian system as a system of ordinary differential equations

In this section, we express the variational particle method (37)–(38) as a system of ordinary differential equations. This will allow us to introduce some useful notation for our general framework, and to verify the Hamiltonian structure of the semi-discrete system.

4.1 Commuting diagrams with degrees of freedom

One practical approach to build commuting projection operators is to introduce one additional layer in the diagram (7), consisting of coefficient spaces $C^\ell = \mathbb{R}^{N_\ell}$ corresponding to the choice of specific bases for the finite-dimensional spaces $V^\ell_h$ with dimension $N_\ell$. This approach is somehow parallel to the geometric construction of [24] where commuting de Rham complexes are described for differential forms. As we consider here a a finite element setting, we will follow similar principles but our construction does not involve differential forms.

In this diagram the main novel ingredient is the degrees of freedom $\sigma^\ell = (\sigma^\ell_i)_{1 \leq i \leq N_\ell}$, which must be unisolvent for the finite-dimensional spaces $V^\ell_h$ in the usual sense that they must be one-to-one when restricted to these spaces. The spaces $V^\ell$ then denote the domains of these degrees of freedom, and as above we consider a conforming discretization in the sense that $V^\ell_h \subset V^\ell$. The other discrete entities can then be determined from the degrees of freedom.

- The “interpolation” operators $\mathcal{I}^\ell$ are characterized by the right-inverse property $\sigma^\ell \mathcal{I}^\ell g = g$ for all $g \in C^\ell$. In particular, the basis functions $\Lambda^\ell_i \in V^\ell_h$ defined by the usual duality relations

$$\sigma^\ell_i(\Lambda^\ell_j) = \delta_{i,j} \quad \text{for} \quad 1 \leq i, j \leq N_\ell$$

(59)

correspond to $\Lambda^\ell_i = \mathcal{I}^\ell e^\ell_i$ where $e^\ell_i = (\delta_{i,j})_{1 \leq j \leq N_\ell}$ is a canonical basis vector of $C^\ell$. It is sometimes convenient to stack the basis functions into column vectors $\Lambda^\ell = (\Lambda^\ell_i)_{1 \leq i \leq N_\ell}$,
and to use a matrix notation for stacked functionals evaluated on vectors of functions. With this convention, the duality relation (59) reads

\[ \sigma^\ell(\Lambda^\ell) = I_{N_\ell} \quad \text{with} \quad \sigma^\ell(\Lambda^\ell) = (\sigma^\ell_i(\Lambda^\ell_j))_{1 \leq i, j \leq N_\ell}. \] (60)

- The matrices \( D^\ell \in \mathbb{R}^{N_{\ell+1} \times N_\ell} \) correspond to the differential operators \( d^0 = \text{grad}, d^1 = \text{curl} \), and \( d^2 = \text{div} \) in the respective bases, namely

\[ D^\ell = \sigma^{\ell+1}(d^\ell \Lambda^\ell) = (\sigma^{\ell+1}_i(d^\ell \Lambda^\ell_j))_{1 \leq i \leq N_{\ell+1}, 1 \leq j \leq N_\ell} \] (61)

so that we have \( \sigma^{\ell+1}(d^\ell G) = \sigma^{\ell+1}(g^\top d^\ell \Lambda^\ell) = D^\ell g \) for all \( G = g^\top \Lambda^\ell \in V^\ell_h \) with \( g \in \mathcal{C}^\ell \).

- The projection operators are defined as \( \Pi^\ell = T^\ell \sigma^\ell : G \rightarrow \sum_i \sigma^\ell_i(G) \Lambda^\ell_i \), that is,

\[ \Pi^\ell G := (\sigma^\ell_i(G))^\top \Lambda^\ell \quad \text{for} \quad G \in V^\ell, \] (62)

and they are characterized by the relations

\[ \sigma^\ell_i(\Pi^\ell G) = \sigma^\ell_i(G) \quad \text{for} \quad 1 \leq i \leq N_\ell, \] (63)

indeed we have \( \sigma^\ell(\Pi^\ell G) = \sigma^\ell((\sigma^\ell(G))^\top \Lambda^\ell) = \sigma^\ell(\Lambda^\ell) \sigma^\ell(G) = \sigma^\ell(G) \) for all \( G \in V^\ell \).

This setting proves particularly useful in practice, as it allows to restate the commuting diagram properties (7) as a linear relation between degrees of freedom.

**Lemma 2.** The following properties are equivalent:

(i) the projection operators (62) satisfy the commuting diagram properties (7),

\[ \Pi^{\ell+1} d^\ell G = d^\ell \Pi^\ell G \quad \text{for all} \quad G \in V^\ell, \] (64)

(ii) there exists a matrix \( D^\ell \in \mathbb{R}^{N_{\ell+1} \times N_\ell} \) such that

\[ \sigma^{\ell+1}(d^\ell G) = D^\ell \sigma^\ell(G) \quad \text{for all} \quad G \in V^\ell. \] (65)

Moreover if (65) holds, then the matrix \( D^\ell \) coincides with (61).

**Proof.** The proof is a matter of elementary computations. For instance, (65) yields

\[ \sigma^{\ell+1}(d^\ell \Pi^\ell G) = D^\ell \sigma^\ell(\Pi^\ell G) = D^\ell \sigma^\ell(G) = \sigma^{\ell+1}(d^\ell G) = \sigma^{\ell+1}(\Pi^{\ell+1} d^\ell G) \]

where we have used twice the characterization (63).  \( \square \)
4.2 The semi-discrete Hamiltonian system in matrix form

The introduction of a third layer in the commuting diagram offers the possibility to rewrite the semi-discrete scheme \([37, 38]\) as a system of ordinary differential equations in matrix form. To do so we collect all the dynamic variables in a global vector

\[
U = \begin{pmatrix} X \\ V \\ E \\ B \end{pmatrix}
\]

where the (column) block-vectors \(X = X_N = (X_p)_{p=1, \ldots, N}\) and \(V = V_N = (V_p)_{p=1, \ldots, N} \in (\mathbb{R}^3)^N\) collect all the particle positions and velocities as in Section 2.4, while the vectors \(E = \sigma^2(E_h) \in \mathbb{R}^{N_2}\) and \(B = \sigma^1(B_h) \in \mathbb{R}^{N_1}\) collect the coefficients of the electric and magnetic fields in their respective bases. Using these degrees of freedom, we observe that the coupling fields \((39)\) read

\[
\begin{align*}
E^S_{\alpha}(X_p) &= \int_{\Omega} E_h(x) \cdot \Pi^2(e_{\alpha} S X_p)(x) \, dx = \sum_{i,j=1}^{N_2} \sigma^2_i(E_h) \sigma^2_{i,j} \sigma^2_j(e_{\alpha} S X_p) \\
B^S_{\alpha}(X_p) &= \int_{\Omega} B_h(x) \cdot \Pi^1(e_{\alpha} S X_p)(x) \, dx = \sum_{i,j=1}^{N_1} \sigma^1_i(B_h) \sigma^1_{i,j} \sigma^1_j(e_{\alpha} S X_p)
\end{align*}
\]

where \(\mathbb{M}^\ell\) is the standard finite-element mass matrix in the corresponding basis of \(V_h^\ell, \ell = 1, 2,\)

\[
\mathbb{M}^\ell_{i,j} = \int_{\Omega} \Lambda^\ell_i(x) \cdot \Lambda^\ell_j(x) \, dx, \quad 1 \leq i, j \leq N_\ell.
\]  

(66)

The value of the coupling fields at the particle positions may then be expressed as block-vectors,

\[
E^S(X) = S^2(X) \mathbb{M}^2 E \quad \text{and} \quad B^S(X) = S^1(X) \mathbb{M}^1 B \quad \text{in} \quad (\mathbb{R}^3)^N,
\]

(67)

where \(S^\ell(X) \in (\mathbb{R}^3)^{N \times N_\ell}\) denotes the matrix with \((3 \times 1)\) blocks

\[
S^\ell(X)_{p,i} = (\sigma^\ell_1(e_{\alpha} S X_p) \sigma^\ell_2(e_{\alpha} S X_p) \sigma^\ell_3(e_{\alpha} S X_p))^T \quad \text{for} \quad 1 \leq p \leq N, \quad 1 \leq i \leq N_\ell.
\]  

(68)

We finally let \(\tau(b) = ((e_{\alpha} \times e_{\beta}) \cdot b)_{1 \leq \alpha, \beta \leq 3} \in \mathbb{R}^{3 \times 3}\) be the rotation matrix

\[
\tau(b) = \begin{pmatrix} 0 & b_3 & -b_2 \\ -b_3 & 0 & b_1 \\ b_2 & -b_1 & 0 \end{pmatrix}
\]

such that \(v \times b = \tau(b)v\) for all \(v, b \in \mathbb{R}^3,\)

