Geometric methods for the physics of magnetised plasmas

Eric Sonnendrücker
Max-Planck-Institut für Plasmaphysik
and
Zentrum Mathematik, TU München

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Abstract

Many models in plasma physics have been shown to exhibit a Hamiltonian structure and can be derived from an action principle. This is true for the equations of motion of a particle in a given electromagnetic field, which is a finite dimensional Hamiltonian system, for which symplectic numerical integrators have been derived with a large success and a well developed theory. Many other, more complex models for plasma physics, disregarding dissipative effects, also fit into an infinite dimensional non canonical hamiltonian geometric structure. This geometric structure provides the basis for the conservation of some fundamental physics invariants like energy, momentum and some Casimir invariants like Gauss' law and div B=0. Therefore preserving it in asymptotic models, like for example the Gyrokinetic model for strongly magnetised plasmas, or numerical approximations can be very helpful. New numerical methods, like mimetic Finite Differences and Finite Element Exterior Calculus based on the discretisation of objects coming from differential geometry allow in a natural way to preserve the geometric structure of the continuous equations. Schemes derived on these concepts allow on the one hand to rederive very good well-known schemes that have previously been found in ad hoc way, like the Yee scheme for Maxwell's equations or charge conserving Particle In Cell methods. These concepts will be introduced and applied to some classical models from plasma physics: Maxwell's equations, a cold plasma model and the Vlasov-Maxwell equations.

Chapter 1

Introduction

1.1 The physics background

The context of this lecture is about analytical and numerical modeling of plasmas, which are globally neutral gases of charged particles, in particular those where there is a non negligible, and even sometimes very strong, external or self-consistent magnetic field. As we will see, this adds additional challenges compared to the purely electrostatic case. Examples of such plasmas are typically found in astrophysics and in magnetic fusion experiments.

In this lecture we will be considering a few models illustrating the different aspects we would like to emphasise. We will restrict ourselves for the sake of simplicity to non relativistic problems, which are mostly relevant for the physics problems we want to address. First the equations of motion of a charged particle of charge q and mass m in a given static electromagnetic field:

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v}, \tag{1.1}$$

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \frac{q}{m}(\mathbf{E} + \mathbf{v} \times \mathbf{B}). \tag{1.2}$$

The other main model considered on its own, will be the Maxwell equations with given sources:

$$-\frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} + \nabla \times \mathbf{B} = \mu_0 \mathbf{J}, \quad \text{(Ampère's law)} \tag{1.3}$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0, \quad \text{(Faraday's law)} \tag{1.4}$$

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}, \quad \text{(Gauss's law)} \tag{1.5}$$

$$\nabla \cdot \mathbf{B} = 0, \quad \text{(magnetic Gauss's law)} \tag{1.6}$$

in the international unit system, ϵ_0, μ_0, c being respectively the permittivity and the permeability of free space and the speed of light, verifying $\epsilon_0 \mu_0 c^2 = 1$.

Our main model for the self-consistent evolution of a plasma will be the Vlasov-Maxwell model. We are neglecting the collisions throughout this lecture as they need to be modeled separately, using in geometric models the metriplectic Ansatz [15], where the full model is composed of a conservative, symplectic, part, and a dissipative part (the collisions). The

Vlasov equation describing the evolution of the phase space density of each species of particles f_s reads

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s + \frac{q_s}{m_s}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_{\mathbf{v}} f_s = 0, \tag{1.7}$$

and is coupled with Maxwell's equations

$$\begin{aligned} -\frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} + \nabla \times \mathbf{B} &= \mu_0 \mathbf{J}, \\ \frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} &= 0, \\ \nabla \cdot \mathbf{E} &= \frac{\rho}{\varepsilon_0}, \\ \nabla \cdot \mathbf{B} &= 0. \end{aligned}$$

The source terms for Maxwell's equation, the charge density $\rho(\mathbf{x}, t)$ and the current density $\mathbf{J}(\mathbf{x}, t)$ can be expressed from the distribution functions of the different species of particles $f_s(\mathbf{x}, \mathbf{v}, t)$ using the relations

$$\begin{aligned} \rho(\mathbf{x}, t) &= \sum_s q_s \int f_s(\mathbf{x}, \mathbf{v}, t)\, \mathrm{d}\mathbf{v}, \\ \mathbf{J}(\mathbf{x}, t) &= \sum_s q_s \int f_s(\mathbf{x}, \mathbf{v}, t)\mathbf{v}\, \mathrm{d}\mathbf{v}. \end{aligned}$$

The Vlasov-Maxwell equations, when the needed collisions are added, are considered to yield a very accurate description of the evolution of a plasma for all problems of interests. But in some cases, simpler models are also useful as they provide a faster time to solution in a computer code. Often fluid models, obtained by taking a few velocity moments of the Vlasov equations, provide a good description. We will also consider in this lecture a simpler cold plasma model, which reads:

$$-\frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} + \nabla \times \mathbf{B} = \mu_0 \mathbf{J}, \tag{1.8}$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0, \tag{1.9}$$

$$\frac{\partial \mathbf{J}}{\partial t} = (\epsilon_0 \omega_p^2)\mathbf{E} - \mathbf{J} \times \omega_c, \tag{1.10}$$

where $\omega_p(\mathbf{x})$ and $\omega_c(\mathbf{x})$ are the given space dependent plasma frequency and cyclotron frequency that characterise the plasma.

The aim of the lecture is first to derive geometric numerical approximation of these models, starting with the ordinary differential equations for the motion of charged particles that will enable us to introduce geometric methods. Then we will introduce the tools of differential geometry that will be needed to properly describe our partial differential equations at the continuous level, so that a natural geometric discretisation in space can be performed leading us to a a very large semi-discrete system that has a generally non canonical Hamiltonian structure and that can then be discretised using the classical geometric methods presented in the first part.

We will at the end of the lecture derive the gyrokinetic model, which is an asymptotic reduction of the full kinetic Vlasov-Maxwell model in a strong and slowly varying external

magnetic field that is valid for studying low frequency phenomena that are well below the gyrofrequency. This model will be an example of geometric asymptotic reduction, where all the approximations are made on the Lagrangian so that the resulting models keeps the non canonical hamiltonian structure and has exact invariants, which are close to the original invariants of the Vlasov-Maxwell system in the considered regime.

1.2 What are geometric methods?

Classical numerical analysis is based on the fundamental notions of consistency and stability. First one tries to find a numerical approximation of a mathematical operator, which is close enough to this operator and converges to it when the discretisation parameter goes to zero. This yields consistency. And then one needs to make sure that the sensivity to the data is not too large, which enables to prove that the approximate solution stays close enough to the exact solution, when the discretisation parameter is small enough and for short enough times, for time dependent problems. This is related to stability. We then get error estimates of the form $\|u(t) - u_h(t)\| \leq C(T)h^p$ for an order p method.

However, if the original system has a specific structure or some symmetries or invariants, for example energy or volume or other conservation laws. Classical numerical tools do not guarantee anything about these invariants. This is where geometric methods come into play. Their aim is to construct approximation that exactly preserve some invariant, which is in general different from but close to the physical invariant. And these invariants are preserved exactly in the numerical scheme, i.e. to round-off in actual simulations. These properties help in getting much better long time simulations and are also a key property for the correct behaviour of strongly non linear simulations. For example in gravitation problems, standard numerical methods like Runge-Kutta do not conserve energy: with explicit Runge-Kutta methods the orbit becomes larger than the actual orbit for explicit method and smaller for implicit methods that are dissipative. Of course higher order methods enable to keep closer to right orbit for a longer time. On the other hand energy preserving or symplectic integrator stay close to the exact orbit for all time, even though the phase error can become large especially for low order methods. An example where local conservation properties play an essential role is nonlinear conservation laws where it is well-known that only locally conservative methods can accurately capture shock formation and get the correct shock velocity. For Partial Differential Equations (PDEs), geometric methods are based on having an exact expression of Stokes theorem on all the parts of the grid: e.g. in 3D for any edge $C = [A, B]$ of the grid

$$\int_C \nabla\phi \cdot \, \mathrm{d}\boldsymbol{\ell} = \int_{\partial C} \phi = \phi(B) - \phi(A),$$

on any face of the grid

$$\int_S \nabla \times \, \mathbf{A} \cdot \, \mathrm{d}\mathbf{S} = \int_{\partial S} \mathbf{A} \cdot \, \mathrm{d}\boldsymbol{\ell},$$

and on any volume of the grid

$$\int_V \nabla \cdot \, \mathbf{B} \, \mathrm{d}V = \int_{\partial V} \mathbf{B} \cdot \, \mathrm{d}\mathbf{S}.$$

These relation can be discretised exactly by using adequate discrete objects, which are not only point values like in classical numerical methods, but also edge integrals, face integrals

and volume integrals. Then approximations will be needed to properly related objects of this kind in the physics models. *The methods that have these features are called geometric because the natural tools for describing them are those of differential geometry.*

The classical language of vector calculus gives the same name to geometrically different objects and hence is not precise enough to automatically derive an appropriate geometric discretisation. Indeed in a 3 dimensional space a scalar field can either be a 0-form or a 3 form and a vector field can either be a 1-form or a 2-form. For this reason, some formalism from differential geometry is necessary to be able to systematically find the correct geometric discretisation. However, we will try to make this lecture as accessible as possible to practitioners and only introduce the concepts and tools that are needed to find the geometric discrete representation of a field, without introducing more abstractions than necessary.

Chapter 2

Variational principles

2.1 Motion of a particle in a electrostatic field

2.1.1 Newton's equations of motion

Consider a given electrostatic field $\mathbf{E} = -\nabla\phi$. The equations of motion of a particle of charge q and mass m can be derived from Newton's law:

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v} \tag{2.1}$$

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -\frac{q}{m}\nabla\phi. \tag{2.2}$$

These equations depend on the coordinate system, even though the motion of a particle between two points can be seen geometrically as a path (a curve) that is a geometric object, that is the same independently of the coordinate system used to represent it. Is there also a way to obtain a geometric description of the motion, which is independent of the coordinate system being used?

2.1.2 Coordinate system and motion

Consider $U \subset \mathbb{R}^n$ an n-dimensional space endowed with an origin O and a, possibly position dependent, coordinate system $(\mathbf{e}_1, \ldots, \mathbf{e}_n)$. Then any point M in U is characterised by the vector $\mathbf{r} = \overrightarrow{OM}$ and its coordinates $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_n)^\top$, such that

$$\mathbf{r} = \sum_{i=1}^{n} \alpha_i \mathbf{e}_i.$$

We use the $(\,)^\top$ notation to indicate that $\boldsymbol{\alpha}$ is a column vector.

Examples:

1. Cartesian coordinates in $\mathbb{R}^2$: $\mathbf{e}_x = (1,0)^\top$, $\mathbf{e}_y = (0,1)^\top$. Then $\mathbf{r} = x\mathbf{e}_1 + y\mathbf{e}_2$ so that its coordinates are $\alpha_1 = x$, and $\alpha_2 = y$.

2. Polar coordinates in $\mathbb{R}^2$: $\mathbf{e}_r = (\cos\theta, \sin\theta)^\top$, $\mathbf{e}_\theta = (-\sin\theta, \cos\theta)^\top$. Then $\mathbf{r} = r\mathbf{e}_1$ and its coordinates are $\alpha_1 = r$, $\alpha_2 = 0$.

A motion in U can be viewed as curve parametrised by time, also called a path:

$$\gamma = \{\mathbf{r}(t) : \ t_0 \leq t \leq t_1\}.$$

The curve is the geometric object and the path its parametrisation. A same curve can correspond to several different parametrisations.

The velocity vector and the acceleration vector of the motion at the point $\mathbf{r}(t)$ are defined by

$$\dot{\mathbf{r}} = \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}(t), \qquad \ddot{\mathbf{r}}(t) = \frac{\mathrm{d}^2\mathbf{r}}{\mathrm{d}t^2}.$$

In cartesian coordinates the components of the velocity vector are simply $(\dot{x}, \dot{y})$ as the basis vectors are constant, but in curvilinear coordinates the basis vector also needs to be derived. For example in polar coordinates

$$\dot{\mathbf{r}}(t) = \frac{\mathrm{d}r}{\mathrm{d}t}\mathbf{e}_r + r(t)\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{e}_r = \dot{r}(t)\mathbf{e}_r + r(t)\begin{pmatrix} -\dot{\theta}(t)\sin\theta(t) \\ \dot{\theta}(t)\cos\theta(t) \end{pmatrix} = \dot{r}(t)\mathbf{e}_r + r(t)\dot{\theta}(t)\mathbf{e}_\theta,$$

so that the components of the velocity vector are $(\dot{r}, r\dot{\theta})$.

Notations: The vector containing the derivatives of a scalar function F with respect to the variables q_i, the gradient, has two classical notations in the literature:

$$\nabla_{\mathbf{q}} F = \frac{\partial F}{\partial \mathbf{q}} = \begin{pmatrix} \frac{\partial F}{\partial q_1} \\ \vdots \\ \frac{\partial F}{\partial q_n} \end{pmatrix}.$$

We will use both in this lecture. $\nabla_{\mathbf{q}}$ (or $\frac{\partial}{\partial \mathbf{q}}$) can be though of as a column vector with components $\frac{\partial}{\partial q_1}, \ldots, \frac{\partial}{\partial q_n}$. For two vectors $\mathbf{F}, \mathbf{G}$, we denote by $\mathbf{FG}$ their tensor product which is the matrix with components $(F_i G_j)_{i,j}$. So for a vector field

$$\mathbf{F}(\mathbf{q}) = \begin{pmatrix} F_1(q_1, \ldots, q_n) \\ \vdots \\ F_n(q_1, \ldots, q_n) \end{pmatrix}.$$

$\nabla_{\mathbf{q}}\mathbf{F}$ is considered to be the tensor product of the vector $\nabla_{\mathbf{q}}$ and the vector $\mathbf{F}$. This writes explicitly

$$\nabla_{\mathbf{q}}\mathbf{F} = \frac{\partial \mathbf{F}}{\partial \mathbf{q}} = \begin{pmatrix} \frac{\partial F_1}{\partial q_1} & \cdots & \frac{\partial F_n}{\partial q_1} \\ \vdots & & \vdots \\ \frac{\partial F_1}{\partial q_n} & \cdots & \frac{\partial F_n}{\partial q_n} \end{pmatrix} = (D\mathbf{F})^\top,$$

where $(D\mathbf{F})$ is the Jacobian matrix of $\mathbb{F}$.

2.1.3 Derivation of the Euler-Lagrange equations

We define the Lagrangian $L = K - U$ of a mechanical system as being the difference of the kinetic energy of the particle $K = \frac{1}{2}m|\dot{\mathbf{r}}|^2$, and the potential energy $U(\mathbf{r})$. Expression the Lagrangian in cartesian coordinates, we find

$$L(\mathbf{x}, \dot{\mathbf{x}}) = \frac{1}{2}m|\dot{\mathbf{x}}|^2 - q\phi(\mathbf{x}). \tag{2.3}$$

Let γ be any path (curve) starting at a point $\mathbf{r}_0$ and ending at a point $\mathbf{r}_1$ parametrised by $\mathbf{x}(t)$, $t_0 \leq t \leq t_1$ with $\mathbf{x}(t_0) = \mathbf{r}_0$ and $\mathbf{r}(t_1) = \mathbf{x}_1$. We then define the action integral as $\mathcal{A}(\gamma) = \int_\gamma L$. For practical calculation, we define the action integral in some coordinate system

$$\mathcal{A}[\mathbf{q}] = \int_{t_0}^{t_1} L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t)\, \mathrm{d}t. \tag{2.4}$$

Hamilton's least action principle states that the motion of a mechanical system coincides with extremal paths of the action integral. In order to find the extremal paths, we shall consider small variations of the action integral along an arbitrary direction $\mathbf{h}(t)$ at each point, with $\mathbf{h}(t)$ bounded, and define the directional derivative of a functional $F : \mathbb{R}^n \to \mathbb{R}$, for $\mathbf{q}, \mathbf{h} \in \mathbb{R}^n$ we define

$$\delta F(\mathbf{q}; \mathbf{h}) = \mathbf{h} \cdot \nabla_{\mathbf{q}} F(\mathbf{q}) = \mathbf{h} \cdot \frac{\partial F}{\partial \mathbf{q}}(\mathbf{q}) = \lim_{\epsilon \to 0} \frac{F[\mathbf{q} + \epsilon \mathbf{h}] - F[\mathbf{q}]}{\epsilon} = \left. \frac{\mathrm{d}}{\mathrm{d}\epsilon} \right|_{\epsilon=0} F[\mathbf{q} + \epsilon \mathbf{h}].$$

Let ϵ be a small parameter. Then, performing a Taylor expansion in ϵ of the Lagrangian on the displaced path

$$\begin{aligned} L(\mathbf{q}(t) + \epsilon \mathbf{h}(t), \dot{\mathbf{q}}(t) + \epsilon \dot{\mathbf{h}}(t), t) = L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t) + \epsilon \mathbf{h} \cdot \nabla_{\mathbf{q}} L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t) \\ + \epsilon \frac{\mathrm{d}\mathbf{h}}{\mathrm{d}t} \cdot \nabla_{\dot{\mathbf{q}}} L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t) + O(\epsilon^2) \end{aligned}$$

Note that $\nabla_{\dot{\mathbf{q}}}$ is the gradient with respect to the variables in $\dot{\mathbf{q}}$ which is considered independent from $\mathbf{q}$. Then we get

$$\frac{\mathcal{A}[\mathbf{x} + \epsilon \mathbf{y}] - \mathcal{A}[\mathbf{x}]}{\epsilon} = \frac{1}{\epsilon} \int_{t_0}^{t_1} \left[L(\mathbf{q}(t) + \epsilon \mathbf{h}(t), \dot{\mathbf{q}}(t) + \epsilon \dot{\mathbf{h}}(t), t) - L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t) \right] \mathrm{d}t, \tag{2.5}$$

$$= \int_{t_0}^{t_1} \mathbf{y} \cdot \left[\nabla_{\mathbf{q}} L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t) - \frac{\mathrm{d}}{\mathrm{d}t} \nabla_{\dot{\mathbf{q}}} L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t) \right] \tag{2.6}$$

$$+ \left[\mathbf{h}(t) \cdot \nabla_{\dot{\mathbf{q}}} L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t) \right]_{t_0}^{t_1} + O(\epsilon). \tag{2.7}$$

integrating the second term by parts and using that the boundary term vanishes as the path extremities are fixed, so that $\mathbf{h}(t_0) = \mathbf{h}(t_1) = 0$. Taking the limit when $\epsilon \to 0$, we find that the extrema of the action integral are achieved when

$$\frac{\mathrm{d}}{\mathrm{d}t} \nabla_{\dot{\mathbf{q}}} L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t) = \nabla_{\mathbf{q}} L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t).$$

These equations are called the *Euler-Lagrange equations of the action principle* that also read, using the alernative notation for the gradients:

$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{\mathbf{q}}}(\mathbf{q}(t), \dot{\mathbf{q}}(t), t) = \frac{\partial L}{\partial \mathbf{q}}(\mathbf{q}(t), \dot{\mathbf{q}}(t), t). \tag{2.8}$$

We observe that this derivation of the Euler-Lagrange equations which are the equations of motion is purely geometric and consists in finding the path that minimises the variations and is true for any coordinate system $\mathfrak{q}$, provided of course the Lagrangian is properly defined with respect to these coordinates. The choice of the coordinate system, or parametrisation, appears in the definition of the Lagrangian.