(69)

and we denote by \(\mathbb{R}(b(X)) \in (\mathbb{R}^{3 \times 3})^{N \times N}\) the block-diagonal rotation matrix with blocks

\[
\mathbb{R}(b(X))_{p,p} = \tau(b(X_p)).
\]  

(70)

Then the particle trajectory equations \([38]--[39],\)

\[
\begin{aligned}
\frac{dX_p}{dt} &= V_p \\
\frac{dV_p}{dt} &= \frac{q_p}{m_p} \left( E^S(X_p) + V_p \times B^S(X_p) \right)
\end{aligned}
\]

for \(p = 1, \ldots, N\)

(71)
can be written in the block-matrix form

\[
\begin{align*}
\frac{dX}{dt} &= V, \\
\frac{dV}{dt} &= \mathcal{W}\begin{pmatrix} S^2(X) \mathbb{M}^2 E + \mathcal{R}^1(X, B) V \end{pmatrix},
\end{align*}
\]

(72)

where \( \mathcal{W}_m = \text{diag}(\frac{q_p}{m_p} : p \in [1, N]) \) is the diagonal weighting matrix carrying the particles charge to mass ratios, and where we have denoted

\[
\mathcal{R}^1(X, B) = \mathcal{R}(B^S(X)) = \mathcal{R}(S^1(X) \mathbb{M}^1 B)
\]

in \((\mathbb{R}^{3 \times 3})^{N \times N}\)

(73)

the block-diagonal rotation matrix associated with the coupling magnetic field. Observe that its diagonal blocks read

\[
\mathcal{R}_p(X, B) = \mathcal{R}(S_1(X) M_1 B)
\]

with \(C = \mathbb{D}^1\) the matrix of the operator curl: \(V^1_h \to V^2_h\), see (61), \(S^2(X)\) the matrix defined in (68) and \(\mathcal{W}_q\) the diagonal weighting matrix carrying the particles charges. Finally the weak Faraday equation is tested against the basis functions \(\Lambda^1_i\). By definition of the weak curl operator (13) this yields

\[
\mathbb{M}^1 \frac{dB}{dt} + C^\top \mathbb{M}^2 E = 0
\]

(75)

with \(\mathbb{M}^1\) and \(\mathbb{M}^2\) the mass matrices recalled in (66).

Finally, rewriting the discrete Hamiltonian \(H_h(X_N, V_N, E_h, B_h)\) as a function of the array variables

\[
H(U) = \frac{1}{2} V^\top \mathcal{W}_m V + \frac{1}{2} E^\top \mathbb{M}^2 E + \frac{1}{2} B^\top \mathbb{M}^1 B,
\]

(76)

with \(\mathcal{W}_m\) the diagonal weighting matrix carrying the particle masses, see (41), we obtain for the corresponding derivatives

\[
\nabla U H(U) = \begin{pmatrix} \nabla X H \\ \langle V \rangle H \\ \nabla E H \\ \nabla B H \end{pmatrix} (U) = \begin{pmatrix} 0 \\ \mathcal{W}_m V \\ \mathbb{M}^2 E \\ \mathbb{M}^1 B \end{pmatrix}
\]

which allows us to rewrite the equations (37)–(39) as a system of ODEs

\[
\frac{dU}{dt} = J(U) \nabla U H(U)
\]

(77)

with a structure matrix given by

\[
J(U) = \begin{pmatrix} 0 & \mathbb{W}^1_m & 0 & 0 \\ -\mathbb{W}^1_m & \mathcal{R}(X, B) \mathcal{W}_m^{-1} & \mathbb{W}_m^{-1} s^2(X) & 0 \\ 0 & -s^2(X)^\top \mathbb{W}_m^{-1} & 0 & C (\mathbb{M}^1)^{-1} \\ 0 & 0 & -\mathbb{M}^1^{-1} C^\top & 0 \end{pmatrix}
\]

(78)
In particular, System (77) may be rewritten in the form of a Poisson system
\[
\frac{dU}{dt} = \{U, H\}(U)
\] (79)
with a discrete bracket defined as \{F, G\}(U) := (\nabla_U F)^\top J(U) \nabla_U G, that is,
\[
\{F, G\}(U) = (\nabla_F X)^\top \mathcal{W}_m \nabla Y G - (\nabla_F X)^\top \mathcal{W}_m \nabla Y G \\
+ (\nabla_F X)^\top \mathcal{W}_m [\mathcal{R}^1(X, B)] \nabla Y G \\
+ (\nabla_F X)^\top \mathcal{W}_m \mathcal{S}^2(X) \nabla E G - (\nabla_F X)^\top \mathcal{S}^2(X) \nabla E G \\
+ (\nabla_F X)^\top \mathcal{C}(M^1)^{-1} \nabla B G - (\nabla_F X)^\top (M^1)^{-1} C^\top \nabla E G.
\] (80)

Note that this is just the matrix form of the discrete bracket \{F, G\} given in (13), where \(F_h\) and \(G_h\) are the same functionals as \(F\) and \(G\) but seen as functions of the finite element fields \(E_h, B_h\).

Compared with the Poisson matrix found in [23, Eq. (4.29)], we observe that the main difference lies in the fact that the particle-field coupling blocks now involve the degrees of freedom of the smoothed particles through the matrices \(S^2\) and \(S^1\) which involve the generic commuting diagram operators \(\Pi^2\) and \(\Pi^1\), see (68) and (73). In particular, the similarity of both matrices allows us to easily verify the Poisson structure of the semi-discrete system (37)–(39).

4.3 Proof of Theorem 1

Since we have rewritten our equations in a matrix form, it suffices to show that \(J\) is a Poisson matrix in the sense of [18, Def. VII.2.4], i.e., that it is skew-symmetric and it satisfies the matrix Jacobi identity. This will show that (80) is a (non-canonical) Poisson bracket and that (79), namely (77), is a Poisson system.

Using that weighting matrices like \(\mathcal{W}_m\) are diagonal, and that \(\mathcal{R}^1(X, B)\) is skew-symmetric, we easily verify that \(J = -J^\top\). To verify the matrix Jacobi identity, we then observe that \(J\) has the same form as the one involved in the original GEMPIC scheme, see [23, Eq. (4.29)], with \(\mathcal{C}M^{-1}_1\) and \(\mathcal{A}^1(X)M^{-1}_1\) replaced by \((M^1)^{-1} C^\top\) and \(S^2(X)\), respectively (the mass and curl matrices being defined for different spaces, due to the different ansatz in the fields). We also note that \(\mathcal{R}^1\) plays the role of the magnetic rotation matrix \(\mathcal{B}\) in [23], with smoothed coupling terms as already observed. In particular, we may follow the same reasoning to verify that it satisfies the Jacobi identity, which amounts to verifying that the analog of Eqs. (4.34) and (4.38) hold in our case. Using the block-diagonal matrix \(\mathcal{R}^1(X, B)\) defined by (73), and taking \((p, \alpha), (p, \beta),\) and \((p, \gamma)\) as multi-indices corresponding to \(b, c,\) and \(d\), Equation (4.34) becomes (for \(q_p \neq 0\))
\[
\frac{\partial \mathcal{R}^1(X, B)(p, \alpha), (p, \beta)}{\partial x_{p, \gamma}} + \frac{\partial \mathcal{R}^1(X, B)(p, \beta), (p, \alpha)}{\partial x_{p, \gamma}} + \frac{\partial \mathcal{R}^1(X, B)(p, \gamma), (p, \alpha)}{\partial x_{p, \beta}} = 0 \quad \forall p, \alpha, \beta, \gamma.
\] (81)

Using the expression \(\mathcal{R}^1(X, B)(p, \alpha), (p, \beta) = \mathbf{\sigma}^1(e_\alpha \times e_\beta S_{X_p})^\top M^1\mathbf{B}\) seen above, this amounts to
\[
\mathbf{B}^\top M^1 \mathbf{\sigma}^1(e_\alpha \times e_\beta (\partial_\gamma S_{X_p}) + e_\beta \times e_\gamma (\partial_\alpha S_{X_p}) + e_\gamma \times e_\alpha (\partial_\beta S_{X_p})) = 0.
\]

By antisymmetry, we see that the function in parentheses vanishes if two of the components coincide, so that we may assume w.l.o.g. that \((\alpha, \beta, \gamma) = (1, 2, 3)\). Then this function is just \(\nabla S_{X_p}\) and the above equation amounts to
\[
0 = \mathbf{B}^\top M^1 \mathbf{\sigma}^1(\nabla S_{X_p}) = \int_\Omega B_h \cdot \Pi^1(\nabla S_{X_p}) = \int_\Omega B_h \cdot \nabla \Pi^0(S_{X_p}) = - \int_\Omega (\text{div}_w B_h) \Pi^0(S_{X_p}),
\]

20
where we have used the commuting diagram property and the admissibility of the shape function $S$. The desired equality then follows from the discrete magnetic Gauss law, see (40).

The second equality to verify is the analog of Equation (4.37) from [23], which reads here (given the above matrix correspondence and correcting a typo on the sign of the right-hand side)

$$
\frac{\partial S^2(X)(p,\alpha)}{\partial x_{p,\beta}} - \frac{\partial S^2(X)(p,\beta)}{\partial x_{p,\alpha}} = -\sum_{j=1}^{N_1} \frac{\partial R^1(X,B)(p,\alpha),(p,\beta)}{\partial B_j} ((M^1)^{-1}C^\top)_{j,i} \quad \forall p,\alpha,\beta,i.
$$

(82)

By antisymmetry of $R^1$, we see that both sides vanish for $\alpha = \beta$, so let us assume w.l.o.g. that $(\alpha,\beta) = (1,2)$. Then $R^1(X,B)(p,\alpha),(p,\beta) = \sigma^1(e_3 S X_p)^\top M^1 B$ and by differentiating these entries and those of the matrix $S^2$, see (68), the equality becomes

$$
\sigma^2_i(e_1(\partial_2 S X_p)) - \sigma^2_i(e_2(\partial_1 S X_p)) = (C\sigma^1(e_3 S X_p))_i \quad \text{for } i = 1, \ldots, N_1.
$$

In vector terms this writes $\sigma^2(\text{curl}(e_3 S X_p)) = C\sigma^1(e_3 S X_p)$, which directly follows from the commuting diagram property as seen in Lemma 2. Thus (82) holds, which shows that $J$ satisfies the Jacobi identity and is indeed a Poisson matrix.

4.4 Propagation in time

Based on its Poisson structure, geometric time propagation schemes can be derived for our variational system in the same way in [23]. More precisely, a variational integrator can be derived from a Hamiltonian splitting, that yields a scheme that is explicit in time. We refer to [23, Sec. 5.1] where the resulting equations are detailed for the weak Ampère case and delta shape functions. This kind of splitting has originally been proposed for the Vlasov–Maxwell system in [19, 35] as a Hamiltonian splitting and later been constructed from a fully discrete action principle in [36]. On the other hand, energy-conserving time propagators can be derived by an antisymmetric splitting of the Poisson matrix combined with a suitable discrete-gradient time propagation of the substeps as explained in [21]. In our numerical experiments, we consider the energy- and Gauss-conserving discrete-gradient method from [21], which demonstrates the best the conservation properties of the phase-space discretization, and the Hamiltonian splitting from [23] due to its simplicity.

5 Generalization and application to the strong Faraday model

Before turning to the description of particular discretizations of Maxwell’s equations, it may be useful to pause for a moment and make some comments on the above findings. In our variational derivation we have explicitly required that (7) was a commuting diagram, and by doing so we have made two implicitly assumptions: first, we have considered that the discrete sequence involved strong differential operators, which corresponds to a conforming discretization. Second, we have referred to the operators $\Pi^\ell$ as projection operators. Although these are standard properties to assume, they played no particular role in our analysis, be it in the variational derivation of Section 2 or in the proof of its Hamiltonian structure. In particular, our results
where the discrete differential operators \( \sim \text{grad}, \sim \text{curl}, \sim \text{div} \) no longer need to coincide with the exact ones (in particular, the discrete spaces \( \tilde{V}_h^\ell \) need not be conforming in \( H^1, H(\text{curl}) \) and \( H(\text{div}) \), and the \( \tilde{\Pi}^\ell \) no longer need to be projection operators. In this generalized setting the only assumptions are that:

(i) the solid diagram in (83) commutes,

(ii) the lower discrete differential are adjoint to the upper ones in the sense of (13), namely \( \int_{\Omega} \tilde{\varphi}_h \text{div} \tilde{F}_h = -\int_{\Omega} \text{grad} \tilde{\varphi}_h \cdot \tilde{F}_h \) must hold for all \( \tilde{\varphi}_h \in \tilde{V}_h^0 \) and \( \tilde{F}_h \in \tilde{V}_h^1 \), and so on.

Our variational derivation then applies verbatim, starting from the discrete Lagrangian

\[
\tilde{L}_h(\mathbf{X}_N, \mathbf{X}_N', \mathbf{V}_N, \mathbf{A}_h, \mathbf{A}_h', \tilde{\varphi}_h) = \sum_{p=1}^{N} \left( (m_p \mathbf{V}_p + q_p \bar{A}^S(\mathbf{X}_p)) \cdot \mathbf{X}_p' - \left( \frac{m_p}{2} \mathbf{V}_p^2 + q_p \bar{\phi}^S(\mathbf{X}_p) \right) \right) + \frac{1}{2} \int_{\Omega} |\text{grad} \tilde{\phi}_h(\mathbf{x}) + \bar{A}_h'(\mathbf{x})|^2 d\mathbf{x} - \frac{1}{2} \int_{\Omega} |\text{curl} \tilde{\mathbf{A}}_h(\mathbf{x})|^2 d\mathbf{x}
\]

with particle arrays \( \mathbf{X}_N, \mathbf{X}_N', \mathbf{V}_N \in (\mathbb{R}^3)^N \), discrete fields \( \tilde{\mathbf{A}}_h, \tilde{\mathbf{A}}'_h \in \tilde{V}_h^2 \), \( \tilde{\varphi}_h \in \tilde{V}_h^3 \) and coupling potentials defined as in (16). The resulting variational equations, analog to (37)–(40), read

\[
\begin{align*}
-\partial_t \tilde{\mathbf{E}}_h + \text{curl} \tilde{\mathbf{B}}_h &= \tilde{\Pi}^2 \bar{J}_N^S \\
\partial_t \tilde{\mathbf{B}}_h + \text{curl} \tilde{\mathbf{E}}_h &= 0
\end{align*}
\]

and

\[
\begin{align*}
\frac{d\mathbf{X}_p}{dt} &= \mathbf{V}_p \\
\frac{d\mathbf{V}_p}{dt} &= \frac{q_p}{m_p} (\bar{E}^S(\mathbf{X}_p) + \mathbf{V}_p \times \bar{B}^S(\mathbf{X}_p))
\end{align*}
\]

with coupling fields defined similarly as in (39). Our analysis then shows that these general equations preserve both the corresponding discrete Gauss laws and the Hamiltonian, and that they have a discrete Poisson structure. This allows to extend our results to a wider range of discrete settings, including the structure-preserving DG-type Conga discretizations developed in [10, 11] where both \( \mathbf{E} \) and \( \mathbf{B} \) are represented in broken finite element spaces. Our results also apply to the discrete ansatz (11) corresponding to a strong Faraday equation. For this case we may consider a conforming (strong) discretization of the form (7), and set

\[
\tilde{V}_h^0 := V_h^0, \quad \tilde{V}_h^1 := V_h^1, \quad \tilde{V}_h^2 := V_h^2, \quad \tilde{V}_h^3 := V_h^3
\]

so that the ansatz (11) takes a form similar to the one (12) considered above, namely

\[
\tilde{\mathbf{B}}_h \in \tilde{V}_h^1 \xrightarrow{\text{grad}} \tilde{\mathbf{E}}_h, \tilde{\mathbf{A}}_h \in \tilde{V}_h^2 \xrightarrow{\text{curl}} \tilde{\varphi}_h \in \tilde{V}_h^3.
\]
A commuting diagram involving the spaces can then be obtained as follows: define the commuting (upper) discrete differential operators as the weak operators, i.e.
\[ \tilde{\text{grad}} := \text{grad}_w, \quad \tilde{\text{curl}} := \text{curl}_w, \quad \tilde{\text{div}} := \text{div}_w, \]
use the strong ones for the adjoint (lower) operators,
\[ \tilde{\text{grad}}^* := \text{grad}, \quad \tilde{\text{curl}}^* := \text{curl}, \quad \tilde{\text{div}}^* := \text{div}. \]
and for the projection operators \( \tilde{\Pi} \ell \) simply take the \( L^2 \) projections on the discrete spaces,
\[ \langle \tilde{\Pi} \ell G, G_h \rangle = \langle G, G_h \rangle \quad \text{for} \quad G \in V^\ell, \ G_h \in V^\ell_h. \]
The commutation property is indeed easily verified: For the \( \text{grad} \) operator, using the embedding \( \text{div} : V^1_h = V^2_h \rightarrow V^3_h = V^0_h \) and the characterization of \( L^2 \) projections, we can write
\[ \langle \tilde{\Pi} \ell \text{grad} \psi, \tilde{C}_h \rangle = \langle \text{grad} \psi, \tilde{C}_h \rangle = -\langle \psi, \text{div} \tilde{C}_h \rangle = -\langle \tilde{\Pi}^0 \psi, \text{div} \tilde{C}_h \rangle = \langle \tilde{\text{grad}} \tilde{\Pi}^0 \psi, \tilde{C}_h \rangle \]
for all \( \psi \in V^0 \) and \( \tilde{C}_h \in V^1_h \), which shows that \( \tilde{\Pi} \ell \text{grad} = \text{grad} \tilde{\Pi}^0 \) holds on \( V^0 \) (which may be taken here as \( H^1(\Omega) \)). The same argument also applies for the operators \( \text{curl} \) and \( \text{div} \). With this construction one recovers the Hamiltonian particle method of [23], with general shape functions. The discrete Poisson matrix thus takes the same form, with particle-field coupling terms encoded in block matrices \( \lambda^\ell(X) \in (\mathbb{R}^3)^{N \times N} \), \( \ell = 1, 2 \), with generic \((3 \times 1)\) blocks
\[ \lambda^\ell(X)_{p,i} = \int_\Omega A^\ell_i(x) \cdot S_{X_p}(x) \, dx \quad \text{for} \quad 1 \leq p \leq N, \quad 1 \leq i \leq N_\ell \]
which extend the corresponding matrices in [23] to the case of a general shape function \( S \).