Definition 1 *The generalised momentum is defined from the Lagrangien by*

$$\mathbf{p}(t) = \frac{\partial L}{\partial \dot{\mathbf{q}}}(\mathbf{q}(t), \dot{\mathbf{q}}(t), t).$$

The Euler-Lagrange equations can then also be written equivalently

$$\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = \frac{\partial L}{\partial \dot{\mathbf{q}}}(\mathbf{q}(t), \dot{\mathbf{q}}(t), t). \tag{2.9}$$

Example 2: In cartesian coordinates, for the Lagrangian (2.3), $L(\mathbf{x}, \dot{\mathbf{x}}) = \frac{1}{2}m|\dot{\mathbf{x}}|^2 - q\phi(\mathbf{x})$, where $\mathbf{q} = \mathbf{x}$, we get the Euler-Lagrange equations

$$\frac{\mathrm{d}(m\dot{\mathbf{x}})}{\mathrm{d}t} = -q\nabla\phi.$$

Then setting $\mathbf{v} = \dot{\mathbf{x}}$, we recover (2.1)–(2.2). Moreover the generalised momentum is the physical momentum

$$\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{x}}} = m\mathbf{v}.$$

Example 2: Consider now a parametrisation in polar coordinates (r, θ). The basis vectors are then

$$\mathbf{e}_r = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}, \quad \mathbf{e}_\theta = \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix}.$$

Then a point on a curve will be of the form $\mathbf{r}(t) = r(t)\mathbf{e}_r(t)$ so that $\dot{\mathbf{r}} = \dot{r}\mathbf{e}_r + r\dot{\theta}\mathbf{e}_\theta$ and the kinetic energy is $\frac{1}{2}m|\dot{\mathbf{r}}|^2 = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2)$. Assuming that we have a central force field, *i.e.* that the potential only depends on r, the Lagrangian in polar coordinates writes, denoting by $\mathbf{q} = (r, \theta)^\top$ and $\dot{\mathbf{q}} = (\dot{r}, \dot{\theta})^\top$

$$L(\mathbf{q}, \dot{\mathbf{q}}) = L(r, \theta, \dot{r}, \dot{\theta}) = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) - q\phi(r). \tag{2.10}$$

The generalised momentum is in this case

$$\frac{\partial L}{\partial \dot{\mathbf{q}}} = \begin{pmatrix} m\dot{r} \\ mr^2\dot{\theta} \end{pmatrix},$$

and the Euler-Lagrange equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} m\dot{r} \\ mr^2\dot{\theta} \end{pmatrix} = \frac{\partial L}{\partial \mathbf{q}} = \begin{pmatrix} mr\dot{\theta}^2 - q\frac{\mathrm{d}\phi(r)}{\mathrm{d}r} \\ 0 \end{pmatrix}.$$

Remark 1 *We observe here a general feature of the Euler-Lagrange equations. If a coordinate does not appear in the Lagrangian (here θ), then the corresponding component of the generalised momentum $\frac{\partial L}{\partial \dot{\theta}}$ is a constant of motion. Such a coordinate is called* cyclic.

2.1.4 Hamilton's canonical equations

Definition 2 *Given a Lagrangian $L(\mathbf{q}, \dot{\mathbf{q}}, t)$ such that the equation defining the canonical momentum $\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{q}}}$ defines, for a given $\mathbf{q}$, an invertible bijection between $\mathbf{p}$ and $\dot{\mathbf{q}}$, we can define the associated Hamiltonian by*

$$H(\mathbf{q}, \mathbf{p}, t) = \mathbf{p} \cdot \dot{\mathbf{q}} - L(\mathbf{q}, \dot{\mathbf{q}}, t). \tag{2.11}$$

The transform going from L to H is called a Legendre transform.

Example: Consider a Lagrangian based on a general quadratic kinetic energy $L(\mathbf{q}, \dot{\mathbf{q}}) = \frac{1}{2}\dot{\mathbf{q}} \cdot M(\mathbf{q})\dot{\mathbf{q}} - U(\mathbf{q})$, where $M(\mathbf{q})$ is a symmetric positive definite matrix. Then $\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{q}}} = M(\mathbf{q})\dot{\mathbf{q}}$. So that $\dot{\mathbf{q}} = M(\mathbf{q})^{-1}\mathbf{p}$, establishing the needed bijection between $\mathbf{p}$ and $\dot{\mathbf{q}}$. In the case if the electrostatic one particle Lagrangian (2.3), we just have $\mathbf{p} = m\dot{\mathbf{x}}$, which is also clearly an invertible transform.

Theorem 1 *The Euler-Lagrange equations derived from the Lagrangian L are equivalent to the Hamilton equations*

$$\frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} = \nabla_{\mathbf{p}} H \tag{2.12}$$

$$\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = -\nabla_{\mathbf{q}} H \tag{2.13}$$

with $H(\mathbf{q}, \mathbf{p}, t) = \mathbf{p} \cdot \dot{\mathbf{q}} - L(\mathbf{q}, \dot{\mathbf{q}}, t)$

Proof. Considering that $\dot{\mathbf{q}}$ is a function of $(\mathbf{q}, \mathbf{p})$ and using the chain rule and the definition $\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{q}}}$, the partial derivatives of H defined by (2.11) verify:

$$\frac{\partial H}{\partial q_i} = \sum_{j=1}^{d} (p_j \frac{\partial \dot{q}_j}{\partial q_i}) - \frac{\partial L}{\partial q_i} - \sum_{j=1}^{d} \frac{\partial \dot{q}_j}{\partial q_i} \frac{\partial L}{\partial \dot{q}_j} = -\frac{\partial L}{\partial q_i}$$

$$\frac{\partial H}{\partial p_i} = \dot{q}_i + \sum_{j=1}^{d} \left(p_j \frac{\partial \dot{q}_j}{\partial p_i} - \frac{\partial \dot{q}_j}{\partial p_i} \frac{\partial L}{\partial \dot{q}_j} \right) = \dot{q}_i$$

where we used $p_j = \frac{\partial L}{\partial \dot{q}_j}$ in both. The second equality directly yields (2.12), and the first equation induces that the Euler-Lagrange equation $\frac{\mathrm{d}p_i}{\mathrm{d}t} = \frac{\partial L}{\partial q_i}$ is equivalent to $\frac{\mathrm{d}p_i}{\mathrm{d}t} = -\frac{\partial H}{\partial q_i}$, which yields (2.13). ∎

Let us observe that Hamilton's equation can also be written denoting by $\mathbf{z} = (q_1, \ldots, q_n, p_1, \ldots, p_n)$, the $2n$ variables together

$$\frac{\mathrm{d}\mathbf{z}}{\mathrm{d}t} = \mathcal{J} \nabla_{\mathbf{z}} H, \quad \text{with } \mathcal{J} = \mathcal{J}_c = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix} \tag{2.14}$$

where I_n is the n-dimensional identity matrix. This is called a *canonical Hamiltonian system.* Then for any functional $G : \mathbb{R}^n \to \mathbb{R}$, we have

$$\frac{\mathrm{d}G(\mathbf{z}(t))}{\mathrm{d}t} = \nabla_{\mathbf{z}} G \cdot \frac{\mathrm{d}\mathbf{z}}{\mathrm{d}t} = (\nabla_{\mathbf{z}} G)^\top \mathcal{J} \nabla_{\mathbf{z}} H = \nabla_{\mathbf{q}} G \cdot \nabla_{\mathbf{p}} H - \nabla_{\mathbf{p}} G \cdot \nabla_{\mathbf{q}} H.$$

Definition 3 *The* canonical Poisson bracket *of two functionals $F, G : \mathbb{R}^n \to \mathbb{R}$ is defined by*

$$\{F, G\} = \nabla_{\mathbf{q}} F \cdot \nabla_{\mathbf{p}} G - \nabla_{\mathbf{p}} F \cdot \nabla_{\mathbf{q}} G.$$

It is then straightforward to prove the following

Proposition 1 *Hamilton's equation* (2.12)–(2.13) *are equivalent to*

$$\frac{\mathrm{d}G(\mathbf{z}(t))}{\mathrm{d}t} = \{G, H\}, \quad \forall G \in C^1(\mathbb{R}^n).$$

Theorem 2 *If the Hamiltonian does not depend explicitly on t i.e. if* $\frac{\partial H}{\partial t} = 0$*, it is conserved by Hamilton's equations:*

$$\frac{\mathrm{d}}{\mathrm{d}t} H(\mathbf{q}, \mathbf{p}) = 0.$$

Proof. Using the chain rule and (2.12)–(2.13), we find

$$\frac{\mathrm{d}}{\mathrm{d}t} H(\mathbf{q}, \mathbf{p}) = \frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} \cdot \nabla_{\mathbf{q}} H + \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} \cdot \nabla_{\mathbf{p}} H = \nabla_{\mathbf{p}} H \cdot \nabla_{\mathbf{q}} H - \nabla_{\mathbf{q}} H \cdot \nabla_{\mathbf{p}} H = 0.$$

■

Definition 4 *The flow of a differential equation is the mapping* $\varphi_t : \mathbb{R}^n \to \mathbb{R}^n$, $\mathbf{z}(0) \mapsto \mathbf{z}(t)$.

An important aspect of Hamiltonian systems is that their flow preserve the volume. Denoting by $\mathbf{z} = (\mathbf{q}, \mathbf{p})$, the $2n$ variables all together. We observe that $\nabla_{\mathbf{z}} \cdot (\nabla_{\mathbf{p}} H, -\nabla_{\mathbf{q}} H)^\top = \nabla_{\mathbf{q}} \cdot \nabla_{\mathbf{p}} H - \nabla_{\mathbf{p}} \cdot \nabla_{\mathbf{q}} H = 0$. The Jacobian of the flow of the differential systems satisfying this property is conserved. This is know as the preservation of volume and Liouville's theorem.

In order to prove this theorem, we will need a Lemma on trace free matrix differential equations

Lemma 1 *Assume* Z *and* $A(Z)$ *are* $n \times n$ *matrices such that* $\operatorname{tr} A = 0$ *and that*

$$\frac{\mathrm{d}Z}{\mathrm{d}t} = A(Z)Z. \tag{2.15}$$

Then $\frac{\mathrm{d}(\det Z)}{\mathrm{d}t} = 0$*. The determinant of the matrix* Z *is an invariant of the flow.*

Proof.

$$\frac{\mathrm{d}}{\mathrm{d}t}(\det Z)(t) = \lim_{\epsilon \to 0} \frac{\det Z(t+\epsilon) - \det Z(t)}{\epsilon}.$$

But as Z satisfies (2.15),

$$\begin{aligned} Z(t+\epsilon) &= Z(t) + \epsilon A(Z(t))Z(t) + O(\epsilon^2) \\ &= (I + \epsilon A(Z(t)))Z(t) + O(\epsilon^2), \end{aligned}$$

so that

$$\begin{aligned} \det Z(t+\epsilon) &= \det(I + \epsilon A(Z(t))) \det Z(t) + O(\epsilon^2) \\ &= (1 + \epsilon \operatorname{tr} A(Z) + O(\epsilon^2)) \det Z(t) + O(\epsilon^2), \end{aligned}$$

from which it follows that

$$\frac{\mathrm{d}(\det Z)}{\mathrm{d}t} = \operatorname{tr} A(Z) = 0.$$

■

Theorem 3 (Liouville) *The flow of the differential equation*

$$\frac{\mathrm{d}\mathbf{z}}{\mathrm{d}t} = \mathbf{F}(\mathbf{z}) \tag{2.16}$$

conserves volume, i.e. the Jacobian $\det D_{\mathbf{y}} \mathbf{z}$*, if and only if* $\nabla \cdot \mathbf{F} = 0$*. This implies that if* ρ *is a solution of*

$$\frac{\partial \rho}{\partial t} + \mathbf{F} \cdot \nabla_{\mathbf{z}} \rho = 0,$$

then

$$\int_{\varphi_t(\Omega)} \rho(t, \mathbf{z}) \, \mathrm{d}\mathbf{z} = \int_{\Omega} \rho(t, \mathbf{y}) \, \mathrm{d}\mathbf{y}.$$

Proof. The flow of the differential equation maps an initial condition $\mathbf{y} \in \mathbb{R}^n$ to the value at time t, that we shall denote $\mathbf{z}(t;\mathbf{y})$ to highlight the dependence on the initial condition as well as the dependence on time. Then taking the derivative with respect to y_j of the i^{th} component of (2.16), we find

$$\frac{\partial^2 z_i}{\partial t \partial y_j} = \frac{\partial}{\partial y_j}(F_i(\mathbf{z}(t;\mathbf{y}))) = \sum_{k=1}^{n} \frac{\partial z_k}{\partial y_j}\frac{\partial F_i}{\partial z_k}.$$

Hence the Jacobian matrix of $\mathbf{z}$ with respect to $\mathbf{y}$ denoted by $D_{\mathbf{y}}\mathbf{z}$ verifies the differential equation

$$\frac{\mathrm{d}D_{\mathbf{y}}\mathbf{z}}{\mathrm{d}t} = D_{\mathbf{z}}\mathbf{F}(\mathbf{t};\mathbf{y})D_{\mathbf{y}}\mathbf{z}.$$

Moreover $\operatorname{tr} D_{\mathbf{z}}\mathbf{F}(\mathbf{t};\mathbf{y}) = \nabla \cdot \mathbf{F} = 0$. This is exactly the setting of Lemma 1, so that the Jacobian of the flow $\det D_{\mathbf{y}}\mathbf{z}$ is conserved.

Making the change of variables $\mathbf{z} = \mathbf{z}(t;\mathbf{y}) = \varphi_t(\mathbf{y})$, whose Jacobian is one, due to the previous relation, we get the equality of the integrals. ∎

A last stronger property of the Hamiltonian flow is that it is symplectic:

Definition 5 *A linear transformation $A : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ is called symplectic if $A^\top \mathcal{J} A = \mathcal{J}$.*

Theorem 4 *A canonical hamiltonian flow is symplectic,* i.e *if $\mathbf{z}(t;\mathbf{y})$ is a solution of* (2.14) *with initial condition $\mathbf{y}$ then the linear transformation $D_{\mathbf{y}}\mathbf{z}$ is symplectic.*

Proof. As we saw in the previous proof $D_{\mathbf{y}}\mathbf{z}$ is a solution of the matrix differential equation:

$$\frac{\mathrm{d}D_{\mathbf{y}}\mathbf{z}}{\mathrm{d}t} = D_{\mathbf{z}}\mathbf{F}(\mathbf{t};\mathbf{y})D_{\mathbf{y}}\mathbf{z}.$$

with now because of the structure of $\mathbf{F}$

$$D_{\mathbf{z}}\mathbf{F}(\mathbf{t};\mathbf{y}) = \begin{pmatrix} \nabla_{\mathbf{q}}\nabla_{\mathbf{p}}H & \nabla_{\mathbf{p}}\nabla_{\mathbf{p}}H \\ -\nabla_{\mathbf{q}}\nabla_{\mathbf{q}}H & -\nabla_{\mathbf{q}}\nabla_{\mathbf{p}}H \end{pmatrix}.$$

Hence

$$\frac{\mathrm{d}}{\mathrm{d}t}(D_{\mathbf{y}}\mathbf{z}^\top \mathcal{J} D_{\mathbf{y}}\mathbf{z}) = \frac{\mathrm{d}}{\mathrm{d}t}(D_{\mathbf{y}}\mathbf{z}^\top)\mathcal{J}D_{\mathbf{y}}\mathbf{z} + D_{\mathbf{y}}\mathbf{z}^\top \mathcal{J}\frac{\mathrm{d}}{\mathrm{d}t}(D_{\mathbf{y}}\mathbf{z}).$$

This yields by explicit computation, using the differential equation above verified by $D_{\mathbf{y}}\mathbf{z}$ and the explicit form of $D_{\mathbf{z}}\mathbf{F}(\mathbf{t};\mathbf{y})$

$$\frac{\mathrm{d}}{\mathrm{d}t}(D_{\mathbf{y}}\mathbf{z})^\top \mathcal{J} D_{\mathbf{y}}\mathbf{z}) = (D_{\mathbf{y}}\mathbf{z})^\top(\nabla_{\mathbf{z}}\nabla_{\mathbf{z}}H)D_{\mathbf{y}}\mathbf{z} - (D_{\mathbf{y}}\mathbf{z})^\top(\nabla_{\mathbf{z}}\nabla_{\mathbf{z}}H)D_{\mathbf{y}}\mathbf{z} = 0,$$

where we denote the Hessian matrix of H by

$$\nabla_{\mathbf{z}}\nabla_{\mathbf{z}}H = \begin{pmatrix} \nabla_{\mathbf{q}}\nabla_{\mathbf{q}}H & \nabla_{\mathbf{q}}\nabla_{\mathbf{p}}H \\ \nabla_{\mathbf{q}}\nabla_{\mathbf{p}}H & \nabla_{\mathbf{p}}\nabla_{\mathbf{p}}H \end{pmatrix}.$$

From this it follows that

$$(D_{\mathbf{y}}\mathbf{z}(t))^\top \mathcal{J} D_{\mathbf{y}}\mathbf{z}(t) = (D_{\mathbf{y}}\mathbf{z}(0))^\top \mathcal{J} D_{\mathbf{y}}\mathbf{z}(0) = \mathcal{J},$$

as $\mathbf{z}(0) = \mathbf{y}$ so that $D_{\mathbf{y}}\mathbf{z}(0)$ is the identity matrix. ∎

2.2 Motion of a particle in an electromagnetic field

2.2.1 Newton's equations of motion

Consider a given electromagnetic field $\mathbf{E}(t,\mathbf{x}), \mathbf{B}(t,\mathbf{x})$. The equations of motion of a particle of charge q and mass m can be derived from Newton's law, the acceleration being given by the Lorentz force

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v} \tag{2.17}$$

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \frac{q}{m}(\mathbf{E} + \mathbf{v} \times \mathbf{B}). \tag{2.18}$$

2.2.2 Action principle

Introducing the scalar potential ϕ and the vector potential $\mathbf{A}$ such that

$$\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} - \nabla\phi, \qquad \mathbf{A} = \nabla \times \mathbb{A}.$$

The previous equations of motion can be derived from an action principle involving the following Lagrangian:

$$L(\mathbf{x}, \dot{\mathbf{x}}) = (q\mathbf{A} + \frac{1}{2}m\dot{\mathbf{x}}) \cdot \dot{\mathbf{x}} - q\phi. \tag{2.19}$$

We have in this case

$$\nabla_{\mathbf{x}} L = q(\nabla_{\mathbf{x}}\mathbf{A} \cdot \dot{\mathbf{x}} - \nabla_{\mathbf{x}}\phi), \quad \nabla_{\dot{\mathbf{x}}} L = q\mathbf{A} + m\dot{\mathbf{x}}.$$

So that the Euler-Lagrange equations $\frac{\mathrm{d}}{\mathrm{d}t}\nabla_{\dot{\mathbf{x}}} L = \nabla_{\mathbf{x}} L$ become at $(\mathbf{x}(t), \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t}(t))$

$$q(\frac{\partial \mathbf{A}}{\partial t} + \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} \cdot \nabla_{\mathbf{x}}\mathbf{A}) + m\frac{\mathrm{d}^2\mathbf{x}}{\mathrm{d}t^2} = q(\nabla_{\mathbf{x}}\mathbf{A} \cdot \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} - \nabla_{\mathbf{x}}\phi). \tag{2.20}$$

Now, a straightforward computation component by component shows that

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} \cdot \nabla_{\mathbf{x}}\mathbf{A} - \nabla_{\mathbf{x}}\mathbf{A} \cdot \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = (\nabla \times \mathbf{A}) \times \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t},$$

so that defining $\mathbf{v} = \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t}$, (2.20) becomes

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \frac{q}{m}\left(-\frac{\partial \mathbf{A}}{\partial t} - \nabla_{\mathbf{x}}\phi + \mathbf{v} \times (\nabla \times \mathbf{A})\right) = \frac{q}{m}(\mathbf{E} + \mathbf{v} \times \mathbf{B}),$$

where we recognise the Newton equation (2.18).