6 Application to tensor-product spline and Fourier field solvers

In this section, we apply the above method to the case of tensor-product finite element spaces defined on cartesian domains. Following the interpolation / histogram approach of [16, 24], we review a general method for designing commuting diagrams, which is based on geometric degrees of freedom that can then be associated to finite element spaces of various types. In this article, we detail two applications, one using splines and another one using truncated Fourier spaces.

6.1 Geometric degrees of freedom with commuting properties

Let us equip the cartesian domain \( \Omega = [0, L]^3 \) with a tensor-product grid using \( M_\alpha \) nodes along each dimension \( \alpha \),
\[ x_m = (x_{1,m_1}, x_{2,m_2}, x_{3,m_3}) \quad \text{with} \quad m \in [1, M] := \prod_{\alpha=1}^{3} [1, M_\alpha]. \]
On this mesh, we consider evaluation functionals defined on the various geometric elements:
- point evaluations on the nodes
\[ \mathcal{P}_m(G) := G(x_m), \]
• edge integrals along some dimension \(1 \leq \alpha \leq 3\),

\[
\mathcal{E}_{\alpha,m}(G) := \int_{e_{\alpha,m}} G \quad \text{with} \quad \mathbf{e}_{\alpha,m} = [\mathbf{x}_{m-e_{\alpha}}, \mathbf{x}_m],
\]

(90)

• face integrals normal to some dimension \(1 \leq \alpha \leq 3\),

\[
\mathcal{F}_{\alpha,m}(G) := \int_{f_{\alpha,m}} G \quad \text{with} \quad \mathbf{f}_{\alpha,m} = [\mathbf{e}_{\alpha+1,m-e_{\alpha-1}}, \mathbf{e}_{\alpha+1,m}],
\]

(91)

• and cell integrals

\[
\mathcal{C}_m(G) := \int_{c_m} G \quad \text{with} \quad \mathbf{c}_m = [\mathbf{f}_{1,m-e_{1}}, \mathbf{f}_{1,m}],
\]

(92)

where we have denoted by \([a, b]\) the convex hull of \(a \cup b\). A set of “geometric” degrees of freedom can then be derived from these local functionals:

\[
\begin{align*}
\hat{\sigma}_m^0(\varphi) &:= \mathcal{H}_m(\varphi) & \text{for} \ \varphi \in V^0 \\
\hat{\sigma}_{\alpha,m}^1(C) &:= \mathcal{E}_{\alpha,m}(C \cdot e_{\alpha}) & \text{for} \ C \in V^1 \\
\hat{\sigma}_{\alpha,m}^2(F) &:= \mathcal{F}_{\alpha,m}(F \cdot e_{\alpha}) & \text{for} \ F \in V^2 \\
\hat{\sigma}_m^3(g) &:= \mathcal{C}_m(g) & \text{for} \ g \in V^3
\end{align*}
\]

(93)

If these degrees of freedom are associated to spaces \(V_h^\ell, 0 \leq \ell \leq 3\), of respective dimensions

\[
N_0 = N_3 = M \quad \text{and} \quad N_1 = N_2 = 3M, \quad \text{with} \quad M := M_1M_2M_3,
\]

(94)

and for which they are unisolvent, then they define a unique set of dual basis functions \(\hat{\Lambda}^\ell\) according to [59], which may also be called “geometric”: for the space \(V_0^0\) for example these basis functions correspond to the interpolatory basis associated with the nodes \(\mathbf{x}_m\), for the space \(V_3^3\) they correspond to histopolation basis functions, and for the intermediate spaces they involve a combination of both. A key property of this construction is the following.

**Lemma 3.** The degrees of freedom defined by (93) are well-defined on the domains

\[
\begin{align*}
V^0 &= W_{\text{per},1,2,3}^1, \\
V^1 &= W_{\text{per},2,3}^1 \times W_{\text{per},3,1}^1 \times W_{\text{per},1,2}^1, \\
V^2 &= W_{\text{per},1}^1 \times W_{\text{per},2}^1 \times W_{\text{per},3}^1, \\
V^3 &= L_{\text{per}}^1,
\end{align*}
\]

where we have denoted by \(L_{\text{per}}^1\) the space of \(L\)-periodic and locally \(L^1\) functions, and by

\[
\begin{align*}
W_{\text{per},1,2,3}^1 := \{G \in L_{\text{per}}^1 : \partial_1 \partial_2 \partial_3 G \in L_{\text{per}}^1\} \\
W_{\text{per},\alpha,\beta}^1 := \{G \in L_{\text{per}}^1 : \partial_\alpha \partial_\beta G \in L_{\text{per}}^1\} \\
W_{\text{per},\alpha}^1 := \{G \in L_{\text{per}}^1 : \partial_\alpha G \in L_{\text{per}}^1\}
\end{align*}
\]

(95)

anisotropic Sobolev spaces of \(W^{s,1}\) type. Moreover if the \(\sigma^\ell\) are unisolvent on the spaces \(V_h^\ell\), then the resulting projection operators \(\hat{\Pi}^\ell\) characterized by the relations (93), namely

\[
\begin{align*}
\hat{\sigma}_m^0(\hat{\Pi}^0 \varphi) &= \hat{\sigma}_m^0(\varphi) \\
\hat{\sigma}_{\alpha,m}^1(\hat{\Pi}^1 C) &= \hat{\sigma}_{\alpha,m}^1(C) \\
\hat{\sigma}_{\alpha,m}^2(\hat{\Pi}^2 F) &= \hat{\sigma}_{\alpha,m}^2(F) \\
\hat{\sigma}_m^3(\hat{\Pi}^3 g) &= \hat{\sigma}_m^3(g)
\end{align*}
\]

for all \(\alpha \in [1, 3]\), \(m \in [1, M]\),

satisfy the commuting diagram property

\[
d^\ell \Pi^\ell G = \Pi^{\ell+1} d^\ell G \quad \text{for all} \ G \in V^\ell.
\]
Proof. The fact that these degrees of freedom are well-defined on the above domains follows from standard Sobolev inequalities, see e.g. [1, Rem. 13]. The commuting diagram properties are then easy to verify by applying the Stokes formula and Lemma 2. For the gradient for instance, we consider some $\varphi \in V^0$ and compute

$$\hat{\sigma}^1_{m,\alpha}(\text{grad} \, \varphi) = \int_{e_{m,\alpha}} e_\alpha \cdot \text{grad} \, \varphi = \varphi(x_m) - \varphi(x_{m-e_\alpha}) = \hat{\sigma}^0_m(\varphi) - \hat{\sigma}^0_{m-e_\alpha}(\varphi).$$

According to Lemma 2, this specifies the gradient matrix $\hat{\sigma}^0 \in \mathbb{R}^{N_1 \times N_0}$ such that

$$\hat{\sigma}^1(\text{grad} \, \varphi) = \hat{\sigma}^0 \hat{\sigma}^0(\varphi)$$

and also implies $\text{grad} \, \hat{\Pi}^0 \varphi = \hat{\Pi}^1 \text{grad} \, \varphi$. The same argument works for the other operators. \(\square\)

In the construction above, we see that the commuting properties rely only on the geometric nature of the degrees of freedom, and not on the tensor-product structure of the grid. However, this tensor-product structure allows us to specify the form of the differential matrices. Setting $\varphi = \hat{\Lambda}^k_\ell$ in the proof of Lemma 3, we find indeed the following representation of $\hat{\Pi}^0$

$$\hat{\Pi}^0 = \begin{pmatrix} 1 & 0 & \ldots & 0 & -1 \\ -1 & 1 & 0 \\ 0 & -1 & 1 & 0 \\ \vdots & \ddots & \ddots & \ddots \\ 0 & -1 & 1 & 0 \\ 0 & -1 & 1 \\ \end{pmatrix} \in \mathbb{R}^{M_\alpha \times M_\alpha}, \quad \alpha \in [1, 3]$$

(96)

and the Kronecker matrix product is defined as $(e \otimes b \otimes a)_{m,n} = e_{m_3,n_3} b_{m_2,n_2} a_{m_1,n_1}$. In the same way, we find

$$\hat{\Pi}^1 = \begin{pmatrix} 0_M & -d_3 \otimes l_{M_2} \otimes l_{M_1} & l_{M_3} \otimes d_2 \otimes l_{M_1} \\ -l_{M_3} \otimes d_2 \otimes l_{M_1} & 0_M & -l_{M_2} \otimes d_1 \otimes l_{M_1} \\ -l_{M_3} \otimes d_2 \otimes l_{M_1} & l_{M_3} \otimes d_2 \otimes l_{M_1} & 0_M \\ \end{pmatrix}$$

and

$$\hat{\Pi}^2 = (\hat{\Pi}^0)^\top \quad (98)$$

where $0_M$ denotes the zero square matrix of size $M = M_1 M_2 M_3$. In practice, the basis functions $\hat{\Lambda}^\ell_\ell$ defined by the geometric degrees of freedom according to (59) may not be the most convenient to use, either because they have no simple expression, or because some other basis $\Lambda^\ell_\ell$ has better locality properties, or leads to simpler discrete Maxwell equations. One then needs to determine the coefficients of the geometric projections in this new practical basis, which amounts to finding degrees of freedom $\sigma^\ell_\ell$ that are dual to the practical basis functions and lead to the same projection operator $\Pi^\ell = \hat{\Pi}^\ell$ as the geometric ones. Using the stacked vector notation introduced in Section 4.1 for the geometric basis $\hat{\Lambda}^\ell$ and the practical basis $\Lambda^\ell$, these new degrees of freedom $\sigma^\ell$ are characterized by the relations

$$(\sigma^\ell(G))^\top \Lambda^\ell = \Pi^\ell G = \hat{\Pi}^\ell G = (\sigma^\ell(G))^\top \Lambda^\ell \quad \text{for all } G \in V^\ell.$$
Introducing the matrix $K^\ell = \hat{\sigma}^\ell(A^\ell) = (\hat{\sigma}^\ell_m(\Lambda^\ell_k))_{1 \leq m,k \leq N^\ell}$ such that $A^\ell = (K^\ell)^\top \hat{K}^\ell$, this yields

$$\sigma^\ell(G) = (K^\ell)^{-1} \hat{\sigma}^\ell(G),$$

which gives a practical formula for computing the coefficients of the geometric projections in the practical basis. Accordingly, the differential matrices in this new basis read

$$D^\ell = \sigma^\ell+1(d^\ell A^\ell) = \left( \sum_{i,n} (\ell+1)^{-1}\sigma^\ell+1(i_n^{\ell+1} (d^\ell \hat{\Lambda}^\ell_{m,j} A^\ell_m)) \right)_{i,j} = (K^\ell)^{-1} \hat{D}^\ell K^\ell.$$

Note that $K^0$ is a Vandermonde matrix when $A^0$ is a monomial basis. For this reason the matrices $K^\ell$ are sometimes referred to as a generalized Vandermonde matrices.

### 6.2 Compatible finite elements based on B-splines

Compatible finite elements based on splines on a Cartesian grid have been studied by Buffa, Sangalli, Vázquez and co-authors, see e.g. [8, 9], and in [23] they have been used to implement the strong Faraday GEMPIC formulation. Here we describe how spline spaces can be used in conjunction with the geometric degrees of freedom described in Section 6.1.

For simplicity, we consider periodic boundaries and regular knot sequences with $M_\alpha$ knots per dimension. Denoting by $N_{p,x,k}^\alpha$ the univariate B-spline of degree $p$ along $x_\alpha$, associated with the knots $(kh_\alpha, \ldots, (k+p+1)h_\alpha)$ where $h_\alpha = \frac{L_\alpha}{M_\alpha}$, see e.g. [31], the first space in the sequence consists of tensor-product splines of multi-variate degree $(p_1, p_2, p_3)$, namely

$$V^0_h = S_{p_1,p_2,p_3} := \text{Span} \left( \{ \Lambda^0_k : k \in \llbracket 1, M \rrbracket \} \right) \quad \text{with} \quad \Lambda^0_k(x) := \prod_{\alpha=1}^3 N_{p_\alpha,x_\alpha,k_\alpha}^\alpha(x_\alpha)$$

and the full sequence reads

$$V^0_h \xrightarrow{\text{grad}} V^1_h = \begin{pmatrix} S_{p_1-1,p_2,p_3} \\ S_{p_1-1,p_2,p_3} \\ S_{p_1,p_2-1,p_3-1} \end{pmatrix} \quad \text{curl} \quad V^2_h = \begin{pmatrix} S_{p_1,p_2-1,p_3-1} \\ S_{p_1,p_2-1,p_3-1} \\ S_{p_1-1,p_2-1,p_3-1} \end{pmatrix} \quad \text{div} \quad V^3_h = S_{p_1-1,p_2-1,p_3-1}.$$

The fact that this is indeed a sequence follows from the well-known relation

$$\frac{d}{dx_\alpha} N_{p_\beta,x_\beta,k_\beta}^\beta = \frac{1}{h_\alpha} \left( N_{p_\beta,k_\beta}^{p-1} - N_{p_\beta,k_\beta+1}^{p-1} \right).$$

Introducing for convenience the scaled $B$-splines along $x_\alpha$,

$$D_{p_\beta,x_\beta,k_\beta}^\beta = \frac{1}{h_\alpha} N_{p_\beta,x_\beta,k_\beta}^{p-1}$$

yields a particularly simple formula for the derivative operator in the corresponding basis. In particular, it makes it convenient to equip the vector-valued spaces $V^1_h, V^2_h$ with the basis functions

$$\Lambda^1_{\alpha,k}(x) := e_{\alpha} D_{p_\alpha,x_\alpha,k_\alpha}^\alpha(x_\alpha) \prod_{\beta \neq \alpha} N_{p_\beta,x_\beta,k_\beta}^\beta(x_\beta) \quad \text{for} \quad \alpha \in \llbracket 1, 3 \rrbracket, \ k \in \llbracket 1, M \rrbracket,$$

$$\Lambda^2_{\alpha,k}(x) := e_{\alpha} N_{p_\alpha,x_\alpha,k_\alpha}^\alpha(x_\alpha) \prod_{\beta \neq \alpha} D_{p_\beta,x_\beta,k_\beta}^\beta(x_\beta) \quad \text{for} \quad \alpha \in \llbracket 1, 3 \rrbracket, \ k \in \llbracket 1, M \rrbracket,$$
and the last, scalar-valued space $V^3_h$ with

$$\Lambda^3_k(x) := \prod_{\alpha=1}^{3} D^{p_{\alpha}}_{\alpha,k_{\alpha}}(x) \quad \text{for } k \in [1,M].$$

In practice, B-splines are appealing because of their minimal support property, however they are not dual to the geometric degrees of freedom defined in [93] so that new degrees of freedom must be computed as described at the end of Section 6.1. For the nodal degrees of freedom, the change of basis matrix reads

$$\mathbb{K}^0_{m,k} = \hat{\sigma}^0_m(\Lambda^0_k) = \Lambda^0_k(x_m)$$

and a common choice of interpolation nodes $x_m$ consists of Greville points, which coincide with the knot sequence for regular splines of odd degrees, and with their midpoints for even degrees. More generally, we observe that $\mathbb{K}^0$ is invertible as long as the degrees of freedom $\hat{\sigma}^0$ are unisolvent, which holds iff the grid satisfies the spline interpolation condition, see e.g. [31, Th. 4.61]. Using the tensor-product structure and the locality of the B-splines, we see that the relation (102), writing e.g. interior products (46) based on the directional averaging operator (57) may be evaluated using the relation (102), writing e.g.