2.2.3 Hamilton's equations

We start by defining the generalised momentum

$$\mathbf{p} = \nabla_{\dot{\mathbf{x}}} L(\mathbf{x}, \dot{\mathbf{x}}) = q\mathbf{A}(t, \mathbf{x}) + m\dot{\mathbf{x}}. \tag{2.21}$$

Hence $\dot{\mathbf{x}} = \mathbf{p}/m - (q/m)\mathbf{A}(t,\mathbf{x})$ So that the Hamiltonian, in canonical coordinates $(\mathbf{x},\mathbf{p})$ is defined by

$$H(\mathbf{x},\mathbf{p}) = \mathbf{p}\cdot\dot{\mathbf{x}} - L(\mathbf{x},\dot{\mathbf{x}}) = \mathbf{p}\cdot\Big(\frac{\mathbf{p}}{m} - \frac{q}{m}\mathbf{A}\Big) - \Big(q\mathbf{A} + \frac{1}{2}(\mathbf{p}-q\mathbf{A})\Big)\cdot\frac{1}{m}(\mathbf{p}-q\mathbf{A}) + q\phi$$
$$= \frac{1}{2m}(\mathbf{p}-q\mathbf{A})\cdot(\mathbf{p}-q\mathbf{A}) + q\phi,$$

and Hamilton's equations in canonical coordinates become

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \nabla_{\mathbf{p}}H = \frac{1}{m}(\mathbf{p}-q\mathbf{A}), \tag{2.22}$$
$$\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = -\nabla_{\mathbf{x}}H = \frac{q}{m}(\nabla_{\mathbf{x}}\mathbf{A})\cdot(\mathbf{p}-q\mathbf{A}) - q\nabla_{\mathbf{x}}\phi. \tag{2.23}$$

Remark 2 *We observe that when* $\mathbf{A}=0$, $H = |\mathbf{p}|^2/(2m) + q\phi(t,\mathbf{x})$ *is the sum of a term depending only on* $\mathbf{p}$ *and a term depending only on* $\mathbf{x}$ *(not on* $\mathbf{p}$*). Such a Hamiltonian is called* separable*, which is a very convenient property when designing numerical schemes, as we shall see later. This is not the case in general, when* $\mathbf{A}$ *does not vanish.*

2.2.4 The phase-space Lagrangian

Canonical coordinates have the advantage of yielding a constant symplectic structure and the simple form of Hamilton's canonical equations of motion, but on the other hand we loose the physical velocity as a variable and other nice properties. In some cases it might be more convenient to loose the canonical form and stay with the physical velocity. This can be done by considering, both $\mathbf{x}$ and $\mathbf{v}$ as independent variables in the Lagrangian (2.19) can then be replaced by the so-called *phase-space Lagrangian*. We assume here that both potentials $\mathbb{A}$ and ϕ are time independent

$$L(\mathbf{x},\mathbf{v},\dot{\mathbf{x}},\dot{\mathbf{v}},t) = (q\mathbf{A}(\mathbf{x}) + m\mathbf{v})\cdot\dot{\mathbf{x}} - (\frac{1}{2}m|\mathbf{v}|^2 + q\phi(\mathbf{x})). \tag{2.24}$$

We notice that this corresponds to $\mathbf{p}\cdot\dot{\mathbf{x}} - H$ expressed in the $(\mathbf{x},\mathbf{v})$ variables. Moreover this Lagrangian does neither explicitly depend on $\dot{\mathbf{v}}$ nor on t. In the $(\mathbf{x},\mathbf{v})$ variables, the Hamiltonian $H(\mathbf{x},\mathbf{v}) = \frac{1}{2}m|\mathbf{v}|^2 + q\phi(\mathbf{x})$ is separable.

Let us now express the Euler-Lagrange equations for $\mathbf{q} = (\mathbf{x},\mathbf{v})$. First as the Lagrangian does not depend explicitly on $\dot{\mathbf{v}}$, $\frac{\mathrm{d}}{\mathrm{d}t}\nabla_{\dot{\mathbf{v}}}L = \nabla_{\mathbf{v}}L$ writes

$$0 = \nabla_{\mathbf{v}}L = m\dot{\mathbf{x}} - m\mathbf{v},$$

and then $\frac{\mathrm{d}}{\mathrm{d}t}\nabla_{\dot{\mathbf{x}}}L = \nabla_{\mathbf{x}}L$ writes

$$\frac{\mathrm{d}}{\mathrm{d}t}(q\mathbf{A} + m\mathbf{v}) = q\nabla_{\mathbf{x}}\mathbf{A}\cdot\dot{\mathbf{x}} - q\nabla_{\mathbf{x}}\phi.$$

This is identical to (2.20) replacing $\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t}$ by $\mathbf{v}$, so that from the Euler-Lagrange equations, we directly obtain the equations of motion (2.17)–(2.18). Then, observing that $\nabla_{\mathbf{x}}H = q\nabla_{\mathbf{x}}\phi$, $\nabla_{\mathbf{v}}H = m\mathbf{v}$ and $\mathbf{v}\times\mathbf{B} = \mathbb{B}(\mathbf{x})\mathbf{v}$, with

$$\mathbb{B}(\mathbf{x}) = \begin{pmatrix} 0 & B_3 & -B_2 \\ -B_3 & 0 & B_1 \\ B_2 & -B_1 & 0 \end{pmatrix},$$

we see that

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \frac{1}{m}\nabla_{\mathbf{v}} H, \tag{2.25}$$

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \mathbb{B}(\mathbf{x})\nabla_{\mathbf{v}} H - q\nabla_{\mathbf{x}} H, \tag{2.26}$$

which can also be written in matrix form

$$\begin{pmatrix} \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} \\ \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} \end{pmatrix} = \begin{pmatrix} 0 & \frac{1}{m} I_n \\ -\frac{1}{m} I_n & \frac{q}{m^2}\mathbb{B}(\mathbf{x}) \end{pmatrix} \begin{pmatrix} \nabla_{\mathbf{x}} H \\ \nabla_{\mathbf{v}} H \end{pmatrix}, \quad \text{or grouping the variables } \frac{\mathrm{d}\mathbf{z}}{\mathrm{d}t} = \mathcal{J}(\mathbf{z})\nabla_{\mathbf{z}} H. \tag{2.27}$$

This corresponds to a non canonical Hamiltonian system, with a Poisson bracket defined by

$$\{F, G\} = \nabla_{\mathbf{z}} F \cdot \mathcal{J} \cdot \nabla_{\mathbf{z}} G = (\nabla_{\mathbf{z}} F)^\top \mathcal{J} (\nabla_{\mathbf{z}} G). \tag{2.28}$$

The matrix $\mathcal{J}$ is called *Poisson matrix*.

Definition 6 *A* Poisson bracket $\{.,.\}$ *is a bilinear form satisfying for any smooth functionals* F, G, H

(i) $\{F, G\} = -\{G, F\}$, *(skew-symmetry)*

(ii) $\{FG, H\} = F\{G, H\} + G\{F, H\}$, *(Leibniz rule)*

(iii) $\{\{F, G\}, H\} + \{\{G, H\}, F\} + \{\{H, F\}, G\} = 0$. *Jacobi identity*

Proposition 2 *If* $\nabla \cdot \mathbf{B} = 0$*, then the bracket defined by* (2.28) *is a Poisson bracket.*

Proof. It is obviously bilinear as the gradients are. It is skew-symmetric because $\mathcal{J}$ is skew-symmetric. The Leibniz rule is verified by construction

$$\{FG, H\} = (\nabla_{\mathbf{z}}(FG))^\top \mathcal{J}(\nabla_{\mathbf{z}} H) = F(\nabla_{\mathbf{z}} G)^\top \mathcal{J}(\nabla_{\mathbf{z}} H) + G(\nabla_{\mathbf{z}} F)^\top \mathcal{J}(\nabla_{\mathbf{z}} H) = F\{G, H\} + G\{F, H\}.$$

Jacobi's identity is more complex and depends on the components of $\mathcal{J}$. We shall now first verify that the Jacobi identity holds for the canonical bracket, for three smooth functions F, G and H of the variables $(\mathbf{q}, \mathbf{p})$

$$\begin{aligned}
&\{\{F, G\}_c, H\}_c = \nabla_{\mathbf{q}}(\nabla_{\mathbf{q}} F \cdot \nabla_{\mathbf{p}} G - \nabla_{\mathbf{p}} F \cdot \nabla_{\mathbf{q}} G) \cdot \nabla_{\mathbf{p}} H - \nabla_{\mathbf{p}}(\nabla_{\mathbf{q}} F \cdot \nabla_{\mathbf{p}} G - \nabla_{\mathbf{p}} F \cdot \nabla_{\mathbf{q}} G) \cdot \nabla_{\mathbf{q}} H \\
&= (\nabla_{\mathbf{q}}\nabla_{\mathbf{q}} F \cdot \nabla_{\mathbf{p}} G + \nabla_{\mathbf{q}}\nabla_{\mathbf{p}} G \cdot \nabla_{\mathbf{q}} F) \cdot \nabla_{\mathbf{p}} H - (\nabla_{\mathbf{q}}\nabla_{\mathbf{p}} F \cdot \nabla_{\mathbf{q}} G + \nabla_{\mathbf{q}}\nabla_{\mathbf{q}} G \cdot \nabla_{\mathbf{p}} F) \cdot \nabla_{\mathbf{p}} H \\
&- (\nabla_{\mathbf{p}}\nabla_{\mathbf{q}} F \cdot \nabla_{\mathbf{p}} G + \nabla_{\mathbf{p}}\nabla_{\mathbf{p}} G \cdot \nabla_{\mathbf{q}} F) \cdot \nabla_{\mathbf{q}} H + (\nabla_{\mathbf{p}}\nabla_{\mathbf{p}} F \cdot \nabla_{\mathbf{q}} G + \nabla_{\mathbf{p}}\nabla_{\mathbf{q}} G \cdot \nabla_{\mathbf{p}} F) \cdot \nabla_{\mathbf{q}} H \\
&= \underbrace{\nabla_{\mathbf{p}} H \cdot \nabla_{\mathbf{q}}\nabla_{\mathbf{q}} F \cdot \nabla_{\mathbf{p}} G}_{1} + \underbrace{\nabla_{\mathbf{p}} H \cdot \nabla_{\mathbf{q}}\nabla_{\mathbf{p}} G \cdot \nabla_{\mathbf{q}} F}_{2} + \underbrace{\nabla_{\mathbf{q}} H \cdot \nabla_{\mathbf{p}}\nabla_{\mathbf{p}} F \cdot \nabla_{\mathbf{q}} G}_{3} + \underbrace{\nabla_{\mathbf{q}} H \cdot \nabla_{\mathbf{p}}\nabla_{\mathbf{q}} G \cdot \nabla_{\mathbf{p}} F}_{4} \\
&- \underbrace{\nabla_{\mathbf{p}} H \cdot \nabla_{\mathbf{q}}\nabla_{\mathbf{q}} G \cdot \nabla_{\mathbf{p}} F}_{5} - \underbrace{\nabla_{\mathbf{p}} H \cdot \nabla_{\mathbf{q}}\nabla_{\mathbf{p}} F \cdot \nabla_{\mathbf{q}} G}_{6} - \underbrace{\nabla_{\mathbf{q}} H \cdot \nabla_{\mathbf{p}}\nabla_{\mathbf{p}} G \cdot \nabla_{\mathbf{q}} F}_{7} - \underbrace{\nabla_{\mathbf{q}} H \cdot \nabla_{\mathbf{p}}\nabla_{\mathbf{q}} F \cdot \nabla_{\mathbf{p}} G}_{8}
\end{aligned}$$

In the same way

$$\begin{aligned}
&\{\{G, H\}_c, F\}_c = \\
&\underbrace{\nabla_{\mathbf{p}} F \cdot \nabla_{\mathbf{q}}\nabla_{\mathbf{q}} G \cdot \nabla_{\mathbf{p}} H}_{5} + \underbrace{\nabla_{\mathbf{p}} F \cdot \nabla_{\mathbf{q}}\nabla_{\mathbf{p}} H \cdot \nabla_{\mathbf{q}} G}_{9} + \underbrace{\nabla_{\mathbf{q}} F \cdot \nabla_{\mathbf{p}}\nabla_{\mathbf{p}} G \cdot \nabla_{\mathbf{q}} H}_{7} + \underbrace{\nabla_{\mathbf{q}} F \cdot \nabla_{\mathbf{p}}\nabla_{\mathbf{q}} H \cdot \nabla_{\mathbf{p}} G}_{10} \\
&- \underbrace{\nabla_{\mathbf{p}} F \cdot \nabla_{\mathbf{q}}\nabla_{\mathbf{q}} H \cdot \nabla_{\mathbf{p}} G}_{11} - \underbrace{\nabla_{\mathbf{p}} F \cdot \nabla_{\mathbf{q}}\nabla_{\mathbf{p}} G \cdot \nabla_{\mathbf{q}} H}_{4} - \underbrace{\nabla_{\mathbf{q}} F \cdot \nabla_{\mathbf{p}}\nabla_{\mathbf{p}} H \cdot \nabla_{\mathbf{q}} G}_{12} - \underbrace{\nabla_{\mathbf{q}} F \cdot \nabla_{\mathbf{p}}\nabla_{\mathbf{q}} G \cdot \nabla_{\mathbf{p}} H}_{2}
\end{aligned}$$

and

$$\{\{H,F\}_c,G\}_c =$$
$$\underbrace{\nabla_{\mathbf{p}}G\cdot\nabla_{\mathbf{q}}\nabla_{\mathbf{q}}H\cdot\nabla_{\mathbf{p}}F}_{11}+\underbrace{\nabla_{\mathbf{p}}G\cdot\nabla_{\mathbf{q}}\nabla_{\mathbf{p}}F\cdot\nabla_{\mathbf{q}}H}_{8}+\underbrace{\nabla_{\mathbf{q}}G\cdot\nabla_{\mathbf{p}}\nabla_{\mathbf{p}}H\cdot\nabla_{\mathbf{q}}F}_{12}+\underbrace{\nabla_{\mathbf{q}}G\cdot\nabla_{\mathbf{p}}\nabla_{\mathbf{q}}F\cdot\nabla_{\mathbf{p}}H}_{6}$$
$$-\underbrace{\nabla_{\mathbf{p}}G\cdot\nabla_{\mathbf{q}}\nabla_{\mathbf{q}}F\cdot\nabla_{\mathbf{p}}H}_{1}-\underbrace{\nabla_{\mathbf{p}}G\cdot\nabla_{\mathbf{q}}\nabla_{\mathbf{p}}H\cdot\nabla_{\mathbf{q}}F}_{6}-\underbrace{\nabla_{\mathbf{q}}G\cdot\nabla_{\mathbf{p}}\nabla_{\mathbf{p}}F\cdot\nabla_{\mathbf{q}}H}_{3}-\underbrace{\nabla_{\mathbf{q}}G\cdot\nabla_{\mathbf{p}}\nabla_{\mathbf{q}}H\cdot\nabla_{\mathbf{p}}F}_{9}$$

When adding the three terms, we observe that the terms with the same number cancel, so that the sum is zero and Jacobi's identity is verified for the Poisson bracket.

Let us now make the change of variables $\mathbf{q}=\mathbf{x}$, $\mathbf{p}=\mathbf{P}(\mathbf{x},\mathbf{v})$. In our case we have $P(\mathbf{x},\mathbf{v})=m\mathbf{v}+q\mathbf{A}(\mathbf{x})$, but we will do the computation for a general function P, such that the change of variables is a C^1 diffeomorphism (*i.e* its Jacobian matrix is continuous an invertible). For a smooth scalar valued function $\tilde{F}(\mathbf{q},\mathbf{p})$, we define $F(\mathbf{x},\mathbf{v})=\tilde{F}(\mathbf{x},\mathbf{P}(\mathbf{x},\mathbf{v}))$, so that

$$\begin{pmatrix}\nabla_{\mathbf{x}}F\\ \nabla_{\mathbf{v}}F\end{pmatrix}=\begin{pmatrix}\nabla_{\mathbf{q}}\tilde{F}+\nabla_{\mathbf{x}}\mathbf{P}\nabla_{\mathbf{p}}\tilde{F}\\ \nabla_{\mathbf{v}}\mathbf{P}\nabla_{\mathbf{p}}\tilde{F}\end{pmatrix}=\begin{pmatrix}I_n & \nabla_{\mathbf{x}}\mathbf{P}\\ 0 & \nabla_{\mathbf{v}}\mathbf{P}\end{pmatrix}\begin{pmatrix}\nabla_{\mathbf{q}}\tilde{F}\\ \nabla_{\mathbf{p}}\tilde{F}\end{pmatrix}.$$

We observe that the inverse matrix

$$\begin{pmatrix}I_n & \nabla_{\mathbf{x}}\mathbf{P}\\ 0 & \nabla_{\mathbf{v}}\mathbf{P}\end{pmatrix}^{-1}=\begin{pmatrix}I_n & -(\nabla_{\mathbf{x}}\mathbf{P})(\nabla_{\mathbf{v}}\mathbf{P})^{-1}\\ 0 & (\nabla_{\mathbf{v}}\mathbf{P})^{-1}\end{pmatrix},$$

so that, remembering that

$$\mathcal{J}_c=\begin{pmatrix}0 & I_n\\ -I_n & 0\end{pmatrix}$$

we have

$$\left\{\tilde{F},\tilde{G}\right\}_c=\begin{pmatrix}\nabla_{\mathbf{q}}\tilde{F}\\ \nabla_{\mathbf{p}}\tilde{F}\end{pmatrix}^{\top}\mathcal{J}_c\begin{pmatrix}\nabla_{\mathbf{q}}\tilde{F}\\ \nabla_{\mathbf{p}}\tilde{F}\end{pmatrix}=\begin{pmatrix}\nabla_{\mathbf{x}}F\\ \nabla_{\mathbf{v}}F\end{pmatrix}^{\top}\begin{pmatrix}I_n & \nabla_{\mathbf{x}}\mathbf{P}\\ 0 & \nabla_{\mathbf{v}}\mathbf{P}\end{pmatrix}^{-\top}\mathcal{J}_c\begin{pmatrix}I_n & \nabla_{\mathbf{x}}\mathbf{P}\\ 0 & \nabla_{\mathbf{v}}\mathbf{P}\end{pmatrix}^{-1}\begin{pmatrix}\nabla_{\mathbf{x}}F\\ \nabla_{\mathbf{v}}F\end{pmatrix}$$
$$=\begin{pmatrix}\nabla_{\mathbf{x}}F\\ \nabla_{\mathbf{v}}F\end{pmatrix}^{\top}\begin{pmatrix}I_n & 0\\ -(\nabla_{\mathbf{v}}\mathbf{P})^{-\top}(\nabla_{\mathbf{x}}\mathbf{P})^{\top} & (\nabla_{\mathbf{v}}\mathbf{P})^{-\top}\end{pmatrix}\begin{pmatrix}0 & I_n\\ -I_n & 0\end{pmatrix}\begin{pmatrix}I_n & -(\nabla_{\mathbf{x}}\mathbf{P})(\nabla_{\mathbf{v}}\mathbf{P})^{-1}\\ 0 & (\nabla_{\mathbf{v}}\mathbf{P})^{-1}\end{pmatrix}\begin{pmatrix}\nabla_{\mathbf{x}}F\\ \nabla_{\mathbf{v}}F\end{pmatrix}$$
$$=\begin{pmatrix}\nabla_{\mathbf{x}}F\\ \nabla_{\mathbf{v}}F\end{pmatrix}^{\top}\begin{pmatrix}0 & (\nabla_{\mathbf{v}}\mathbf{P})^{-1}\\ -(\nabla_{\mathbf{v}}\mathbf{P})^{-\top} & (\nabla_{\mathbf{v}}\mathbf{P})^{-\top}(\nabla_{\mathbf{x}}\mathbf{P})(\nabla_{\mathbf{v}}\mathbf{P})^{-1}-(\nabla_{\mathbf{v}}\mathbf{P})^{-\top}(\nabla_{\mathbf{x}}\mathbf{P})^{\top}(\nabla_{\mathbf{v}}\mathbf{P})^{-1}\end{pmatrix}\begin{pmatrix}\nabla_{\mathbf{x}}F\\ \nabla_{\mathbf{v}}F\end{pmatrix}$$
$$=\begin{pmatrix}\nabla_{\mathbf{x}}F\\ \nabla_{\mathbf{v}}F\end{pmatrix}^{\top}\mathcal{J}\begin{pmatrix}\nabla_{\mathbf{x}}F\\ \nabla_{\mathbf{v}}F\end{pmatrix}=\{F,G\}$$

Indeed, in our case $\nabla_{\mathbf{x}}\mathbf{P}=\frac{1}{m}I_n$ and $\nabla_{\mathbf{v}}\mathbf{P}=q\nabla_{\mathbf{x}}\mathbf{A}$, so that

$$\begin{pmatrix}0 & (\nabla_{\mathbf{v}}\mathbf{P})^{-1}\\ -(\nabla_{\mathbf{v}}\mathbf{P})^{-\top} & (\nabla_{\mathbf{v}}\mathbf{P})^{-\top}(\nabla_{\mathbf{x}}\mathbf{P})(\nabla_{\mathbf{v}}\mathbf{P})^{-1}-(\nabla_{\mathbf{v}}\mathbf{P})^{-\top}(\nabla_{\mathbf{x}}\mathbf{P})^{\top}(\nabla_{\mathbf{v}}\mathbf{P})^{-1}\end{pmatrix}$$
$$=\begin{pmatrix}0 & \frac{1}{m}I_n\\ -\frac{1}{m}I_n & \frac{q}{m^2}(\nabla_{\mathbf{x}}\mathbf{A}-(\nabla_{\mathbf{x}}\mathbf{A}))^{\top}\end{pmatrix}=\mathcal{J}$$

as $\mathbf{B}=\nabla\times\mathbf{A}$.

It follows that the Poisson bracket is independent of the coordinate system, and the bracket identities are satisfied for our bracket, that corresponds to the canonical bracket written in the physical $(\mathbf{x},\mathbf{v})$ coordinates.

■

Remark 3 *The Jacobi identity is the key element of the Poisson bracket. It follows immediately from it that if I_1 and I_2 are invariants of the motion, then $\{I_1, H\} = \{I_2, H\} = 0$ and then using Jacobi's identity with $F = I_1$, $G = I_2$ it follows that $\{\{I_1, I_2\}, H\} = 0$, so that $\{I_1, I_2\}$ is also an invariant of motion.*

2.3 The Vlasov-Maxwell equations

2.3.1 The model

The non relativistic Vlasov equation for a particle species s of charge q_s and mass q_s reads

$$\frac{\partial f_s}{\partial t} + v \cdot \nabla_x f_s + \frac{q_s}{m_s}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_v f = 0, \tag{2.29}$$

it is coupled non linearly to the Maxwell equations

$$\frac{\partial \mathbf{E}}{\partial t} - c^2 \nabla \times \mathbf{B} = -\mu_0 \mathbf{J}, \tag{2.30}$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0, \tag{2.31}$$

$$\nabla \cdot \mathbf{E} = \rho/\varepsilon_0, \tag{2.32}$$

$$\nabla \cdot \mathbf{B} = 0, \tag{2.33}$$

in addition to initial and boundary conditions. Here ε_0 and μ_0 are the vacuum permittivity and permeability that are related to the speed of light c by $\mu_0 \varepsilon_0 c^2 = 1$. The source for the Maxwell equation, the charge density ρ and the current density J, are obtained from the Vlasov equations by

$$\rho = \sum_s q_s \int f_s \, \mathrm{d}\mathbf{v}, \qquad \mathbf{J} = \sum_s q_s \int f_s \mathbf{v} \, \mathrm{d}\mathbf{v}. \tag{2.34}$$

In order to define an action principle for the Vlasov-Maxwell equations, we shall need to introduce the characteristics of the Vlasov equation. Let us consider the system of differential equations

$$\frac{\mathrm{d}\mathbf{X}_s}{\mathrm{d}t} = \mathbf{V}_s, \tag{2.35}$$

$$\frac{\mathrm{d}\mathbf{V}_s}{\mathrm{d}t} = \frac{q_s}{m_s}(\mathbf{E}(t, \mathbf{X}_s(t)) + \mathbf{V}_s \times \mathbf{B}(t, \mathbf{X}_s(t))), \tag{2.36}$$

with initial conditions $\mathbf{X}(0) = \mathbf{x}_0$, $\mathbf{V}(0) = \mathbf{v}_0$. In order to explicit the dependence of the solution on the initial condition, we shall denote the solution at time t by $\mathbf{X}(t; \mathbf{x}_0, \mathbf{v}_0), \mathbf{V}(t; \mathbf{x}_0, \mathbf{v}_0)$, The are called the *characteristics* of the Vlasov equation (2.29), and if $f_{s,0}$ is the initial value of the distribution function, the solution of the Vlasov equation can then be expressed with the help of the characteristics

$$f(t, \mathbf{X}(t; \mathbf{x}_0, \mathbf{v}_0), \mathbf{V}(t; \mathbf{x}_0, \mathbf{v}_0)) = f_{s,0}(\mathbf{x}_0, \mathbf{v}_0).$$

2.3.2 Action principle

The phase-space Lagrangian for the motion of a single particle of mass m_s and charge q_s in an electromagnetic field is given in standard non canonical coordinates by

$$L_s(\mathbf{x}, \mathbf{v}, \dot{\mathbf{x}}, t) = (m_s\mathbf{v} + q_s\mathbf{A}) \cdot \dot{\mathbf{x}} - (\frac{1}{2}m_s|\mathbf{v}|^2 + q_s\phi).$$

The self consistent field theory is then obtained by plugging this Lagrangian into the following action proposed by Low [12]

$$\mathcal{A}[\mathbf{X}_s, \mathbf{V}_s, \phi, \mathbf{A}] = \sum_s \int f_{s,0}(\mathbf{x}_0, \mathbf{v}_0) L_s(\mathbf{X}_s(t; \mathbf{x}_0, \mathbf{v}_0), \mathbf{V}_s(t; \mathbf{x}_0, \mathbf{v}_0), \frac{\mathrm{d}\mathbf{X}_s}{\mathrm{d}t}(t; \mathbf{x}_0, \mathbf{v}_0))\, \mathrm{d}\mathbf{x}_0\, \mathrm{d}\mathbf{v}_0\, \mathrm{d}t$$
$$+ \frac{\epsilon_0}{2} \int |\nabla\phi + \frac{\partial \mathbf{A}}{\partial t}|^2\, \mathrm{d}\mathbf{x}\, \mathrm{d}t - \frac{1}{2\mu_0} \int |\nabla \times \mathbf{A}|^2\, \mathrm{d}\mathbf{x}\, \mathrm{d}t. \quad (2.37)$$

where the particle distribution functions f_s are taken at the initial time and the characteristics express the evolution of the distribution function, and there are as many $\mathbf{X}_s$, and $\mathbf{V}_s$ as there are particle species.

In this variational principle the characteristics of the Vlasov equation, which are the particles equations of motion are obtained by taking the variation with respect to $\mathbf{X}$ and $\mathbf{V}$, the Poisson equation, is obtained by taking the variations with respect to ϕ and the Ampere equation is obtained by taking the variations with respect to $\mathbf{A}$. The definition of the electromagnetic fields from the potentials

$$\mathbf{E} = -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t}, \qquad \mathbf{B} = \nabla \times \mathbf{A} \quad (2.38)$$

automatically implies the Faraday equation $\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0$ and $\nabla \cdot \mathbf{B} = 0$.

In order to perform the variations, we need to generalise the directional derivative we used in the finite dimensional case to the case where the varied functions live in an infinite dimensional Banach space. This is based on the Fréchet derivative which gives a rigorous definition of the functional derivative used in physics for functions that are in a Banach (including Hilbert) space. Consider a functional J from a Hilbert space V into $\mathbb{R}$. Its Fréchet derivative J', assuming it exists, is a linear form on V, which means that it maps any function from V to a scalar. It can be computed using the Gâteaux formula:

$$J'[u](v) = \lim_{\varepsilon \to 0} \frac{J[u + \epsilon v] - J[u]}{\varepsilon} = \left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} J[u + \epsilon v]. \quad (2.39)$$

Remark 4 *In mathematics, differentiability in Banach spaces is defined based on the Fréchet derivative. Let V, W be two normed spaces (*e.g. *Banach spaces). A function $J : U \subset V \to W$ is called Fréchet differentiable at $u \in U$ if there exists a bounded linear operator $A : V \to W$ such that*

$$\lim_{h \to 0} \frac{\|J(u + h) - J(u) - Ah\|_W}{\|h\|_V} = 0.$$

Then A is the Fréchet derivative of J at u and denoted by $A = J'[u]$. If a function is differentiable, its Fréchet derivative exists and then the Gâteaux derivative also exists and is equal to the Fréchet derivative, but there are cases where the Gâteaux derivative exists but the function is not differentiable in the sense of Fréchet.

Example: Let Ω be an open subset of $\mathbb{R}^n$, $u \in H_0^1(\Omega)$ and consider the functional

$$J[u] = \frac{1}{2}\int_\Omega |\nabla u(\mathbf{x})|^2 \,\mathrm{d}\mathbf{x}.$$

Then for any $v \in H_0^1(\Omega)$

$$\frac{J[u+\epsilon v]-J[u]}{\epsilon} = \frac{1}{2\epsilon}\int_\Omega (|\nabla(u+\epsilon v)|^2 - |\nabla u|^2)\,\mathrm{d}\mathbf{x} = \frac{1}{2\epsilon}\int_\Omega (2\epsilon \nabla u\cdot\nabla v - \epsilon^2|\nabla v|^2)\,\mathrm{d}\mathbf{x} \xrightarrow[\epsilon\to 0]{} \int_\Omega \nabla u\cdot\nabla v\,\mathrm{d}\mathbf{x},$$

so that $J'[u](v) = \int_\Omega \nabla u\cdot\nabla v\,\mathrm{d}\mathbf{x}$. Here we see again that $J'[u]$ is an element of the dual of V and needs to be applied to an element of v. However using Riesz's theorem and the scalar product in $L^2(\Omega)$, $J'[u]$ can be identified to an element of $L^2(\Omega)$ by writing

$$J'[u](v) = \int_\Omega \nabla u\cdot\nabla v\,\mathrm{d}\mathbf{x} = -\int_\Omega \Delta u v\,\mathrm{d}\mathbf{x} = \int_\Omega \frac{\delta J}{\delta u}[u] v\,\mathrm{d}\mathbf{x}$$

so that $\frac{\delta J}{\delta u}[u] = -\Delta u$ almost everywhere. $\frac{\delta J}{\delta u}[u]$ is called the *functional derivative* of J at u. Note that the boundary terms matter. Here we have used that $u \in H_0^1(\Omega)$, setting the boundary terms to 0 in the integration by parts.

We can now compute the variations of action (2.37). Let us start with the variations with respect to $\mathbf{X}_s$, which appears only in one integral. Hence

$$\left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} \mathcal{A}[\mathbf{X}_s + \epsilon\mathbf{Y}, \mathbf{V}_s, \phi, \mathbf{A}] = \int f_{s,0}(\mathbf{x}_0,\mathbf{v}_0)\left(\mathbf{Y}\cdot\nabla_{\mathbf{x}} L_s + \frac{\mathrm{d}\mathbf{Y}}{\mathrm{d}t}\cdot\nabla_{\dot{\mathbf{x}}} L_s\right)\mathrm{d}\mathbf{x}_0\,\mathrm{d}\mathbf{v}_0\,\mathrm{d}t.$$

Integrating in parts in time, assuming the variations vanish at initial and final time we find the usual Euler-Lagrange equations:

$$\frac{\mathrm{d}}{\mathrm{d}t}\nabla_{\dot{\mathbf{x}}} L_s = \nabla_{\mathbf{x}} L_s. \tag{2.40}$$

Applying it to the actual Lagrangian, we can perform the same computation as in (2.20) and in the same way the variations with respect to $\mathbf{V}_s$ yields $\frac{\mathrm{d}\mathbf{X}_s}{\mathrm{d}t} = \mathbf{V}_s$, so that the equations for the characteristics obtained based on the variations of (2.37) with respect to the characteristics yield the classical equations of motion of a particle in an electromagnetic field

$$\frac{\mathrm{d}\mathbf{X}_s}{\mathrm{d}t} = \mathbf{V}_s, \tag{2.41}$$

$$\frac{\mathrm{d}\mathbf{V}_s}{\mathrm{d}t} = \frac{q_s}{m_s}(\mathbf{E} + \mathbf{V}_s\times\mathbf{B}). \tag{2.42}$$

Let us know come to the variations with respect to ϕ, plugging in directly the expression for the single particle Lagrangian, using also that $\mathbf{E} = -\frac{\partial\mathbf{A}}{\partial t} - \nabla\phi$

$$\left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} \mathcal{A}[\mathbf{X}_s, \mathbf{V}_s, \phi+\epsilon\psi, \mathbf{A}] = -\sum_s \int f_{s,0}(\mathbf{x}_0,\mathbf{v}_0) q_s \psi(t,\mathbf{X}_s(t))\,\mathrm{d}\mathbf{x}_0\,\mathrm{d}\mathbf{v}_0\,\mathrm{d}t - \epsilon_0\int \mathbf{E}\cdot\nabla\psi\,\mathrm{d}\mathbf{x}\,\mathrm{d}t.$$

Now using that f_s is conserved along the characteristics $f_{s,0}(\mathbf{x}_0,\mathbf{v}_0) = f_s(t,\mathbf{X}_s(t),\mathbf{V}_s(t))$ and performing the change of variables $x = \mathbf{X}_s(t;\mathbf{x}_0,\mathbf{v}_0)$, $v = \mathbf{V}_s(t;\mathbf{x}_0,\mathbf{v}_0)$ using that the Jacobian of the transformation is one thanks to the Liouville theorem we find:

$$\sum_s \int f_{s,0}(\mathbf{x}_0,\mathbf{v}_0) q_s \psi(t,\mathbf{X}_s(t))\,\mathrm{d}\mathbf{x}_0\,\mathrm{d}\mathbf{v}_0\,\mathrm{d}t = \sum_s q_s \int f_s(t,\mathbf{x},\mathbf{v})\psi(t,\mathbf{x})\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{v}\,\mathrm{d}t = \int \rho\psi\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{v}\,\mathrm{d}t,$$

so that the variations with respect to ϕ vanish when

$$-\epsilon_0 \int \mathbf{E} \cdot \nabla \psi \, \mathrm{d}\mathbf{x} \, \mathrm{d}t = \int \rho \psi \, \mathrm{d}\mathbf{x} \, \mathrm{d}\mathbf{v} \, \mathrm{d}t, \quad \forall \psi \in H^1(\Omega).$$

which is a weak form of the Poisson equation. An integration by parts, assuming that ψ vanishes on the boundary yields the classical form $\epsilon_0 \nabla \cdot \mathbf{E} = \rho$.

Let us finally come to the variations with respect to $\mathbf{A}$, plugging in directly the expression for the single particle Lagrangian, using also that $\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} - \nabla \phi$

$$\left. \frac{\mathrm{d}}{\mathrm{d}\epsilon} \right|_{\epsilon=0} \mathcal{A}[\mathbf{X}_s, \mathbf{V}_s, \phi, \mathbf{A} + \epsilon \check{\mathbf{A}}] = \sum_s \int f_{s,0}(\mathbf{x}_0, \mathbf{v}_0) q_s \check{\mathbf{A}} \cdot \mathbf{V}(t) \, \mathrm{d}\mathbf{x}_0 \, \mathrm{d}\mathbf{v}_0 \, \mathrm{d}t - \epsilon_0 \int \frac{\partial \check{\mathbf{A}}}{\partial t} \cdot \mathbf{E} \, \mathrm{d}\mathbf{x} \, \mathrm{d}t$$
$$- \frac{1}{\mu_0} \int \nabla \times \check{\mathbf{A}} \cdot \nabla \times \mathbf{A} \, \mathrm{d}\mathbf{x} \, \mathrm{d}t$$

Performing again the change of variables $x = \mathbf{X}_s(t; \mathbf{x}_0, \mathbf{v}_0)$, $v = \mathbf{V}_s(t; \mathbf{x}_0, \mathbf{v}_0)$, the integral over f_s yields the current density and we find the weak form of Ampère's equation:

$$\epsilon_0 \int \frac{\partial \check{\mathbf{A}}}{\partial t} \cdot \mathbf{E} \, \mathrm{d}\mathbf{x} \, \mathrm{d}t + \frac{1}{\mu_0} \int \nabla \times \check{\mathbf{A}} \cdot \nabla \times \mathbf{A} \, \mathrm{d}\mathbf{x} \, \mathrm{d}t = \int \mathbf{J} \cdot \check{\mathbf{A}} \, \mathrm{d}\mathbf{x} \, \mathrm{d}t, \quad \forall \check{\mathbf{A}} \in H(curl, \Omega).$$

Multiplying by μ_0 and integrating by parts the two integrals on the left hand side assuming that $\check{\mathbf{A}}$ vanishes at initial and final times as well as its tangential components on the boundary we find the classical form of Ampère's equation:

$$-\frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} + \nabla \times \mathbf{B} = \mu_0 \mathbf{J},$$

using that $\epsilon_0 \mu_0 c^2 = 1$ and that $\mathbf{B} = \nabla \times \mathbf{A}$.

Chapter 3

Numerical methods for hamiltonian systems

We have seen that hamiltonian systems of the form $\frac{\mathrm{d}\mathbf{z}}{\mathrm{d}t} = \mathcal{J}(\mathbf{z})\nabla_{\mathbf{z}}H$ feature at leas two important conservation, the conservation of the Poisson bracket by the flow (see [9] (VII.4)). This is similar to the symplecticity of the flow in the canonical case

$$\{F, G\}(\mathbf{Z}(t;\mathbf{y})) = \{F, G\}(\mathbf{y}),$$

or equivalently

$$(\nabla_{\mathbf{y}}\mathbf{Z})^{\top}\mathcal{J}(\mathbf{y})(\nabla_{\mathbf{y}}\mathbf{Z}) = \mathcal{J}(\mathbf{Z}(t,\mathbf{y})).$$

and the conservation of the hamiltonian H.

Definition 7 *A functional C is called a Casimir of a Poisson bracket if $\{C, F\} = 0$ for all smooth functions F. This is equivalent to $\mathcal{J}\nabla C = 0$.*

Proposition 3 *If a flow conserves the Poisson bracket, then the Casimirs are preserved.*

Proposition 4 *The only flow that preserves the Poisson structure and the hamiltonian is the exact flow.*

This means that when constructing a numerical approximation, one cannot have at the same time the exact preservation of the Poisson structure and of the hamiltonian, but approximations that conserve either of them can be constructed. However when the Poisson structure is conserved it is possible to show that an approximate hamiltonian (which approximates the exact hamiltonian up to the order of the method) is exactly conserved.

3.1 Splitting methods

This section is mostly based on the review article of McLachland and Quispel [13].

We consider a system of differential equations where the right-hand-side can be split in a sum

$$\frac{\mathrm{d}\mathbf{Z}}{\mathrm{d}t} = \mathbf{A}(t, \mathbf{Z}(t)) = \mathbf{A}_1 + \mathbf{A}_2 + \cdots + \mathbf{A}_n \tag{3.1}$$

A splitting method then consists in obtaining an approximate solution of the full system by combining solutions of the reduced system $\frac{\mathrm{d}\mathbf{Z}}{\mathrm{d}t} = \mathbf{A}_i$ for $i = 1, \ldots n$. In the context

of geometric methods, splitting is a particularly useful tool, if each subsystem has itself the desired geometric structure and if for each split part either the exact solution can be obtained, which is often the case in practice, or if a simpler geometric integrator can be found.