$$N_{\alpha,k}^\alpha(x) = \int_{x-h_{\alpha}}^{x} D_{\alpha,k}^\alpha(y) \, dy,$$

see (99), (100), we have

$$\hat{\sigma}_{\alpha,m}^1(\Lambda^1_{\alpha,k}) = \hat{\epsilon}_{\alpha,m}(\Lambda^1_{\alpha,k} \cdot e_{\alpha}) = \int_{(m_{\alpha^{-1}})h_{\alpha}}^{m_{\alpha}h_{\alpha}} D_{\alpha,k_{\alpha}}^\alpha(x) \, dx \prod_{\beta \neq \alpha} N_{\beta,k_{\beta}}^0(m_{\beta}h_{\beta}) = \Lambda^0_k(x_m) = \hat{\sigma}^0_m(\Lambda^0_k)$$

hence the matrix block $\mathbb{K}^{1,\alpha} = (\mathbb{K}^1_{(\alpha,m),(\alpha,k)})_{m,k}$ coincides with $\mathbb{K}^0$, the other blocks of $\mathbb{K}^1$ being clearly zero. Similarly we find that $\mathbb{K}^2$ and $\mathbb{K}^3$ also coincide with $\mathbb{K}^0$, so that (with obvious notation)

$$\begin{cases}
\hat{\sigma}^0(\varphi) = (\mathbb{K}^0)^{-1} \hat{\sigma}(\varphi), \\
\hat{\sigma}^{1,\alpha}(C) = (\mathbb{K}^0)^{-1} \hat{\sigma}^{1,\alpha}(C), \\
\hat{\sigma}^{2,\alpha}(F) = (\mathbb{K}^0)^{-1} \hat{\sigma}^{2,\alpha}(F), \\
\hat{\sigma}^3(g) = (\mathbb{K}^0)^{-1} \hat{\sigma}^3(g).
\end{cases}$$

From relation (99) we also see that the one-dimensional derivative matrices – and hence, every $\mathbb{D}^\ell$ – are the same as for the geometric basis. As for the three-dimensional mass matrices, they are the Kronecker product of the one-dimensional mass matrices which are a circulant matrices with $2p_{\alpha} + 1$ non-zero entries per row in each dimension. Finally we note that the discrete interior products (46) based on the directional averaging operator (57) may be evaluated using the relation (102), writing e.g.

$$I_{e_{\alpha}}^0 \Lambda^1_{\beta,k}(x) = A_{h,\alpha}(\Lambda^1_{\beta,k} \cdot e_{\alpha})(x) = \frac{\delta_{\alpha,\beta}}{2h_{\alpha}} \int_{x_{\alpha} - h_{\alpha}}^{x_{\alpha} + h_{\alpha}} D_{\alpha,k_{\alpha}}^\alpha(x) \prod_{\gamma \neq \alpha} N_{\gamma,k_{\gamma}}^0(x) = \frac{\delta_{\alpha,\beta}}{2h_{\alpha}} (\Lambda^0_k \cdot e_{\alpha} + \Lambda^0_k)(x).$$

6.3 Compatible finite elements based on Fourier spaces

With periodic boundary conditions, another option is to consider a sequence of compatible finite elements made of discrete Fourier spaces. Such spectral elements are very common in particle
solvers, with particle-field interaction usually based on discrete Fourier transforms and FFT algorithms. Here we describe a coupling based on the geometric degrees of freedom described in Section 6.1. To match the dimensions of the grid, we consider spaces with \( M_\alpha = 2K_\alpha + 1 \) modes per dimension, of the form

\[
V^0_h \equiv V^1_h = \text{Span}\left( \{ \Lambda^0_k : k \in \mathbb{Z} \} \right) \quad \text{with} \quad \Lambda^0_k(x) := e^{\frac{2\pi ikx}{L}} = \prod_{\alpha=1}^{3} e^{\frac{2\pi k_{\alpha} x_{\alpha}}{L}},
\]

where we have denoted \( \mathbb{Z} = \prod_{\alpha=1}^{3} \mathbb{Z} \). These discrete spaces clearly form a de Rham sequence, as the derivative of a Fourier mode is the same mode up to a complex scaling factor.

One interesting feature of the canonical modal basis is that it leads to diagonal Maxwell equations. Indeed the differential matrices \( D^\ell \) have the same simple block and Kronecker-product structure as (96)–(98), here with diagonal one-dimensional derivative matrices

\[
d^\alpha = \frac{2\pi}{L_\alpha} \text{diag}(-K_\alpha, \cdots, 0, \cdots, K_\alpha),
\]

and the mass matrices are all diagonal due to the orthogonality of the basis functions, with \( \mathcal{M}^\ell = L^3 M_\ell \) for the chosen normalization.

However, as the modal basis is not dual to the geometric degrees of freedom from Section 6.1, we need to determine the proper change of basis formulas in order to apply the geometric interpolation-histopolation projections \( \hat{\Pi}^\ell \), as we did for the B-splines in the previous section. To do so, it is convenient to consider regular interpolation nodes \( x_m = (m_1 h_1, m_2 h_2, m_3 h_3) \), with \( h_\alpha = \frac{L_\alpha}{M_\alpha} \). The nodal change of basis matrix reads then

\[
\hat{\sigma}^0_{m,k} = \hat{\sigma}^0_m(\Lambda_k) = \Lambda_k(x_m) = \prod_{\alpha=1}^{3} e^{\frac{2\pi k_{\alpha} m_{\alpha}}{M_\alpha}},
\]

which is a standard DFT matrix as well as its inverse,

\[
(\hat{\sigma}^0)^{-1} = \left( \frac{1}{M} \prod_{\alpha=1}^{3} e^{-\frac{2\pi k_{\alpha} m_{\alpha}}{M_\alpha}} \right)_{k,m} = \frac{1}{M} (\hat{\sigma}^0)^* =: \hat{\sigma}
\]

where we remind that \( M = M_1 M_2 M_3 \), see (94). The interpolation operator in the modal basis then takes the well-known form

\[
\hat{\Pi}^0(\varphi) = \sigma^0(\varphi) \top \Lambda^0 \quad \text{with} \quad \sigma^0(\varphi) = \hat{\sigma} \sigma^0(\varphi) = \frac{1}{M} \sum_{m \in [1,M]} \varphi(x_m) \prod_{\alpha=1}^{3} e^{\frac{2\pi k_{\alpha} m_{\alpha}}{M_\alpha}}.
\]

For the other projections in the sequence we proceed similarly as in Section 6.2, noting that

\[
\int_{(m_{\alpha}-1)h_\alpha}^{m_{\alpha} h_\alpha} e^{\frac{2\pi k_{\alpha} x_{\alpha}}{L}} \, dx_\alpha = T^\alpha_{k_{\alpha}} e^{\frac{2\pi k_{\alpha} m_{\alpha}}{M_\alpha}} \quad \text{with} \quad T^\alpha_{k_{\alpha}} := \begin{cases} h_\alpha & \text{if } k_{\alpha} = 0, \\ \frac{1}{2\pi k_{\alpha}} (1 - e^{-\frac{2\pi k_{\alpha} m_{\alpha}}{M_\alpha}}) & \text{else}. \end{cases}
\]
In particular, writing \( T^\alpha := \text{diag} \left( T^\alpha_{k,k} = T^\alpha_k : k \in [-K, K] \right) \) we find \( k^{1,\alpha} = k^0 T^\alpha \) for the matrix block \( k^{1,\alpha} = (k^{1,(\alpha,m), (\alpha,k)})_{m,k} \) and similarly \( k^{2,\alpha} = k^0 T^{\alpha-1} T^{\alpha+1} \) and \( k^{3} = k^0 T^1 T^2 T^3 \). The expression of the different degrees of freedom in the modal Fourier basis reads then

\[
\begin{align*}
\sigma^0(\varphi) &= \mathbb{F} \hat{\sigma}^0(\varphi), \\
\sigma^{1,\alpha}(C) &= (T^\alpha)^{-1} \mathbb{F} \hat{\sigma}^{1,\alpha}(C), \\
\sigma^{2,\alpha}(F) &= (T^{\alpha-1} T^{\alpha+1})^{-1} \mathbb{F} \hat{\sigma}^{2,\alpha}(F), \\
\sigma^{3}(g) &= (T^1 T^2 T^3)^{-1} \mathbb{F} \hat{\sigma}^{3}(g),
\end{align*}
\]

where we note that all the \( T^\alpha \) matrices are clearly diagonal and invertible. To apply the discrete interior products \( \text{avg} \) based on directional averaging \( \text{davg} \), we finally need to evaluate

\[
(A_{h,\alpha} \Lambda^0_k(x)) = \frac{1}{2h_{\alpha}} \int_{x_{\alpha} - h_{\alpha}}^{x_{\alpha} + h_{\alpha}} e^{\frac{2\pi i k x}{L}} \, \text{d}x = \text{sinc} \left( \frac{2\pi k}{M_{\alpha}} \right) \Lambda^0_k(x)
\]

for all \( \alpha \in [1,3] \) and \( k \in [-K, K] \).

7 Numerical illustration in reduced phase space

In this section, we will show some numerical results obtained with the proposed schemes in a reduced phase space. All results are obtained with an implementation of the strong Ampère scheme within the SeLaLib library. We study the variational semi-discretization as derived in Section 2—which is energy conserving—as well as the momentum-preserving semi-discretization as derived in Section 3. For the basis of the finite element field solver, both splines and Fourier modes are considered. The shape function is chosen to be a B-spline of varying degree.

As for the time discretization, we compare a Hamiltonian splitting scheme for both space discretization methods, see Section 4.4. Only when considering the conservation properties we also provide results for the variational scheme with an energy-conserving discrete gradient time discretization. We use a time step of \( \Delta t = 0.05 \), the linear solvers use a tolerance of \( 10^{-15} \) and the nonlinear iterations in the discrete gradient method have a tolerance of \( 10^{-12} \).

7.1 Physical model

For the numerical study we consider a reduced phase space with one periodic spatial and one or two velocity dimensions, namely \( x = x_1 \in [0, L_1], \) \( v = (v_1, v_2) \in \mathbb{R}^2 \), with unknowns of the form

\[
f = f(t, x_1, v_1, v_2), \quad E = (E_1(t, x_1), E_2(t, x_1)), \quad B = B_3(t, x_1).
\]

Moreover, we simulate an electron distribution in a neutralizing ion background, which differs from the multi-species Vlasov–Maxwell system in that the average current is subtracted from the total one in order for the model to be momentum preserving. In particular, the reduced Maxwell system then reads

\[
\begin{align*}
\frac{\partial E_1(t, x_1)}{\partial t} &= -J_1(t, x_1) + \frac{1}{L_1} \int_0^{L_1} J_1(t, y_1) \, \text{d}y_1 \\
\frac{\partial E_2(t, x_1)}{\partial t} + \frac{\partial B_3(t, x_1)}{\partial x_1} &= -J_2(t, x_1) + \frac{1}{L_1} \int_0^{L_1} J_2(t, y_1) \, \text{d}y_1 \\
\frac{\partial B_3(t, x_1)}{\partial t} + \frac{\partial E_2(t, x_1)}{\partial x_1} &= 0.
\end{align*}
\]
In some cases this model will be further reduced to 1d1v phase space by skipping $v_2$, $E_2$ and $B_3$, so that the equation for $E_1$ above remains as the only field equation.

As a first test case, we consider the Weibel instability in 1d2v phase-space as studied in [23] with an initial value of

$$f(t = 0, x_1, v_1, v_2) = \frac{1}{2\pi v_{th,1} v_{th,2}} \exp \left( -\frac{1}{2} \left( \frac{v_1^2}{v_{th,1}^2} + \frac{v_2^2}{v_{th,2}^2} \right) \right), \quad x_1 \in [0, 2\pi/k),$$

$$B_3(t = 0, x_1) = \beta \cos(kx_1),$$

$$E_2(t = 0, x_1) = 0,$$

and $E_1(t = 0, x_1)$ is computed from Poisson’s equation. The parameters are set to $v_{th,1} = 0.02 \sqrt{2}$, $v_{th,2} = \sqrt{12} v_{th,1}$, $k = 1.25$, $\beta = 10^{-4}$. As a reference solution, we use a simulation with a Fourier solver with $K = 30$ modes corresponding to $M = 61$ cells (i.e., grid points), and $N = 10^5$ particles with a piecewise affine spline shape function $S$.

As a second test case, we consider the two-stream instability in 1d1v phase-space with initial value

$$f(t = 0, x_1, v_1) = (1 + \epsilon \cos(kx_1)) \frac{1}{2\sqrt{2\pi}} \left( \exp \left( -\frac{(v_1 + 2.4)^2}{2} \right) - \exp \left( -\frac{(v_1 - 2.4)^2}{2} \right) \right)$$

with parameters $\epsilon = 0.001$ and $k = 0.2$. The initial field $E_1$ is again determined from Gauss’ law. For this test case, the reference solution is also produced with a Fourier solver and a piecewise affine spline as shape function, but the grid resolution is reduced to 31 cells (and 15 modes) while the particle number is increased to $5 \cdot 10^6$. Note that this test case requires a lot more particles to produce qualitative results compared to the Weibel test case.

In Sections 7.2 to 7.4 below we study the influence of different numerical parameters using the relevant energy curves for these two test cases, namely the magnetic and electric energy, plotted in Figures 1 and 2 respectively. In Section 7.5 we finally compare the long-time conservation properties of the schemes, looking at different error curves shown in Figure 3.

### 7.2 Influence of the shape function

We first study the influence of the shape function. Here, we expect two counteracting effects: On the one hand, a higher degree of the shape function yields smoother data for the field solver which can yield better results. On the other hand, higher order smoothing kernels smear out the influence of particles which yields a damping. This latter effect is clearly seen in the simulations with $M = 7$ cells (grid points) of Figures 1a and 2a. For this coarse resolution, low order splines give rather good results whereas higher order shapes lead to a visible damping in the instability growth rate for both test cases. Increasing the number of cells to $M = 15$ while keeping the number of particles constant as in Figures 1b and 2b, we observe both effects: In this case, the degree one spline yields too noisy data for the field solver, while a degree of e.g. seven yields too high damping and an intermediate degree of four yields rather accurate results. Our results also show that when increasing also the number of particles, the choice of the shape function is of lesser importance (cf. Figures 1d and 2d).

### 7.3 Influence of the space semi-discretization

In Figures 1c 1d and 2c 2d we next compare the variational scheme presented in Section 2 with the momentum-preserving variant from Section 3. Here we use the spectral finite element
solver and a Hamiltonian splitting time discretization. With this configuration, the momentum-preserving scheme yields clearly worse results for the coarse resolution runs (in Figures 1c and 2c), as the instability growth rate is damped similarly as with higher order shape functions. With increased resolution (i.e., using twice as many cells and four times as many particles for both test cases), we find that both schemes yield rather good results for various orders of the shape function (in Figures 1d and 2d). Finally, we see in Figure 1f that the long-time accuracy of the variational semi-discretization can be significantly better than that of the momentum-preserving one: here the Weibel instability is run with a small number of particles and we find a qualitatively wrong behavior for the momentum-preserving scheme using a piecewise affine shape function, where other schemes perform correctly. In Figure 2f a similar comparison is done with the two-stream instability, using a higher particle resolution as required for this test case to produce qualitatively correct results. The long-time behavior is then found to be qualitatively good for the different schemes and shapes.

### 7.4 Influence of the finite element solver

In Figures 1e and 2e we then compare the different field solvers, namely the spectral solver and finite element solvers based on splines of degree one to three. Using a piecewise affine spline for the shape function and low resolution runs we find that the accuracy of the low order fem solver is of bad quality and it improves for higher orders and for the spectral solver. This observation holds for the two test cases.

### 7.5 Conservation properties

We now compare the conservation properties of the various methods. For this we consider long times simulations with both the variational and the momentum-preserving discretizations. For the time stepping, we consider in both cases a Hamiltonian splitting as before but we also provide the solution with an energy-conserving discrete gradient propagator for the variational scheme to show that the semi-discretization is indeed energy-conserving. Figures 3a and 3b show the relative error in energy conservation for the various runs. We can see that the energy is conserved up to the tolerance of the linear solvers for the variational scheme with an energy-conserving discrete gradient time propagator. If we use the Hamiltonian splitting instead, there is an energy error but its behavior is oscillatory and decreases with decreased time step. This is the typical behavior for such Poisson integrators. Finally, we see that the energy error is larger for the momentum-preserving scheme, in particular for the low order shape function with a low particle resolution. For the variational scheme, on the other hand, the energy error does not depend on the shape function.

Figure 3c and 3d show the error in momentum for the various methods. We can see that the momentum-preserving scheme indeed preserves momentum up to machine precision. On the other hand, for the variational scheme the error in momentum increases as soon as the nonlinear phase of the simulations starts and later flattens out at a certain level. As this error level seems to be rather independent of the propagator, and is smaller for higher order shape functions, we conjecture that it is dominated by the error in the spatial semi-discretization.

Finally the error in Gauss’ law as a function of time is shown in Figures 3e and 3f for the two test cases, respectively. We can see that all scheme preserve Gauss’ law to machine precision.
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References

[1] Douglas N. Arnold, Richard S. Falk, and Ragnar Winther. Finite element exterior calculus, homological techniques, and applications. *Acta Numerica*, 15:1–155, 2006. doi: 10.1017/S0962492906210018.

[2] Douglas N. Arnold, Richard S. Falk, and Ragnar Winther. Finite element exterior calculus: From hodge theory to numerical stability. *Bulletin of the American Mathematical Society*, 47:281–354, 2010. doi: 10.1090/S0273-0979-10-01278-4.

[3] V. I. Arnold. *Mathematical Methods of Classical Mechanics*. Springer, 1989. ISBN 9781441930873. doi: 10.1007/978-1-4757-2063-1.