Proposition 5 (Lie-Trotter splitting) *Assume that $\mathbf{A}_i$ is at least C^1 and that the flow can be computed exactly for each split part and denote it by $\varphi_t^{(i)}(\mathbf{y}) = \mathbf{Z}(t;\mathbf{y})$. Then*

$$\psi_{\Delta t}(\mathbf{y}) = \varphi_{\Delta t}^{(1)} \circ \varphi_{\Delta t}^{(2)} \circ \cdots \circ \varphi_{\Delta t}^{(n)}(\mathbf{y}) \tag{3.2}$$

is a first order approximation of the exact solution of (3.1)*.*

Proof. By a Taylor expansion in t as $\frac{\mathrm{d}\mathbf{Z}_i}{\mathrm{d}t} = \mathbf{A}_i$ we have

$$\varphi_{\Delta t}^{(i)}(\mathbf{y}) = \mathbf{Z}(\Delta t;\mathbf{y}) = \mathbf{y} + \Delta t \frac{\mathrm{d}\mathbf{Z}(0;\mathbf{y})}{\mathrm{d}t} + O(\Delta t^2) = \mathbf{y} + \Delta t \mathbf{A}_i(0,\mathbf{y}) + O(\Delta t^2).$$

Let us now consider the case of two parts

$$\begin{aligned}
\varphi_{\Delta t}^{(1)} \circ \varphi_{\Delta t}^{(2)}(\mathbf{y}) &= \varphi_{\Delta t}^{(1)}(\varphi_{\Delta t}^{(2)}(\mathbf{y})) = \varphi_{\Delta t}^{(1)}(\mathbf{y} + \Delta t \mathbf{A}_2(0,\mathbf{y}) + O(\Delta t^2)) \\
&= \mathbf{y} + \Delta t \mathbf{A}_2(0,\mathbf{y}) + \Delta t \mathbf{A}_1(0,\mathbf{y}) + O(\Delta t^2)) \\
&= \mathbf{y} + \Delta t \mathbf{A}(0,\mathbf{y}) + O(\Delta t^2) = \psi_{\Delta t}(\mathbf{y}) + O(\Delta t^2)
\end{aligned}$$

By chaining the computation, the same procedure also applies for the case of n parts. ∎

Definition 8 *The* adjoint $\psi_{\Delta t}^*$ *of an discrete flow $\psi_{\Delta t}$ is defined by $\psi_{\Delta t}^* = \psi_{-\Delta t}^{-1}$.*

Definition 9 *A numerical method is called $\psi_{\Delta t}$* symmetric *(or self-adjoint or time-reversible) if $\psi_{-\Delta t}(\psi_{\Delta t}(\mathbf{y})) = \mathbf{y}$.*

Proposition 6 *Given a method $\psi_{\Delta t}$ of order 1, the numerical method $\Phi_{\Delta t} = \psi_{\Delta t/2} \circ \psi_{\Delta t/2}^*$ is symmetric and of order 2.*

Proof. Using the definition of the adjoint we have

$$\Phi_{-\Delta t}(\Phi_{\Delta t}(\mathbf{y})) = \psi_{-\Delta t/2} \circ \psi_{\Delta t/2}^{-1} \circ \psi_{\Delta t/2} \circ \psi_{-\Delta t/2}^{-1}(\mathbf{y}) = \mathbf{y}.$$

It is also clear by using the definition that $\Phi_{\Delta t}^* = (\psi_{\Delta t/2} \circ \psi_{\Delta t/2}^*)^* = \psi_{\Delta t/2} \circ \psi_{\Delta t/2}^* = \Phi_{\Delta t}$, which is the classical definition of self-adjointness.

The proof that it is second order can be found in the book by Hairer, Lubich and Wanner [9]. ∎

Remark 5 *If $\psi_{\Delta t} = \varphi_{\Delta t}^1 \circ \varphi_{\Delta t}^2$ is the composition of two exact flows verifying $\phi_{-\Delta t}^{-1} = \phi_{\Delta t}$ then*

$$\psi_{\Delta t/2} \circ \psi_{\Delta t/2}^* = \varphi_{\Delta t/2}^1 \circ \varphi_{\Delta t/2}^2 \circ \varphi_{\Delta t/2}^2 \circ \varphi_{\Delta t/2}^1 = \varphi_{\Delta t/2}^1 \circ \varphi_{\Delta t}^2 \circ \varphi_{\Delta t/2}^1$$

This is the well known Strang splitting *which is of order 2 and symmetric. Symmetry is a very important property for long time integration as some errors cancel with symmetric methods.*

For this reason, the simplest method of choice for the splitting in n parts, is the symmetric composition

$$\psi_{\Delta t} = \varphi^{(1)}_{\Delta t/2} \circ \cdots \circ \varphi^{(n-1)}_{\Delta t/2} \circ \varphi^{(n)}_{\Delta t} \circ \varphi^{(n-1)}_{\Delta t/2} \circ \cdots \circ \varphi^{(1)}_{\Delta t/2} \tag{3.3}$$

Methods of arbitrary order can be derived by composition of lower order methods [9, 13]. For example, the simplest fourth order method is obtained by combining the symmetric Strang-splitting $\psi_{\Delta t}$ of order 2 above to obtain

$$\Phi_h^{(4,TJ)} = \psi_{\alpha\Delta t} \circ \psi_{\beta\Delta t} \circ \psi_{\alpha\Delta t}, \tag{3.4}$$

with

$$\alpha = 1/(2 - 2^{1/3}), \qquad \beta = -2^{1/3}/(2 - 2^{1/3}).$$

This is called the *triple jump method*. Note that the second coefficient β is negative (see [9], p.44).

McLachland and Quispel [13] claim that this method has a high error constant and suggest to use preferably the Suzuki fractals (see [9], p.44). The one with the least number of stages has 5 stages and reads

$$\Phi_h^{(4,S)} = \psi_{\alpha\Delta t} \circ \psi_{\alpha\Delta t} \circ \psi_{\beta\Delta t} \circ \psi_{\alpha\Delta t} \circ \psi_{\alpha\Delta t}, \tag{3.5}$$

with

$$\alpha = 1/(4 - 4^{1/3}), \qquad \beta = -4^{1/3}/(4 - 4^{1/3}).$$

McLachland and Quispel [13] propose what they consider some good general high-order method p. 407 of their review paper, mentioning however that optimal high order methods can be derived for some specific problems. Let us mention in particular the 6th order method

$$\Phi_h^{(6)} = \psi_{a_1\Delta t} \circ \psi_{a_2\Delta t} \circ \psi_{a_3\Delta t} \circ \psi_{a_4\Delta t} \circ \psi_{a_5\Delta t} \circ \psi_{a_4\Delta t} \circ \psi_{a_3\Delta t} \circ \psi_{a_2\Delta t} \circ \psi_{a_1\Delta t}, \tag{3.6}$$

with $a_1 = 0.1867$, $a_2 = 0.55549702371247839916$, $a_3 = 0.12946694891347535806$, $a_4 = -0.84326562338773460855$, $a_5 = 1 - 2\sum_{i=1}^{4} a_i$.

3.2 Numerical integration of the motion of a charged particle in a static electromagnetic field

Only the exact integrator conserves exactly the energy and the symplectic form. So one needs to chose. When solving numerically a Poisson system of the form

$$\frac{\mathrm{d}\mathbf{Z}}{\mathrm{d}t} = \mathcal{J}(\mathbf{Z})\nabla H,$$

one usually uses a splitting method, where each of the split parts has still a good structure but is simpler to integrate, ideally each split part could be integrated exactly. For example if the hamiltonian can be split into several pieces that can be integrated exactly keeping the full Poisson matrix,

$$\frac{\mathrm{d}\mathbf{Z}}{\mathrm{d}t} = \mathcal{J}(\mathbf{Z})\nabla H_1 + \mathcal{J}(\mathbf{Z})\nabla H_2 + \mathcal{J}(\mathbf{Z})\nabla H_3.$$

we obtain a symplectic integrator.

Another option is to split the Poisson matrix, such that each piece remains antisymmetric and keeping the full hamiltonian

$$\frac{\mathrm{d}\mathbf{Z}}{\mathrm{d}t} = \mathcal{J}_1(\mathbf{Z})\nabla H + \mathcal{J}_2(\mathbf{Z})\nabla H + \mathcal{J}_3(\mathbf{Z})\nabla H$$

and using a discrete gradient method, one can exactly conserve H.

And finally by decomposing the right-hand-side in divergence free parts, where one can construct a volume preserving integrator for each part, one obtains globally a volume preserving integrator.

In our case the system reads

$$\begin{pmatrix} \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} \\ \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} \end{pmatrix} = \begin{pmatrix} 0 & \frac{1}{m} I_n \\ -\frac{1}{m} I_n & \frac{q}{m^2}\mathbb{B}(\mathbf{x}) \end{pmatrix} \begin{pmatrix} \nabla_{\mathbf{x}} H \\ \nabla_{\mathbf{v}} H \end{pmatrix}, \tag{3.7}$$

with the Hamiltonain $H(\mathbf{x}, \mathbf{v}) = \frac{1}{2}m|\mathbf{v}|^2 + q\phi(\mathbf{x})$, and the Poisson matrix

$$\mathcal{J}(\mathbf{x}) = \begin{pmatrix} 0 & \frac{1}{m} I_n \\ -\frac{1}{m} I_n & \frac{q}{m^2}\mathbb{B}(\mathbf{x}) \end{pmatrix}.$$

3.2.1 Hamiltonian splitting

The above Hamiltonian can be split into $H(\mathbf{x}, \mathbf{v}) = H_1(\mathbf{x}) + H_2(\mathbf{v})$ with $H_1(\mathbf{x}) = q\phi(\mathbf{x})$ and $H_2(\mathbf{v}) = \frac{1}{2}m|\mathbf{v}|^2$. Hence splitting the Hamiltonian yields the following two subsystems: keeping only $\mathcal{J}\nabla H_1$

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = 0, \tag{3.8}$$

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \frac{q}{m}\mathbf{E}, \tag{3.9}$$

and keeping only $\mathcal{J}\nabla H_2$

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v}, \tag{3.10}$$

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \frac{q}{m}\mathbf{v} \times \mathbf{B}. \tag{3.11}$$

As in the subsystem (3.8)-(3.9) $\mathbf{E}$ depends only on $\mathbf{x}$ which stays constant due to (3.8). This subsystem can be integrated analytically, with the solution

$$\mathbf{x}(t; \mathbf{x}_0, \mathbf{v}_0) = \mathbf{x}_0, \qquad \mathbf{v}(t; \mathbf{x}_0, \mathbf{v}_0) = \mathbf{v}_0 + \frac{q}{m}\mathbf{E}(\mathbf{x}_0)t \tag{3.12}$$

This is however not the case for the other subsystem (3.10)-(3.11). One option would be use a numerical symplectic integrator for subsystem (3.10)-(3.11) or event for the full system, but this would be implicit. We won't consider this option here.

3.2.2 Divergence free splitting

If we further split the system, we will not conserve the full Poisson structure in each of the subsystems, so it will not be possible to derive a Poisson integrator. However observing that splitting the $\mathbf{x}$ components and the $\mathbf{v}$ components in the right-hand-side of (3.10)-(3.11) we have

$$\nabla_{\mathbf{z}} \cdot \begin{pmatrix} \mathbf{v} \\ 0 \end{pmatrix} = \nabla_{\mathbf{x}} \cdot \mathbf{v} = 0,$$

and

$$\nabla_{\mathbf{z}} \cdot \begin{pmatrix} 0 \\ \frac{q}{m}\mathbf{v} \times \mathbf{B} \end{pmatrix} = \frac{q}{m} \nabla_{\mathbf{v}} \cdot (\mathbf{v} \times \mathbf{B}) = 0,$$

so that each part is divergence free and thus volume preserving. So, let us now consider along with (3.8)-(3.9), the further two subsystems:

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v}, \tag{3.13}$$

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = 0, \tag{3.14}$$

and

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = 0, \tag{3.15}$$

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \frac{q}{m}\mathbf{v} \times \mathbf{B}. \tag{3.16}$$

The analytical solution of (3.13)-(3.14) is

$$\mathbf{x}(t; \mathbf{x}_0, \mathbf{v}_0) = \mathbf{x}_0 + \mathbf{v}_0 t, \qquad \mathbf{v}(t; \mathbf{x}_0, \mathbf{v}_0) = \mathbf{v}_0. \tag{3.17}$$

and as $\mathbf{x}$ is constant along the flow, the solution of (3.16) is a rotation around the axis defined by $\mathbf{B}(\mathbf{x}_0)$, so that we can verify that, denoting by $\omega_0 = q|\mathbf{B}(\mathbf{x}_0)|/m$, $\mathbf{b}_0 = \mathbf{B}(\mathbf{x}_0)/|\mathbf{B}(\mathbf{x}_0)|$, $v_{0,\parallel} = \mathbf{v}_0 \cdot \mathbf{b}_0$, and by $\mathbf{v}_{0,\perp} = \mathbf{b}_0 \times (\mathbf{v}_0 \times \mathbf{b}_0)$, the analytical solution of (3.15)-(3.16) is

$$\mathbf{x}(t; \mathbf{x}_0, \mathbf{v}_0) = \mathbf{x}_0, \qquad \mathbf{v}(t; \mathbf{x}_0, \mathbf{v}_0) = v_{0,\parallel}\mathbf{b}_0 + \cos(\omega_0 t)\mathbf{v}_{0,\perp} + \sin(\omega_0 t)\mathbf{b}_0 \times \mathbf{v}_{0,\perp}. \tag{3.18}$$

Finally combining the flows, (3.12)–(3.17)–(3.18) using one of splittings proposed in the previous section, we obtain a volume preserving approximation of (3.7). This method was recently investigated in [10].

On the other hand, as (3.16) is a 2D rotation, a volume preserving second order numerical integrator can be obtained using the implicit trapezoidal rule. Denoting by $\mathbf{v}_1 = \mathbf{v}(\Delta t; \mathbf{x}_0, \mathbf{x}_0)$, this reads

$$\mathbf{v}_1 - \mathbf{v}_0 = \frac{q\Delta t}{2m}(\mathbf{v}_1 + \mathbf{v}_0) \times \mathbf{B}(\mathbf{x}_0) = \frac{\omega_0 \Delta t}{2}(\mathbf{v}_1 + \mathbf{v}_0) \times \mathbf{b}_0. \tag{3.19}$$

Taking the dot product with $\mathbf{b}_0$, we get $v_{1,\parallel} = v_{0,\parallel}$, then collecting $\mathbf{v}_1$ on the left-hand-side and $\mathbf{v}_0$ on the right-hand-side, we get

$$\mathbf{v}_1 - \frac{\omega_0 \Delta t}{2}\mathbf{v}_1 \times \mathbf{b}_0 = \mathbf{v}_0 + \frac{\omega_0 \Delta t}{2}\mathbf{v}_0 \times \mathbf{b}_0$$

Taking the cross product of this expression with $\mathbf{b}_0$ and using that $v_{1,\|} = v_{0,\|}$ and that for any $\mathbf{v}$, we have $(\mathbf{v} \times \mathbf{b}_0) \times \mathbf{b}_0 = -\mathbf{v} + v_\| \mathbf{b}_0 = -\mathbf{v}_\perp$, we find

$$\mathbf{v}_1 \times \mathbf{b}_0 + \frac{\omega_0 \Delta t}{2} \mathbf{v}_1 = \mathbf{v}_0 \times \mathbf{b}_0 - \frac{\omega_0 \Delta t}{2} \mathbf{v}_0 + (\omega_0 \Delta t) v_{0,\|} \mathbf{b}_0.$$

Then, multiplying this last expression with $\frac{\omega_0 \Delta t}{2}$ and summing with the previous one, we get

$$\begin{aligned}
\left(1 + \frac{\omega_0^2 \Delta t^2}{4}\right) \mathbf{v}_1 &= \left(1 - \frac{\omega_0^2 \Delta t^2}{4}\right) \mathbf{v}_0 + \omega_0 \Delta t \mathbf{v}_0 \times \mathbf{b}_0 + \frac{\omega_0^2 \Delta t^2}{2} v_{0,\|} \mathbf{b}_0 \\
&= \left(1 + \frac{\omega_0^2 \Delta t^2}{4} - \frac{\omega_0^2 \Delta t^2}{2}\right) \mathbf{v}_0 + \omega_0 \Delta t \mathbf{v}_0 \times \mathbf{b}_0 + \frac{\omega_0^2 \Delta t^2}{2} v_{0,\|} \mathbf{b}_0 \\
&= \left(1 + \frac{\omega_0^2 \Delta t^2}{4}\right) \mathbf{v}_0 + \omega_0 \Delta t \mathbf{v}_0 \times \mathbf{b}_0 + \frac{\omega_0^2 \Delta t^2}{2} (\mathbf{v}_0 \times \mathbf{b}_0) \times \mathbf{b}_0
\end{aligned}$$

so that we get, denoting by $\beta = \frac{\omega_0 \Delta t}{2}$, the classical formula for the Boris push [3]

$$\mathbf{v}(\Delta t; \mathbf{x}_0, \mathbf{x}_0) = \mathbf{v}_1 = \mathbf{v}_0 + \frac{2\beta}{1+\beta^2} (\mathbf{v}_0 + \beta \mathbf{v}_0 \times \mathbf{b}_0) \times \mathbf{b}_0. \tag{3.20}$$

Putting it altogether, we obtain a symmetric volume preserving algorithm by combining (3.17), (3.12), and (3.20) on a time step Δt. So starting from $(\mathbf{x}^n, \mathbf{v}^n)$ we get

First operator (3.17) on $\Delta t/2$:	$\mathbf{x}^{(1)} = \mathbf{x}^n + \mathbf{v}^n \Delta t/2,$	$\mathbf{v}^{(1)} = \mathbf{v}^n$
Second operator (3.12) on $\Delta t/2$:	$\mathbf{x}^{(2)} = \mathbf{x}^{(1)},$	$\mathbf{v}^{(2)} = \mathbf{v}^{(1)} + \mathbf{E}(\mathbf{x}^{(1)}) \Delta t/2$
Third operator (3.20) on Δt:	$\mathbf{x}^{(3)} = \mathbf{x}^{(2)},$	$\mathbf{v}^{(3)} = \mathbf{v}^{(2)} + \frac{2\beta}{1+\beta^2} (\mathbf{v}^{(2)} + \beta \mathbf{v}^{(2)} \times \mathbf{b}_0) \times \mathbf{b}_0$
Second operator (3.12) on $\Delta t/2$:	$\mathbf{x}^{(4)} = \mathbf{x}^{(3)},$	$\mathbf{v}^{(4)} = \mathbf{v}^{(3)} + \mathbf{E}(\mathbf{x}^{(3)}) \Delta t/2$
First operator (3.17) on $\Delta t/2$:	$\mathbf{x}^{(5)} = \mathbf{x}^n + \mathbf{v}^{(4)} \Delta t/2,$	$\mathbf{v}^{(5)} = \mathbf{v}^{(4)}.$

Noticing that $\mathbf{x}$ does not evolve between the second and fourth step and $\mathbf{x}^{(1)}$ is an approximation of $\mathbf{x}^{n+1/2}$, the algorithm can be simplified and becomesstarting from $(\mathbf{x}^n, \mathbf{v}^n)$ and indicating only the quantities that are modified at each step:

$$\begin{aligned}
\mathbf{x}^{n+1/2} &= \mathbf{x}^n + \mathbf{v}^n \Delta t/2, \\
\mathbf{v}^- &= \mathbf{v}^n + \mathbf{E}(\mathbf{x}^{n+1/2}) \Delta t/2, \\
\mathbf{v}^+ &= \mathbf{v}^- + \frac{2\beta}{1+\beta^2} (\mathbf{v}^- + \beta \mathbf{v}^- \times \mathbf{b}_0) \times \mathbf{b}_0, \\
\mathbf{v}^{n+1} &= \mathbf{v}^+ + \mathbf{E}(\mathbf{x}^{n+1/2}) \Delta t/2, \\
\mathbf{x}^{n+1} &= \mathbf{x}^{n+1/2} + \mathbf{v}^{n+1} \Delta t/2.
\end{aligned}$$

This is the classical Boris-Buneman algorithm that has been the workhorse for electromagnetic PIC for many years and although it is only second order it has much better long time properties than the fourth order RK4 method. This is due to the fact that it is symmetric and volume preserving as was first proved in [17].