[4] Franck Assous, Patrick Ciarlet, and Simon Labrunie. *Mathematical foundations of computational electromagnetism*. Applied Mathematical Sciences, Vol 198. Springer, 2018.

[5] A. Bossavit. Whitney forms: a class of finite elements for three-dimensional computations in electromagnetism. In *Physical Science, Measurement and Instrumentation, Management and Education - Reviews, IEE Proceedings A*, pages 493–500, 1988.

[6] Alain Bossavit. *Computational electromagnetism: variational formulations, complementarity, edge elements*. Academic Press, 1998.

[7] Haim Brezis. *Functional analysis, Sobolev spaces and partial differential equations*. Springer. Springer, 2010. ISBN 0387709134.

[8] Annalisa Buffa, Giancarlo Sangalli, and Rafael Vázquez. Isogeometric analysis in electromagnetics: B-splines approximation. *Computer Methods in Applied Mechanics and Engineering*, 199(17):1143–1152, 2010. doi: 10.1016/j.cma.2009.12.002.

[9] Annalisa Buffa, Judith Rivas, Giancarlo Sangalli, and Rafael Vázquez. Isogeometric discrete differential forms in three dimensions. *SIAM Journal on Numerical Analysis*, 49:818–844, 2011. doi: 10.1137/100786708.

[10] Martin Campos Pinto and E. Sonnendrücker. Gauss-compatible Galerkin schemes for time-dependent Maxwell equations. *Mathematics of Computation*, 85:2651–2685, 2016.

[11] Martin Campos Pinto and Eric Sonnendrücker. Compatible Maxwell solvers with particles I: conforming and non-conforming 2d schemes with a strong Ampere law. *The SMAI journal of computational mathematics*, 3:53–89, 2017. doi: 10.5802/smai-jcm.20. URL smai-jcm.centre-mersenne.org/item/SMAI-JCM_2017__3__53_0/.

[12] Martin Campos Pinto, Sébastien Jund, Stéphanie Salmon, and Eric Sonnendrücker. Charge conserving FEM-PIC schemes on general grids. *Comptes Rendus Mecanique*, 342(10-11):570–582, 2014. doi: 10.1016/j.crme.2014.06.011.
[13] Nicolas Crouseilles, Lukas Einkemmer, and Erwan Faou. Hamiltonian splitting for the Vlasov–Maxwell equations. *Journal of Computational Physics*, 283:224–240, 2015. doi: 10.1016/j.jcp.2014.11.029.

[14] James W. Eastwood. The virtual particle electromagnetic particle-mesh method. *Computer Physics Communications*, 64(2):252–266, 1991. doi: 10.1016/0010-4655(91)90036-K.

[15] Evstati G. Evstatiev and Bradley A. Shadwick. Variational formulation of particle algorithms for kinetic plasma simulations. *Journal of Computational Physics*, 245:376–398, 2013. doi: 10.1016/j.jcp.2013.03.006.

[16] Marc Gerritsma. Edge functions for spectral element methods. In *Spectral and High Order Methods for Partial Differential Equations*, pages 199–207. Springer, Heidelberg, 2011.

[17] Robert T. Glassey. *The Cauchy problem in kinetic theory*. Society for Industrial and Applied Mathematics (SIAM). Society for Industrial and Applied Mathematics (SIAM), 1996. ISBN 0-89871-367-6.

[18] Ernst Hairer, Christian Lubich, and Gerhard Wanner. *Geometric Numerical Integration*. Springer, 2006.

[19] Yang He, Hong Qin, Yajuan Sun, Jianyuan Xiao, Ruili Zhang, and Jian Liu. Hamiltonian integration methods for Vlasov–Maxwell equations. *Physics of Plasmas*, 22:124503, 2015. doi: 10.1063/1.4938034.

[20] Ralf Hiptmair. Finite elements in computational electromagnetism. *Acta Numerica*, 11: 237–339, 2002.

[21] Katharina Kormann and Eric Sonnendrücker. Energy-conserving time propagation for a structure-preserving particle-in-cell Vlasov–Maxwell solver. *Journal of Computational Physics*, 425:109890, 2020.

[22] Michael Kraus. *Variational Integrators in Plasma Physics*. PhD thesis, Technische Universität München, 2013. [arXiv:1307.5665](https://arxiv.org/abs/1307.5665).

[23] Michael Kraus, Katharina Kormann, Philip J. Morrison, and Eric Sonnendrücker. GEM-PIC: Geometric electromagnetic particle-in-cell methods. *Journal of Plasma Physics*, 83 (4), 2017.

[24] Jasper Kreeft, Artur Palha, and Marc Gerritsma. Mimetic framework on curvilinear quadrilaterals of arbitrary order, 2011.

[25] H. Ralph Lewis. Energy-conserving numerical approximations for Vlasov plasmas. *Journal of Computational Physics*, 6(1):136–141, 1970. doi: 10.1016/0021-9991(70)90012-4.

[26] H. Ralph Lewis. Variational algorithms for numerical simulation of collisionless plasma with point particles including electromagnetic interactions. *Journal of Computational Physics*, 10(3):400–419, 1972. doi: 10.1016/0021-9991(72)90044-7.

[27] Francis E. Low. A Lagrangian Formulation of the Boltzmann-Vlasov Equation for Plasmas. In *Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences*, volume 248, pages 282–287, 1958. doi: 10.1098/rspa.1958.0244.
[28] Jerrold E. Marsden and Alan Weinstein. The Hamiltonian structure of the Maxwell–Vlasov equations. *Physica D: Nonlinear Phenomena*, 4(3):394–406, 1982. doi: 10.1016/0167-2789(82)90043-4.

[29] P. Monk. An analysis of Nédélec’s method for the spatial discretization of Maxwell’s equations. *Journal of Computational and Applied Mathematics*, 47(1):101–121, 1993.

[30] Philip J. Morrison. The Maxwell–Vlasov equations as a continuous Hamiltonian system. *Physics Letters A*, 80(5–6):383–386, 1980. doi: 10.1016/0375-9601(80)90776-8.

[31] Larry Schumaker. *Spline functions: basic theory*. Cambridge University Press. Cambridge University Press, third edition, 2007.

[32] Bradley A. Shadwick, Alexander B. Stamm, and Evstati G. Evstatiev. Variational formulation of macro-particle plasma simulation algorithms. *Physics of Plasmas*, 21(5):055708, 2014. doi: 10.1063/1.4874338.

[33] Jonathan Squire, Hong Qin, and William M. Tang. Geometric integration of the Vlasov–Maxwell system with a variational particle-in-cell scheme. *Physics of Plasmas*, 19:084501, 2012. doi: 10.1063/1.4742985.

[34] Alan Weinstein and Philip J. Morrison. Comments on: The Maxwell–Vlasov equations as a continuous hamiltonian system. *Physics Letters A*, 86(4):235–236, 1981. doi: 10.1016/0375-9601(81)90496-5.

[35] Jianyuan Xiao, Hong Qin, Jian Liu, Yang He, Ruili Zhang, and Yajuan Sun. Explicit high-order non-canonical symplectic particle-in-cell algorithms for Vlasov–Maxwell systems. *Physics of Plasmas*, 22:112504, 2015. doi: 10.1063/1.4935904.

[36] Jianyuan Xiao, Hong Qin, and Jian Liu. Structure-preserving geometric particle-in-cell methods for Vlasov–Maxwell systems. *Plasma Science and Technology*, 20:110501, 2018. doi: 10.1088/2058-6272/aac3d1.
Figure 1: Weibel instability: Time evolution of the magnetic energy for various configurations. In all figures except (e), a spectral finite element solver is used and the degree of the shape function is given in the legend. In (e), the shape function is a spline of degree 1 and the legend indicates the degree of the finite element solver. The number of particles is 1000 in all figures except (d) where it is 4000. Figures (a), (b), and (e) show results with the variational scheme and figures (c),(d), and (f) compare the variational and the momentum-preserving schemes (see legend). All simulations use the Hamiltonian splitting time propagator.
Figure 2: Two-stream instability: Time evolution of the first component of the electric energy for various configurations. In all figures except (e), a spectral finite element solver is used and the degree of the spline shape is given in the legend. In (e), the shape function is a spline of degree 1 and the legend indicates the degree of the finite element solver. The number of particles is 48000 in all figures except (d) where it is 192000. Figures (a), (b), and (e) show results with the variational scheme and figures (c), (d), and (f) compare the variational and the momentum-preserving schemes (see legend). All simulations use the Hamiltonian splitting time propagator.
Figure 3: Conservation properties: energy, momentum and Gauss’ law errors are shown for long-time simulations of the Weibel instability with $N = 1000$ particles (left column) and of the two-stream instability with $N = 48000$ particles (right column). In all the runs, a spectral solver with $K = 7$ modes is used for the field.