This algorithm is very good when $\beta = \frac{\omega_0 \Delta t}{2}$ is small enough, this means when the time step is small compared to the cyclotron period. Then the error committed by the second order approximation of (3.15)–(3.16) is of the order of the splitting error, else it is better to use the exact solution of (3.15)–(3.16), given by (3.18), instead. Then the middle step in the previous algorithm is replaced by

$$\begin{aligned}
\mathbf{v}^+ &= v_\|^- \mathbf{b}_0 + \cos(\omega_0 \Delta t) \mathbf{v}_\perp^- + \sin(\omega_0 \Delta t) \mathbf{b}_0 \times \mathbf{v}_\perp^-, \\
&= (\mathbf{v} \cdot \mathbf{b}_0) \mathbf{b}_0 + \mathbf{b}_0 \times (\cos(\omega_0 \Delta t) \mathbf{v}^- \times \mathbf{b}_0 + \sin(\omega_0 \Delta t) \mathbf{v}^-).
\end{aligned} \tag{3.21}$$

3.2.3 Discrete gradient methods

A general class of methods called *discrete gradient methods* conserves exactly a discrete Hamiltonian for ODEs of the form

$$\frac{\mathrm{d}\mathbf{z}}{\mathrm{d}t} = \mathcal{J}(\mathbf{z})\nabla_{\mathbf{z}} H$$

where $\mathcal{J}$ is a skew-symmetric matrix (not necessarily defining a Poisson bracket). They were proposed by Mc Lachland, Quispel and Robidoux [14].

They are based on a discrete gradient $\bar{\nabla} H(\mathbf{z}^n, \mathbf{z}^{n+1})$ such that

$$(\mathbf{z}^{n+1} - \mathbf{z}^n)^\top \bar{\nabla} H(\mathbf{z}^n, \mathbf{z}^{n+1}) = H(\mathbf{z}^{n+1}) - H(\mathbf{z}^n),$$

Then the scheme $\frac{\mathbf{z}^{n+1}-\mathbf{z}^n}{\Delta t} = \bar{\mathcal{J}}\bar{\nabla} H(\mathbf{z}^n, \mathbf{z}^{n+1})$ conserves H, indeed

$$H(\mathbf{z}^{n+1}) - H(\mathbf{z}^n) = (\mathbf{z}^{n+1} - \mathbf{z}^n)^\top \bar{\nabla} H(\mathbf{z}^n, \mathbf{z}^{n+1}) = \Delta t \bar{\nabla} H^\top \bar{\mathcal{J}}^\top \bar{\nabla} H = 0$$

provided $\bar{\mathcal{J}}$ is a skew-symmetric approximation of $\mathcal{J}(\mathbf{z})$.

Application to our problem: In order to find the above structure with simpler differential equations, from (3.7) we can consider the following split parts, in which the two parts of $\mathcal{J}$ remain antisymmetric

$$\begin{pmatrix} \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} \\ \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} \end{pmatrix} = \begin{pmatrix} 0 & \frac{1}{m} I_n \\ -\frac{1}{m} I_n & 0 \end{pmatrix} \begin{pmatrix} \nabla_{\mathbf{x}} H \\ \nabla_{\mathbf{v}} H \end{pmatrix} = \mathcal{J}_1 \nabla_{\mathbf{z}} H, \tag{3.22}$$

and

$$\begin{pmatrix} \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} \\ \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & \frac{q}{m^2}\mathbb{B}(\mathbf{x}) \end{pmatrix} \begin{pmatrix} \nabla_{\mathbf{x}} H \\ \nabla_{\mathbf{v}} H \end{pmatrix} = \mathcal{J}_2 \nabla_{\mathbf{z}} H, \tag{3.23}$$

the hamiltonian remaining in both cases $H(\mathbf{x}, \mathbf{v}) = \frac{1}{2} m v^2 + q\phi(\mathbf{x})$, which will be conserved in each part of the splitting and so for the full composed method.

The second part can be written equivalently

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = 0, \qquad \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \frac{q}{m}\mathbf{v} \times \mathbf{B}(\mathbf{x}).$$

This is the same as (3.15)–(3.16) for which an exact solution, which conserves the hamiltonian H is given by (3.18). On the other hand, the approximate solution given by (3.20) also conserves the hamiltonian and could also be used in an energy preserving method. Note that as $\nabla_{\mathbf{x}} H$ does not appear in the final system due to the form of $\mathcal{J}_2$ which has 0 on the blocks of the first line and an average gradient for $\nabla_{\mathbf{v}} H$ is $\bar{\nabla}_{\mathbf{v}} H = \frac{m}{2}(\mathbf{v}_1 + \mathbf{v}_0)$, so that (3.19) is indeed a discrete gradient discretisation of (3.15)–(3.16).

Let us now turn to the first subsystem (3.22), which is equivalent to

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v}, \qquad \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \frac{q}{m}\mathbf{E}(\mathbf{x}).$$

Straightforward discrete gradients can be obtained for quadratic hamiltonians, in particular as we have seen $\bar{\nabla}_{\mathbf{v}} H(\mathbf{v}^n, \mathbf{v}^{n+1}) = \frac{m}{2}(\mathbf{v}^{n+1} + \mathbf{v}^n)$, so that the first equation can be discretised by

$$\frac{\mathbf{x}^{n+1} - \mathbf{x}^n}{\Delta t} = \frac{1}{2}(\mathbf{v}^{n+1} + \mathbf{v}^n) \tag{3.24}$$

Now, the second equation of this system is more complex as it involves a general function $\phi(\mathbf{x})$ in the hamiltonian. In this case a general method yielding a discrete gradient is the *Average-vector-field* proposed by Celledoni et al. [5]. Here the $\mathbf{x}$ part of the hamiltonian is $q\phi(\mathbf{x})$ and the second component of $\mathcal{J}_1\nabla_{\mathbf{z}}H$ is $\frac{q}{m}\mathbf{E}(\mathbf{x})$ for which a discrete gradient can be defined over a linear trajectory going from $\mathbf{x}^n$ to $\mathbf{x}^{n+1}$ which reads

$$\bar{\nabla}_{\mathbf{x}}H(\mathbf{x}^n,\mathbf{x}^{n+1}) = q\int_0^1 \mathbf{E}(\mathbf{x}^n+\zeta(\mathbf{x}^{n+1}-\mathbf{x}^n))\ \mathrm{d}\zeta.$$

Indeed in this case

$$(\mathbf{x}^{n+1}-\mathbf{x}^n)\cdot\mathcal{J}_1\bar{\nabla}_{\mathbf{x}}H(\mathbf{x}^n,\mathbf{x}^{n+1}) = q\int_0^1 \frac{\mathrm{d}}{\mathrm{d}\zeta}\phi(\mathbf{x}^n+\zeta(\mathbf{x}^{n+1}-\mathbf{x}^n))\ \mathrm{d}\zeta = q\phi(\mathbf{x}^{n+1})-q\phi(\mathbf{x}^n),$$

So that the second discrete equation reads

$$\frac{\mathbf{v}^{n+1}-\mathbf{v}^n}{\Delta t} = q\int_0^1 \mathbf{E}(\mathbf{x}^n+\zeta(\mathbf{x}^{n+1}-\mathbf{x}^n))\ \mathrm{d}\zeta. \tag{3.25}$$

Note that for the hamiltonian to be conserved, this integral needs to be computed exactly, but this can be done for example when $\mathbf{E}$ is a finite element approximation whose basis functions are polynomials on each cell. Else if ϕ is a smooth analytical function the integral can be approximate to arbitrary accuracy by a high order quadrature rule. In all cases the system (3.24)–(3.25) needs to be solved iteratively using a Picard or a Newton method as it is nonlinearly implicit.

Chapter 4

Some useful notions from differential geometry

In this chapter we introduce the basic notions of differential geometry that will be needed for the Finite Element Exterior Calculus. We follow mostly the definitions from the book of Frankel [8] and the paper by Palha et al. [16] introducing so-called physics compatible discretization techniques.

4.1 Basic notions

The basic object of differential geometry is a manifold $\mathcal{M}$:

Definition 10 *A (differentiable) manifold of dimension n is defined as a collection of p mappings*

$$\begin{aligned}\mathbf{F}_\nu : U_\nu \subset \mathbb{R}^n &\to \mathcal{M},\\ \mathbf{q} &\mapsto \mathbf{F}_\nu(\mathbf{q}) = (x_1^\nu(\mathbf{q}), \ldots, x_n^\nu(\mathbf{q}))\end{aligned}$$

which are at least C^1 diffeomorphisms, that cover $\mathcal{M}$. The sets U_ν are open and the coordinate systems are compatible in the intersection of two such sets.

Each of the mapping $\mathbf{F}_\nu$ defines a local coordinate system (which is global if there is only one mapping). From the mappings we define the Jacobians

$$D\mathbf{F}_\nu(\mathbf{q}) = ((\frac{\partial x_i^\nu}{\partial q_j}))_{1\le i,j\le n}, \qquad D(\mathbf{F}_\nu^{-1})(\mathbf{x}) = ((\frac{\partial q_i}{\partial x_j^\nu}))_{1\le i,j\le n}.$$

Using the chain rule on $\mathbf{F}_\nu^{-1}(\mathbf{F}_\nu(\mathbf{q})) = \mathbf{q}$ one finds that $D(\mathbf{F}_\nu^{-1})(\mathbf{x}) = (D\mathbf{F}_\nu(\mathbf{q}))^{-1}$.

In our application the manifold will just be $\mathbb{R}^n$ with a unique mapping $\mathbf{F}$ defining the coordinate system. Another useful example to understand the notion is the surface of a sphere, which is a two-dimensional manifold, that needs at least two mappings (also called charts in the differential geometry literature, where they are sometimes defined by the inverse of the mapping we are using here) to be completely covered without singular point. See Figure 4.1 for an illustration.

An important goal in differential geometry is to define quantities independently of the local coordinates. Such quantities are called intrinsic.

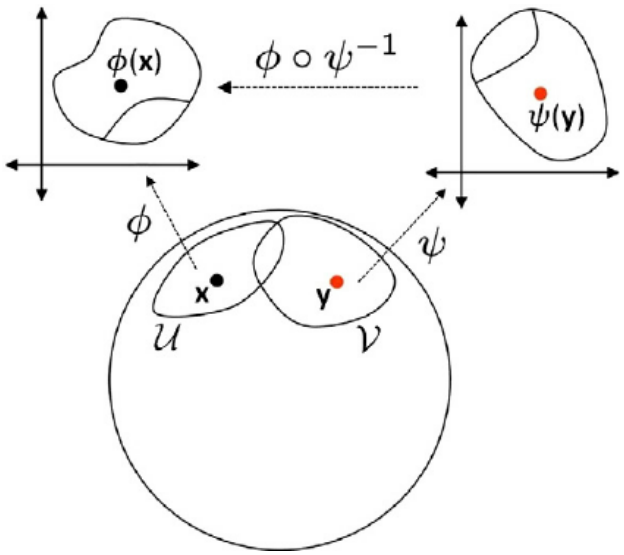

Figure 4.1: Illustration of two charts on a sphere.

Tangent plane and vectors. The first important object that can be associated to a point $\mathbf{x}$ in a manifold is a vector. A vector is intrinsically defined as the tangent at $\mathbf{x}$ to a curve passing through $\mathbf{x}$. In local coordinates a curve γ is parametrized by

$$\begin{aligned}\gamma :&[a,b] \to \mathcal{M} \\ &s \mapsto (x_1(\mathbf{q}(s)), \dots x_n(\mathbf{q}(s)))\end{aligned}$$

and its tangent at $\mathbf{x} = \gamma(c)$, $c \in [a,b]$ is

$$\mathbf{v}(c) = \frac{\mathrm{d}\gamma}{\mathrm{d}s}(c) = \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}s}(c) = \left(\frac{\mathrm{d}x_1}{\mathrm{d}s}(c), \dots, \frac{\mathrm{d}x_n}{\mathrm{d}s}(c) \right)^\top .$$

The collection of all possible curves passing through $\mathbf{x}$ on $\mathcal{M}$ define a vector for each curve and altogether the tangent plane $T_x\mathcal{M}$ at $\mathbf{x}$. If the $\mathcal{M} = \mathbb{R}^n$ as in our main application the tangent plane is also $T_x\mathcal{M} = \mathbb{R}^n$, however this is not always the case as one can figure out by considering the surface of a sphere as a manifold.

Considering not only the vector at a specific point $\mathbf{x} = \gamma(c)$ but all vectors defined by a curve $\mathbf{v}(s) = \frac{\mathrm{d}\gamma}{\mathrm{d}s}(s)$, $s \in [a,b]$ defines a *vector field*. The collection of all points associated to their tangent plane

$$T\mathcal{M} = \{(\mathbf{x}, \mathbf{v}), \quad \mathbf{x} \in \mathcal{M}, \mathbf{v} \in T_x\mathcal{M}\}$$

is called the *tangent bundle*.

The local coordinates defined by the mapping $\mathbf{F}$ also defines a basis of $T_x\mathcal{M}$. Indeed, using the mapping $\mathbf{x}(s) = \mathbf{F}(\mathbf{q}(s))$, we find

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}s} = \sum_{j=1}^{n} \frac{\mathrm{d}q^j}{\mathrm{d}s} \frac{\partial \mathbf{F}}{\partial q_j} = \sum_{j=1}^{n} v^j \frac{\partial \mathbf{F}}{\partial q_j}.$$

The corresponding basis vectors are $\mathbf{t}_j = \frac{\partial \mathbf{F}}{\partial q_j} := \boldsymbol{\partial}_j$. They depend on $\mathbf{x}$ although we generally don't make it explicit in their expression. Geometrically the basis vector $\boldsymbol{\partial}_i$ at a point $\mathbf{x} \in \mathcal{M}$

is associated to the curves passing through $\mathbf{x}$ obtained by letting all q_j $j \neq i$ one constant. These basis vectors are denoted in the modern differential geometry literature by $\boldsymbol{\partial}_j$, that we will use in these notes, or by $\frac{\partial}{\partial q_j}$. So that a vector $\mathsf{v} \in T_x\mathcal{M}$ can be expressed in the local coordinate basis by

$$\mathsf{v} = \sum_{i=1}^{n} v^i \boldsymbol{\partial}_i = (D\mathbf{F})\mathbf{v}.$$

We denote here in serif font v, the geometrical object. One can think of it as the vector expressed in a reference frame, typically cartesian coordinates of $\mathbb{R}^n$ or $\mathbb{R}^{n+m}$ for an object embedded in a higher dimension manifold (as the surface of a sphere). And we denote in bold font the components of a column vector in a local basis $\mathbf{v} = (v^1, \ldots, v^n)^\top$. The last form above is a matrix vector multiplication directly following from the definition of $\boldsymbol{\partial}_i$ as the i^{th} column of the Jacobian matrix $D\mathbf{F}$. As the geometric object is independent of the choice of local coordinates we have

$$\mathsf{v} = (D\mathbf{F})\mathbf{v} = (D\mathbf{F}')\mathbf{v}',$$

if $\mathbf{F}'$ defines another local coordinate system (mapping) in which $\mathbf{v}' = (v'^1, \ldots, v'^n)$ are the components of v. We follow here the convention of denoting the components of a tangent vector with upper indices and the basis vectors in the tangent plane with lower indices. This will lead to the Einstein summation convention, where elements with upper index multiplying elements with lower index are automatically summed: $v^i\boldsymbol{\partial}_i = \sum_{i=1}^n v^i\boldsymbol{\partial}_i$. Vectors or tangent vectors are also called contravariant vectors in the physics literature.

Example: Consider the mapping yielding polar coordinates

$$\mathbf{F}(r, \theta) = \begin{pmatrix} x_1 = r\cos\theta \\ x_2 = r\sin\theta \end{pmatrix}$$

A basis of the tangent plane at any point $\mathbf{x} = (x_1, x_2)$ is given by

$$\boldsymbol{\partial}_r = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}, \quad \boldsymbol{\partial}_\theta = \begin{pmatrix} -r\sin\theta \\ r\cos\theta \end{pmatrix}.$$

Here $\boldsymbol{\partial}_r$ is tangent to the line $\theta = C$ (only r varies) passing through $\mathbf{x}$ and $\boldsymbol{\partial}_\theta$ is tangent to the line $r = C$ (only θ varies) passing through $\mathbf{x}$. Note that this basis is not normalized, as opposed to the classical basis used in polar coordinates $\mathbf{e}_r = (\cos\theta, \sin\theta)^\top$, $\mathbf{e}_\theta = (-\sin\theta, \cos\theta)^\top$. Moreover unlike in cartesian coordinates where the basis vectors of the tangent plane are constants, in polar coordinates, as in any general system of curvilinear coordinates, or local coordinates, they depend on the point of which the tangent plane is considered.

4.2 Cotangent plane and covectors

Even though vectors (tangent vectors) and vector fields are the most intuitive objects for defining dynamics on a manifold, an another object proved to be mathematically more interesting the *covector* p, which is defined as a linear form on the tangent space at $\mathbf{x}$, *i.e.* a linear mapping from $T_x\mathcal{M} \to \mathbb{R}$, so that a covector applied to a vector yields a real number

$\mathsf{p}(\mathsf{v}) \in \mathbb{R}$, and is linear: $\mathsf{p}(\lambda_1\mathsf{v}_1 + \lambda_2\mathsf{v}_2) = \lambda_1\mathsf{p}(\mathsf{v}_1) + \lambda_2\mathsf{p}(\mathsf{v}_2)$. The collection of all covectors at $\mathbf{x}$ is called the *cotangent plane* at $\mathbf{x}$ and denoted by $T^*_x\mathcal{M}$. To a vector field we can then associate a covector at each corresponding point, this defines a covector field, which is more classically called a *differential form* or a *1-form*. In the same way as the tangent bundle, one can define the *cotangent bundle* by

$$T^*\mathcal{M} = \{(\mathbf{x}, \mathbf{p}), \quad \mathbf{x} \in \mathcal{M}, \mathbf{p} \in T^*_x\mathcal{M}\}.$$

The natural basis of $T^*_x\mathcal{M}$ is the dual basis of $\boldsymbol{\partial}_1, \dots, \boldsymbol{\partial}_n$ denoted by $\mathrm{d}q^1, \dots, \mathrm{d}q^n$ or $\mathrm{d}^1, \dots, \mathrm{d}^n$ and defined by $\mathrm{d}^i(\boldsymbol{\partial}_j) = \delta^i_j (= 1$ if $i = j$ and 0 else). From this definition, as the $\boldsymbol{\partial}_j$ are the columns of $D\mathbf{F}$ and $(D\mathbf{F})^{-1}D\mathbf{F} = \mathbb{I}_n$, the d^i are the lines of $(D\mathbf{F})^{-1}$. So the components $\mathbf{p}^\top = (p_1, \dots, p_n)$ of a covector p, which is a geometric object independent of the basis are defined by

$$\mathsf{p} = \sum_{i=1}^n p_i \, \mathrm{d}^i = \mathbf{p}^\top (D\mathbf{F})^{-1}.$$

The components of a covector define a line vector, which multiplies the inverse Jacobian matrix on the left. We therefore denote them using a transpose: $\mathbf{p}^\top$, and their components are denoted classically with a lower index. We can now express in local coordinates how a covector is applied to a vector:

$$\mathsf{p}(\mathsf{v}) = \sum_{i=1}^n p_i \, \mathrm{d}^i(\sum_{j=1}^n v^j \boldsymbol{\partial}_j) = \sum_{i=1}^n p_i v^i = \mathbf{p}^\top (D\mathbf{F})^{-1}(D\mathbf{F})\mathbf{v} = \mathbf{p}^\top \mathbf{v}.$$

We notice that the definition of the covectors is such that their application to a vector can be expressed directly using any local coordinate system without using the mapping $\mathbf{F}$. Indeed $\mathsf{p}(\mathsf{v}) = \mathbf{p}^\top \mathbf{v} = \mathbf{p}'^\top \mathbf{v}'$ independently of the local coordinate system. Because such sums involving a vector and a covector arrive frequently, we will use the Einstein sommation convention denoting by

$$p_i v^i = \sum_{i=1}^n p_i v^i.$$

A sum is implied where the same index appears as a lower index and an upper index in a product, hence implying a duality pairing between a covector and a vector.

4.3 p-forms

We have introduced 1-forms which associate a real number to any vector of the tangent plane $T_x\mathcal{M}$ at some given point $\mathbf{x} \in \mathcal{M}$. We shall use an index x to denote the dependence on a point on the manifold. We can now define the *tensor product* of two 1-forms, which is applied to two vectors $\mathbf{v}$ and $\mathbf{w}$, as

$$\alpha_x \otimes \beta_x(\mathbf{v}, \mathbf{w}) = \alpha_x(\mathbf{v})\beta_x(\mathbf{w})$$

and the *exterior product* of two one forms as

$$\alpha_x \wedge \beta_x(\mathbf{v}, \mathbf{w}) = \alpha_x \otimes \beta_x(\mathbf{v}, \mathbf{w}) - \beta_x \otimes \alpha_x(\mathbf{v}, \mathbf{w}) = \alpha_x(\mathbf{v})\beta_x(\mathbf{w}) - \alpha_x(\mathbf{w})\beta_x(\mathbf{v}).$$

From this definition, it follows that the exterior product of two 1-forms is antisymmetric

$$\alpha_x \wedge \beta_x(\mathbf{v}, \mathbf{w}) = -\beta_x \wedge \alpha_x(\mathbf{v}, \mathbf{w}).$$

The exterior product of two 1-forms should be a 2-form. So this leads to the definition of a 2-form as an antisymmetric element of $T_x^*\mathcal{M} \times T_x^*\mathcal{M}$ and more generally the p-forms are defined as follows:

Definition 11 *A p-form α^p is a p-linear form on $T_x\mathcal{M} \times \cdots \times T_x\mathcal{M}$ (p times), which is alternating, i.e.*

$$\begin{aligned} \alpha_x^p :\ & T_x\mathcal{M} \times \cdots \times T_x\mathcal{M} \to \mathbb{R} \\ & (\mathbf{v}_1, \ldots, \mathbf{v}_p) \mapsto \alpha_x^p(\mathbf{v}_1, \ldots, \mathbf{v}_p) \end{aligned}$$

such that

$$\alpha_x^p(\ldots, \mathbf{v}_i, \ldots, \mathbf{v}_j, \ldots) = -\alpha_x^p(\ldots, \mathbf{v}_j, \ldots, \mathbf{v}_i, \ldots).$$

When two vectors are exchanged, all the others staying the same, the sign of the p-form changes. This is a generalization of anti-symmetry to p variables. This implies in particular, that when a vector appears twice in the arguments the p-form vanishes. We denote a p-form by α^p with an upper right index when we wish to explicit the degree p of the form. When it is useful to recall its dependency on $\mathbf{x}$ we write α_x^p.

Due to the alternating property, in a manifold of dimension n all p-forms for $p > n$ vanish. This can be seen by decomposing all the vectors on a basis, which contains exactly n-elements.

We will denote the space of p-forms on the manifold $\mathcal{M}$ by $\Lambda^p(\mathcal{M})$ for $p = 0, \ldots, n$. The 0-forms are the scalar functions on $\mathcal{M}$. The n-forms in a manifold of dimension n are also well known from linear algebra. Indeed at a point $\mathbf{x}$ of the manifold a n-form is a n-covector defined as an alternating n-linear form, which is the definition of the determinant of n vectors.

Definition 12 *The* exterior *product of a k-form and a l-form is a mapping*

$$\wedge :\ \Lambda^k(\mathcal{M}) \times \Lambda^l(\mathcal{M}) \to \Lambda^{k+l}(\mathcal{M}) \qquad k + l \leq n$$

satisfying the following properties

$$\begin{aligned} &\textit{antisymmetry:} && \alpha^k \wedge \beta^l = (-1)^{kl} \beta^l \wedge \alpha^k && (4.1) \\ &\textit{associativity:} && (\alpha^k \wedge \beta^l) \wedge \gamma^m = \alpha^k \wedge (\beta^l \wedge \gamma^m) && (4.2) \\ &\textit{distributivity:} && (\alpha^k + \beta^k) \wedge \gamma^m = \alpha^k \wedge \gamma^m + \beta^k \wedge \gamma^m && (4.3) \end{aligned}$$

where $\alpha^k \in \Lambda^k(\mathcal{M})$, $\beta^l \in \Lambda^l(\mathcal{M})$, $\gamma^m \in \Lambda^m(\mathcal{M})$.

Note that the wedge product with a 0-form is just a multiplication with a scalar function.

Given a basis $(\mathrm{d}q^1, \ldots, \mathrm{d}q^n)$ of the space of 1-forms $\Lambda^1(\mathcal{M})$, a basis of $\Lambda^p(\mathcal{M})$ is given by all possible combinations of p distinct $\mathrm{d}q^i$ by wedge product. The order is fixed arbitrarily, for example by imposing that the indices are in increasing order:

$$\alpha^p(\mathbf{x}) = \sum_{i_1 < \cdots < i_p} \alpha_{i_1, \ldots, i_p}(\mathbf{x})\, \mathrm{d}q^{i_1} \wedge \cdots \wedge \mathrm{d}q^{i_p}.$$

The dimension of $\Lambda^p(\mathcal{M})$ is thus $\binom{n}{p} = n!/(p!(n-p)!)$

Example: In $\mathbb{R}^3$, the zero forms are the scalar functions. The 1-forms, 2-forms, 3-forms can be expressed in the local basis by

$$\alpha^0(\mathbf{x}) = \alpha(\mathbf{x}), \tag{4.4}$$
$$\alpha^1(\mathbf{x}) = \alpha_1(\mathbf{x})\,\mathrm{d}q^1 + \alpha_2(\mathbf{x})\,\mathrm{d}q^2 + \alpha_3(\mathbf{x})\,\mathrm{d}q^3, \tag{4.5}$$
$$\alpha^2(\mathbf{x}) = \alpha_{23}(\mathbf{x})\,\mathrm{d}q^2 \wedge \mathrm{d}q^3 + \alpha_{31}(\mathbf{x})\,\mathrm{d}q^3 \wedge \mathrm{d}q^1 + \alpha_{12}(\mathbf{x})\,\mathrm{d}q^1 \wedge \mathrm{d}q^2, \tag{4.6}$$
$$\alpha^3(\mathbf{x}) = \alpha_{123}(\mathbf{x})\,\mathrm{d}q^1 \wedge \mathrm{d}q^2 \wedge \mathrm{d}q^3. \tag{4.7}$$

We note that the 1-forms and 2-forms have 3 scalar components and the 0-forms and 3-forms have 1 scalar component. In order to evaluate the basis p-form on vectors, one can use the formulas for determinants

$$\mathrm{d}q^i(\mathbf{v}) = v^i$$
$$\mathrm{d}q^i \wedge \mathrm{d}q^j(\mathbf{v},\mathbf{w}) = \begin{vmatrix} \mathrm{d}q^i(\mathbf{v}) & \mathrm{d}q^i(\mathbf{w}) \\ \mathrm{d}q^j(\mathbf{v}) & \mathrm{d}q^j(\mathbf{w}) \end{vmatrix} = v^i w^j - v^j w^i,$$
$$\mathrm{d}q^1 \wedge \mathrm{d}q^2 \wedge \mathrm{d}q^3(\mathbf{u},\mathbf{v},\mathbf{w}) = \begin{vmatrix} \mathrm{d}q^1(\mathbf{u}) & \mathrm{d}q^1(\mathbf{v}) & \mathrm{d}q^1(\mathbf{w}) \\ \mathrm{d}q^2(\mathbf{u}) & \mathrm{d}q^2(\mathbf{v}) & \mathrm{d}q^2(\mathbf{w}) \\ \mathrm{d}q^3(\mathbf{u}) & \mathrm{d}q^3(\mathbf{v}) & \mathrm{d}q^3(\mathbf{w}) \end{vmatrix} = \begin{vmatrix} u^1 & v^1 & w^1 \\ u^2 & v^2 & w^2 \\ u^3 & v^3 & w^3 \end{vmatrix}.$$

Remark 6 *Following the intuitive definition of the Riemann integral, paving the space into small segments, we observe that 1-forms, which are applied to one single vector, will be naturally integrated along curves, 2-forms, which take 2 vectors, will be naturally integrated on surfaces and 3-forms taking 3 vectors will be naturally integrated on volumes. 0-forms for their part cannot be integrated, one only takes their point values.*

This idea comes back when discretising on a mesh. 0-form degrees of freedom are associated to points of the mesh (e.g. vertices), 1-forms to edges, 2-forms to faces and 3-forms to cells or volumes.

4.4 Riemanian metric

The structures that we have built on our manifold up to now do not allow us to define the length of a vector. For this we need a new structure call Riemannian metric defined as follows:

Definition 13 *A* Riemannian metric *g on a smooth manifold $\mathcal{M}$ is a scalar product (a bilinear symmetric positive definite form) on the tangent spaces $T_x\mathcal{M}$ that varies smoothly with $\mathbf{x}$, i.e.*

$$g_x : T_x\mathcal{M} \times T_x\mathcal{M} \to \mathbb{R}$$

such that g_x is bilinear and

(i) $g_x(\mathbf{v},\mathbf{w}) = g_x(\mathbf{w},\mathbf{v})$, $\forall \mathbf{v},\mathbf{w} \in T_x\mathcal{M}$,

(ii) $g_x(\mathbf{v},\mathbf{v}) \geq 0$ $\forall \mathbf{v} \in T_x\mathcal{M}$,

(iii) $g_x(\mathbf{v},\mathbf{v}) = 0 \Leftrightarrow \mathbf{v} = 0$,

(iv) For any smooth vector fields $\mathbf{v}_x, \mathbf{w}_x$, the mapping $\mathbf{x} \mapsto g_x(\mathbf{v}_x, \mathbf{w}_x)$ is smooth.

In our applications, the tangent planes are $\mathbb{R}^n$, which is equipped with the euclidian scalar product $\cdot$. We can express it in the natural basis of $T_x\mathcal{M}$, $\boldsymbol{\partial}_1, \ldots, \boldsymbol{\partial}_n$:

$$g_x(\mathbf{v}, \mathbf{w}) = \mathsf{v} \cdot \mathsf{w} = \sum_{i,j=1}^{n} v^i w^j \boldsymbol{\partial}_i \cdot \boldsymbol{\partial}_j.$$

Denoting by $g_{ij} = \boldsymbol{\partial}_i \cdot \boldsymbol{\partial}_j$, the scalar product is expressed in the tangent basis $\boldsymbol{\partial}_1, \ldots, \boldsymbol{\partial}_n$ by

$$g_x(\mathbf{v}, \mathbf{w}) = \sum_{i,j=1}^{n} v^i w^j g_{ij} = v^i w^j g_{ij}$$

using the Einstein summation convention. Obviously this reduces to the classical formula $\sum v^i w^i$ when the canonical basis of $\mathbb{R}^n$ is used (corresponding to an identity mapping) as $g_{ij} = \delta_{ij}$ in this case.

The metric enables us to associate a covector to a vector in a unique way. Indeed, given a vector $\mathbf{v} \in T_x\mathcal{M}$, $\mathbf{w} \mapsto g_x(\mathbf{v}, \mathbf{w})$ defines a linear form on $T_x\mathcal{M}$, i.e. an element $\mathsf{p} \in T_x^*\mathcal{M}$ such that $\mathbf{p}(\mathbf{w}) = g_x(\mathbf{v}, \mathbf{w})$. This can be written in local coordinates

$$\mathbf{p}^\top \mathbf{w} = \mathbf{v}^\top G \mathbf{w} \quad \text{or equivalently} \quad p_j w^j = v^i g_{ij} w^j$$

using Einstein's summation convention, that we will use systematically in the sequel, where G is the $n \times n$ matrix with entries g_{ij}. As this is verified for any $\mathbf{w} \in T_x\mathcal{M}$, it follows that $p_i = g_{ij} v^j$ ($\Leftrightarrow \mathbf{p}^\top = \mathbf{v}^\top G$). In particular in cartesian coordinates, where G is the identity matrix, a covector has the same components as the vector it is associated to. Note that due to the definition of g_{ij} with the tangent vectors, G can be expressed using the Jacobian of the mapping $G = (D\mathbf{F})^\top D\mathbf{F}$ and the inverse of G whose coefficients are denoted by g^{ij} verifies $G^{-1} = (D\mathbf{F})^{-1} D\mathbf{F}^{-\top}$, so that

$$g^{ij} = \mathbf{d}^i \cdot \mathbf{d}^j. \tag{4.8}$$

4.5 Exterior derivative

Definition 14 *The* exterior derivative*, denoted by* d *is the unique operator from* $\Lambda^p(\mathcal{M}) \to \Lambda^{p+1}(\mathcal{M})$ *satisfying:*

(i) d *is additive:* $\mathrm{d}(\alpha + \beta) = \mathrm{d}\alpha + \mathrm{d}\beta$,

(ii) $\mathrm{d}\alpha^0$ *is the usual differential of functions,*

(iii) $\mathrm{d}(\alpha^p \wedge \beta^q) = \mathrm{d}\alpha^p \wedge \beta^q + (-1)^p \alpha^p \wedge \mathrm{d}\beta^q$*, (Leibniz rule),*

(iv) $\mathrm{d}^2\alpha = \mathrm{d}(\mathrm{d}\alpha) = 0$.

See Frankel [8] p. 53 for a proof of the uniqueness.

Let us compute exterior derivatives in $\mathbb{R}^3$. For this we shall in particular need $\mathrm{d}\,\mathrm{d}q^i = 0$ and (*iii*) for a scalar function, which is a 0-form ($p = 0$):

$$\mathrm{d}(\alpha^0 \wedge \beta^q) = \mathrm{d}\alpha^0 \wedge \beta^q + \alpha^0\, \mathrm{d}\beta^q.$$

For a 0-form $\alpha^0_x = \alpha(\mathbf{q})$ for some smooth scalar function α, we get

$$\mathrm{d}\alpha^0_x = \frac{\partial\alpha}{\partial q^1}(\mathbf{q})\,\mathrm{d}q^1 + \frac{\partial\alpha}{\partial q^2}(\mathbf{q})\,\mathrm{d}q^2 + \frac{\partial\alpha}{\partial q^3}(\mathbf{q})\,\mathrm{d}q^3.$$

For a 1-form $\alpha^1_{\mathbf{x}} = \alpha_1(\mathbf{q})\,\mathrm{d}q^1 + \alpha_2(\mathbf{q})\,\mathrm{d}q^2 + \alpha_3(\mathbf{q})\,\mathrm{d}q^3$, we have

$$\begin{aligned}
\mathrm{d}\alpha^1_{\mathbf{x}} =& \ \mathrm{d}\alpha_1(\mathbf{q}) \wedge \mathrm{d}q^1 + \mathrm{d}\alpha_2(\mathbf{q}) \wedge \mathrm{d}q^2 + \mathrm{d}\alpha_3(\mathbf{q}) \wedge \mathrm{d}q^3 \\
=& \sum_{i=1}^{3} \left(\frac{\partial\alpha_i}{\partial q^1}(\mathbf{q})\,\mathrm{d}q^1 + \frac{\partial\alpha_i}{\partial q^2}(\mathbf{q})\,\mathrm{d}q^2 + \frac{\partial\alpha_i}{\partial q^3}(\mathbf{q})\,\mathrm{d}q^3 \right) \wedge \mathrm{d}q^i \\
=& \left(\frac{\partial\alpha_2}{\partial q^1} - \frac{\partial\alpha_1}{\partial q^2} \right) \mathrm{d}q^1 \wedge \mathrm{d}q^2 + \left(\frac{\partial\alpha_1}{\partial q^3} - \frac{\partial\alpha_3}{\partial q^1} \right) \mathrm{d}q^3 \wedge \mathrm{d}q^1 \\
&+ \left(\frac{\partial\alpha_3}{\partial q^2} - \frac{\partial\alpha_2}{\partial q^3} \right) \mathrm{d}q^2 \wedge \mathrm{d}q^3
\end{aligned}$$

Note that the components of the exterior derivative of the 1-form are the components of the curl in cartesian coordinates.

For a 2-form $\alpha^2(\mathbf{x}) = \alpha_{23}(\mathbf{q})\,\mathrm{d}q^2 \wedge \mathrm{d}q^3 + \alpha_{31}(\mathbf{q})\,\mathrm{d}q^3 \wedge \mathrm{d}q^1 + \alpha_{12}(\mathbf{q})\,\mathrm{d}q^1 \wedge \mathrm{d}q^2$, we have

$$\begin{aligned}
\mathrm{d}\alpha^2(\mathbf{x}) =& \ \mathrm{d}\alpha_{23} \wedge \mathrm{d}q^2 \wedge \mathrm{d}q^3 + \mathrm{d}\alpha_{31} \wedge \mathrm{d}q^3 \wedge \mathrm{d}q^1 + \mathrm{d}\alpha_{12} \wedge \mathrm{d}q^1 \wedge \mathrm{d}q^2 \\
=& \left(\frac{\partial\alpha_{23}}{\partial q^1} + \frac{\partial\alpha_{31}}{\partial q^2} + \frac{\partial\alpha_{12}}{\partial q^3} \right) \mathrm{d}q^1 \wedge \mathrm{d}q^2 \wedge \mathrm{d}q^3.
\end{aligned}$$

Here we recognize the formula for the divergence in cartesian coordinates. And finally for a 3-form $\alpha^{(3)}(\mathbf{x}) = \alpha_{123}(\mathbf{q})\,\mathrm{d}q^1 \wedge \mathrm{d}q^2 \wedge \mathrm{d}q^3$, we get $\mathrm{d}\alpha^{(3)} = 0$.

4.6 Interior product

Definition 15 *The* interior product *of a p-form α^p and a vector $\mathbf{v}$ is the $(p-1)$-form denoted by $\mathrm{i}_{\mathbf{v}}\alpha^p$ such that*

$$\mathrm{i}_{\mathbf{v}}\alpha^p(\mathbf{v}_1, \ldots, \mathbf{v}_{p-1}) = \alpha^p(\mathbf{v}, \mathbf{v}_1, \ldots, \mathbf{v}_{p-1}). \tag{4.9}$$

For a 0-form $\mathrm{i}_{\mathbf{v}}\alpha^0 = 0$.

Proposition 7 *The interior product $\mathrm{i}_{\mathbf{v}} : \Lambda^p(\mathcal{M}) \to \Lambda^{p-1}(\mathcal{M})$ is an* anti-derivation*, i.e. it verifies the Leibniz rule*

$$\mathrm{i}_{\mathbf{v}}(\alpha^p \wedge \beta^q) = (\mathrm{i}_{\mathbf{v}}\alpha^p) \wedge \beta^q + (-1)^p \alpha^p \wedge (\mathrm{i}_{\mathbf{v}}\beta^q). \tag{4.10}$$

Note that this is the same property as property *(iii)* of the exterior derivative which is also an anti-derivation. The difference between an anti-derivation and a standard derivation (property of derivatives) is the $(-1)^p$ factor in front of the second term.

4.7 Orientation and twisted forms

In an n-dimensional vector space two bases are related by a transformation matrix P such that, $\det P \neq 0$. From that one can define two classes of bases, those that have the same

orientation are related by a transformation matrix with a positive sign and those that have a different orientation by a transformation matrix with a negative sign. The orientation of a vector space is chosen by arbitrarily choosing a basis, which defines the positive orientation. This is classically done in $\mathbb{R}^3$ with the right-hand rule.

Definition 16 *We say that a n-dimensional manifold $\mathbf{M}_n$ is orientable, if it can be covered with coordinate patches having all the same orientation.*

A classical example of non orientable manifold is the moebius band.

We shall denote by $o(\boldsymbol{\partial}_1, \ldots, \boldsymbol{\partial}_n)$ the orientation of a basis defined by a local coordinate system, $o(\boldsymbol{\partial}_1, \ldots, \boldsymbol{\partial}_n)$ can take the values $+1$ or -1.

The orientation is used to define *twisted forms* sometimes also called *pseudo-forms*, which are defined not to depend on the orientation of the local coordinate system. To achieve this, the orientation is part of the definition of the twisted-form: In a positively oriented local coordinate system $\tilde{\alpha}^p = \alpha^p$ and in a negatively oriented local coordinate system $\tilde{\alpha}^p = -\alpha^p$.

An important twisted form is the *volume form*, which is a twisted n-form represented in a local coordinate system $(q^1, \ldots, q^n)$ on a riemannian manifold of dimension n by

$$\mathrm{vol}^n = o(\boldsymbol{\partial}_1, \ldots \boldsymbol{\partial}_n)\sqrt{g}\, \mathrm{d}q^1 \wedge \cdots \wedge \mathrm{d}q^n,$$

where $\sqrt{g} = \det(D\mathbf{F})$ is the Jacobian of the mapping defining the local coordinate system. Indeed as $G = (D\mathbf{F})^\top D\mathbf{F}$, $g := \det G = (\det(D\mathbf{F}))^2$.

Remark 7 *As the metric can be used to associate a 1-form to a vector, the volume form along with the interior product defines a (n-1)-form associated to a vector: Given a vector* $\mathbf{v}$ $\mathrm{i}_{\mathbf{v}}\mathrm{vol}^n$ *defines a (n-1)-form.*

In particular in a three dimensional manifold for a vector $\mathbf{u}$

$$\mathrm{i}_{\mathbf{u}}\mathrm{vol}^3(\mathbf{v}, \mathbf{w}) = \mathrm{vol}^3(\mathbf{u}, \mathbf{v}, \mathbf{w}) = \sqrt{g} \begin{vmatrix} u^1 & v^1 & w^1 \\ u^2 & v^2 & w^2 \\ u^3 & v^3 & w^3 \end{vmatrix}$$

4.8 Scalar product of p-forms and Hodge $\star$ operator

Given a metric g on an n-dimensional manifold $\mathcal{M}$, we can define a scalar product of the exterior product of p 1-form basis functions in the following way ([11] Section 3.3):

$$\langle \mathrm{d}q^{i_1} \wedge \cdots \wedge \mathrm{d}q^{i_p}, \mathrm{d}q^{j_1} \wedge \cdots \wedge \mathrm{d}q^{j_p} \rangle = \det(\mathrm{d}q^{i_m} \cdot \mathrm{d}q^{j_n})_{m,n} = \det(g^{i_m, j_n})_{m,n}, \tag{4.11}$$

where the last equality follows from the definition of the metric (4.8). Now for two generic p-forms written in local coordinates

$$\alpha_x^p = \sum_{i_1 < \cdots < i_p} \alpha_{i_1 \ldots i_p} \mathrm{d}q^{i_1} \wedge \cdots \wedge \mathrm{d}q^{i_p}, \quad \beta_x^p = \sum_{j_1 < \cdots < j_p} \beta_{j_1 \ldots j_p} \mathrm{d}q^{j_1} \wedge \cdots \wedge \mathrm{d}q^{j_p},$$

it follows by multilinearity, that we define the scalar product of two p-forms at $\mathbf{x}$ on $T_x\mathcal{M}$ by

$$\begin{aligned} \langle \alpha_x^p, \beta_x^p \rangle &= \sum_{i_1 < \cdots < i_p} \alpha_{i_1 \ldots i_p} \beta_{j_1 \ldots j_p} \langle \mathrm{d}q^{i_1} \wedge \cdots \wedge \mathrm{d}q^{i_p}, \mathrm{d}q^{j_1} \wedge \cdots \wedge \mathrm{d}q^{j_p} \rangle \\ &= \sum_{i_1 < \cdots < i_p} \alpha_{i_1 \ldots i_p} \beta_{j_1 \ldots j_p} \det(g^{i_m, j_n})_{m,n}, \qquad (4.12) \\ &= \sum_{i_1 < \cdots < i_p} \alpha_{i_1 \ldots i_p} \beta^{i_1 \ldots i_p}. \qquad (4.13) \end{aligned}$$

The last expression comes from the appropriate definition of index raising for p-forms as follows

$$\beta^{i_1\dots i_p} = \sum_{k_1,\dots,k_p} g^{i_1k_1}\dots g^{i_pk_p}\beta_{k_1\dots k_p}. \tag{4.14}$$

Beware that here, in order to capture all the terms in the determinant, the sum is over all possible $k_1,\dots,k_n$, not only those in increasing order. For a permutation σ of the indices $\beta_{\sigma(k_1\dots k_p)} = \mathrm{sgn}(\sigma)\beta_{k_1\dots k_p}$, $\mathrm{sgn}(\sigma)$ being 1 for an even permutation and -1 for an odd permutation, so that all needed terms can be defined from those in increasing order that are known. For repeated indices the coefficient is zero. We observe that for 1-forms this yields the classical index raising formula.

We now define the Hodge $\star$ of α^p at $\mathbf{x}$ and denote by $\star\alpha^p_x$ the pseudo $(n-p)$-form

$$\star\alpha^p_x = \tilde{\alpha}^{n-p}_x = \sum_{j_1<\dots<j_{n-p}} \alpha^*_{j_1\dots j_{n-p}}\,\mathrm{d}q^{j_1}\wedge\dots\wedge\,\mathrm{d}q^{j_{n-p}},$$

with $\alpha^*_{j_1\dots j_{n-p}} = \sqrt{|g|}\alpha^{k_1\dots k_p}\epsilon_{k_1\dots k_pj_1\dots j_{n-p}}$ using the index raising formula (4.14) and where $\epsilon_{i_1\dots i_n}$ assumes each index appears only once and $\epsilon_{i_1\dots i_n} = 1$ for an even permutation of $(1,\dots,n)$ and $\epsilon_{i_1\dots i_n} = -1$ for an odd permutation.

As an example, let us compute the Hodge $\star$ of general 1-forms and 2-forms in cartesian coordinates:

$$\star(\alpha_1\,\mathrm{d}q^1 + \alpha_2\,\mathrm{d}q^2 + \alpha_3\,\mathrm{d}q^3) = \alpha_1\,\mathrm{d}q^2\wedge\,\mathrm{d}q^3 + \alpha_2\,\mathrm{d}q^3\wedge\,\mathrm{d}q^1 + \alpha_3\,\mathrm{d}q^1\wedge\,\mathrm{d}q^2.$$

An important example is the Hodge of the constant 0-form 1, which is the twisted volume form vol^n:

$$\star 1 = \sqrt{|g|}\epsilon_{12\dots n}\,\mathrm{d}q^1\wedge\dots\wedge\,\mathrm{d}q^n = \mathrm{vol}^n.$$

Note also that the Hodge $\star$ of a twisted p-form defines a (n-p)-form.

Let us also recall that applying twice the Hogde operator to a p-form in a manifold of dimension n yields

$$\star\star\,\alpha^p = (-1)^{p(n-p)}\alpha^p. \tag{4.15}$$

We observe that for n odd, in particular for $n=3$, we always have $\star\star\,\alpha^p = \alpha^p$.

From this definition of the Hodge $\star$ it follows that for two p-forms α^p and β^p

$$\alpha^p\wedge\star\beta^p = \sum_{k_1<\dots<k_p}\alpha_{k_1\dots k_p}\beta^{k_1\dots k_p}\mathrm{vol}^n = \langle\alpha^p,\beta^p\rangle\mathrm{vol}^n,$$

using the scalar product of p-forms (4.13).

Integrating over the manifold we can then define the following scalar product on $\Lambda^p(\mathcal{M})$

$$(\alpha^p,\beta^p) = \int\langle\alpha^p_x,\beta^p_x\rangle\mathrm{vol}^n = \int\alpha^p\wedge\star\beta^p. \tag{4.16}$$

Given this scalar product and its associated norm we define the Hilbert spaces

$$L^2\Lambda^p(\mathcal{M}) = \{\alpha^p\in\Lambda^p(\mathcal{M})\mid(\alpha^p,\alpha^p)<+\infty\},$$

$$H\Lambda^p(\mathcal{M}) = \{\omega^p\in L^2\Lambda^p(\mathcal{M}),\,\mathrm{d}\omega^p\in L^2\Lambda^{p+1}(\Omega)\}.$$

These Hilbert spaces of differential forms form the so-called de Rham complex, which is at the heart of the FEEC theory

$$0 \to H\Lambda^0(\mathcal{M}) \overset{\mathrm{d}}{\to} H\Lambda^1(\mathcal{M}) \overset{\mathrm{d}}{\to} \cdots \overset{\mathrm{d}}{\to} H\Lambda^n(\mathcal{M}) \to 0. \tag{4.17}$$

In a three dimensional manifold the de Rham complex can also be express in the classical vector analysis language:

$$0 \to H^1(\Omega) \overset{\mathrm{grad}}{\to} H(\mathrm{curl}, \Omega) \overset{\mathrm{curl}}{\to} H(\mathrm{div}, \Omega) \overset{\mathrm{div}}{\to} L^2(\Omega) \to 0.$$

4.9 Pullback of differential forms

Consider a smooth map $\boldsymbol{\varphi} : \mathcal{M} \to \mathcal{M}'$, where $\mathcal{M}$ and $\mathcal{M}'$ are two manifolds, not necessarily of the same dimension.

Through this map a vector in the tangent plane $\mathsf{v} \in T_x\mathcal{M}$ induces a vector $\boldsymbol{\varphi}_*\mathsf{v} = (D\boldsymbol{\varphi})\mathbf{v} \in T_{\boldsymbol{\varphi}(\mathbf{x})}\mathcal{M}'$ in the tangent plane at $\boldsymbol{\varphi}(\mathbf{x})$ of $\mathcal{M}'$ called the *push-forward* of v. From this, one can for a p-form $\omega_{x'}$ at a point $\mathbf{x}' \in \mathcal{M}'$ associate a p-form at the pre-image of $\mathbf{x}'$ on $\mathcal{M}$ denoted by $\boldsymbol{\varphi}^*\omega$ and called *pull-back* of the p-form ω. It is defined by

$$(\boldsymbol{\varphi}^*\omega)_x(\mathbf{v}_1, \ldots, \mathbf{v}_p) = \omega_{\boldsymbol{\varphi}(\mathbf{x})}((D\boldsymbol{\varphi})_x\mathbf{v}_1, \ldots, (D\boldsymbol{\varphi})_x\mathbf{v}_p). \tag{4.18}$$

Very important and convenient properties of the pullback are that they respect exterior products and differentiation

$$\boldsymbol{\varphi}^*(\alpha \wedge \beta) = (\boldsymbol{\varphi}^*\alpha) \wedge (\boldsymbol{\varphi}^*\beta), \qquad \mathrm{d}(\boldsymbol{\varphi}^*\alpha) = \boldsymbol{\varphi}^*(\,\mathrm{d}\alpha). \tag{4.19}$$

An important special case is when $\mathcal{M}'$ is a submanifold of $\mathcal{M}$ and $\boldsymbol{\varphi}$ the inclusion, then the pullback is the trace map. With this definition we can write the Stokes theorem

$$\int_{\mathcal{M}} \mathrm{d}\omega = \int_{\partial\mathcal{M}} \mathrm{tr}\,\omega.$$

Green formula and codifferential operator Using the Leibniz rule, (iii) of definition 8, and the Stokes theorem, we can derive a Green type integration by parts formula for differential forms

$$\int_{\mathcal{M}} \mathrm{d}\alpha^{p-1} \wedge \beta^{n-p} = (-1)^p \int_{\mathcal{M}} \alpha^{p-1} \wedge\, \mathrm{d}\beta^{n-p} + \int_{\partial\mathcal{M}} \mathrm{tr}\,\alpha^{p-1} \wedge \mathrm{tr}\,\beta^{n-p}, \qquad \forall \alpha^{p-1} \in \Lambda^{p-1}(\mathcal{M}),\ \beta^{n-p} \in \Lambda^{n-p}(\mathcal{M}). \tag{4.20}$$

Let us now introduce the coderivative operator $\mathrm{d}^* : \Lambda^p(\mathcal{M}) \to \Lambda^{p-1}(\mathcal{M})$ defined by

$$\star\mathrm{d}^*\alpha^p = (-1)^p\,\mathrm{d}\star\alpha^p. \tag{4.21}$$

We can then express the Green formula (4.20) using the scalar product on differential forms (4.16). Indeed setting $\beta^{n-p} = \star\gamma^p$, (4.20) becomes

$$\int_{\mathcal{M}} \mathrm{d}\alpha^{p-1} \wedge \star\gamma^p = (-1)^p \int_{\mathcal{M}} \alpha^{p-1} \wedge\, \mathrm{d}\star\gamma^p + \int_{\partial\mathcal{M}} \mathrm{tr}\,\alpha^{p-1} \wedge \mathrm{tr}\,\star\gamma^p,$$

and so using the definition of the codifferential and of the scalar product (4.16) this can be written equivalently

$$(\,\mathrm{d}\alpha^{p-1}, \gamma^p) = (\alpha^{p-1},\, \mathrm{d}^*\gamma^p) + \int_{\partial\mathcal{M}} \mathrm{tr}\,\alpha^{p-1} \wedge \mathrm{tr} \star\gamma^p. \tag{4.22}$$

Hence, the codifferential is the formal adjoint of the exterior derivative. It is the adjoint if the boundary terms vanish. This explains the notation.

4.10 Maxwell's equations with differential forms

There is a natural interpretation of physics objects with differential forms. In many cases it is more natural than with vectors. For example a force is naturally defined through the work it performs along a curve, which leads to its being a 1-form. The magnetic intensity is measured as a flux through a loop and thus is naturally a 2-form.

In classical vector analysis, Maxwell's equations read

$$-\frac{\partial \mathbf{D}}{\partial t} + \nabla \times \mathbf{H} = \mathbf{J}, \tag{4.23}$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0, \tag{4.24}$$

$$\nabla \cdot \mathbf{D} = \rho, \tag{4.25}$$

$$\nabla \cdot \mathbf{B} = 0. \tag{4.26}$$

These relations are supplemented by the material constitutive relations $\mathbf{D} = \varepsilon\mathbf{E}$, $\mathbf{B} = \mu\mathbf{H}$, where ε is the permittivity tensor (in vacuum it is the constant ε_0), and μ is the permeability tensor of the material (in vacuum it is the constant μ_0). $\mathbf{H}$ and $\mathbf{E}$ are respectively the magnetic field and the electric field, whereas $\mathbf{B}$ is the called magnetic flux intensity or magnetic induction and $\mathbf{D}$ is the electric displacement field.

Given that the curl corresponds to the exterior derivative applied to a 1-form and the divergence to the exterior derivative applied to a 2-form, we find a natural way of writing Maxwell's equations in terms of differential forms

$$-\frac{\partial \mathbf{d}^2}{\partial t} + \mathrm{d}\mathbf{h}^1 = \mathbf{j}^2 \tag{4.27}$$

$$\frac{\partial \mathbf{b}^2}{\partial t} + \mathrm{d}\mathbf{e}^1 = 0, \tag{4.28}$$

$$\mathrm{d}\mathbf{d}^2 = \rho^3, \tag{4.29}$$

$$\mathrm{d}\mathbf{b}^2 = 0. \tag{4.30}$$

The constitutive relations associate 2-forms to 1-forms and thus need to be described by a Hodge $\star$ operator in the differential forms description:

$$\mathbf{d}^2 = \star\mathbf{e}^1, \qquad \mathbf{h}^1 = \star\mathbf{b}^2. \tag{4.31}$$

As the Hodge operator associates twisted forms to straight forms and conversely, it follows from this that either the forms in Ampere's equations (4.27) are twisted forms and the forms in Faraday's equation (4.28) are straight forms other the other way. Mathematically both

options are possible, but physically the sources ρ^3 and $\mathbf{j}^2$ are charge and current densities which should be twisted see e.g. [4, 7]. Therefore, we will consider that $\mathbf{h}^1$, $\mathbf{d}^2$, $\mathbf{j}^2$ and ρ^3 are twisted forms and $\mathbf{e}^1$ and $\mathbf{b}^2$ are straight forms. The electrostatic scalar potential ϕ and the vector potential $\mathbf{A}$ also play an important role in electromagnetism, they can be describe respectively by the 0-form ϕ^0 and the 1-form $\mathbf{a}^1$ and are then related to the electric field and magnetic induction by

$$\mathbf{e}^1 = -\,\mathrm{d}\phi^0 - \frac{\partial \mathbf{a}^1}{\partial t}, \qquad \mathbf{b}^2 = \,\mathrm{d}\mathbf{a}^1. \tag{4.32}$$

Note that taking the exterior derivative of the first equation yields Faraday's law (4.28):

$$\mathrm{d}\mathbf{e}^1 = -\,\mathrm{d}\mathrm{d}\phi^0 - \frac{\partial\,\mathrm{d}\mathbf{a}^1}{\partial t} = -\frac{\partial \mathbf{b}^2}{\partial t},$$

and taking the exterior derivative of the first equation yields (4.30)

$$\mathrm{d}\mathbf{b}^2 = \,\mathrm{d}\mathrm{d}\mathbf{a}^1 = 0.$$

Another important physical object related to Maxwell's equations is the Lorentz force involving $\mathbf{E} + \mathbf{v} \times \mathbf{B}$. The velocity vector being a *vector*, this quantity is naturally expressed in the language of differential forms as $\mathbf{e}^1 - \mathrm{i}_{\mathbf{v}}\mathbf{b}^2$.

Remark 8 *It is important to note here that the exterior derivative and the time derivative here are independent of the metric and thus Maxwell's equations* (4.27)-(4.30) *as well as the equation defining the potentials* (4.32) *have the same form in any coordinate system. The metric only appears in the Hodge operator* (4.31)*, which relates the 1-form and 2-form expressions of the electric and magnetic fields.*

A geometric discretisation should aim at preserving these properties. There are at least two classical strategies to discretise the geometric form of Maxwell's equations. The first one is based on Finite Difference in the framework of the so-called Discrete Exterior Calculus (DEC) [6]. In this framework dual grids are constructed, the straight forms being discretised on the primal grid and the twisted forms on the dual grid. The discrete Hodge operators defines a projection from one grid to the other. The second one is called Finite Element Exterior Calculus (FEEC) [2, 1]. It is constructed on compatible Finite Elements spaces for each degree of forms and a unique grid. The straight forms are approximated in a strong sense, yielding relations between the coefficients in the basis expressions of the discrete differential forms. The twisted forms are approximated in the same Finite Element spaces but in weak form. This can be naturally expressed using the codiferential. Indeed using (4.31), Ampere's equations can also be written

$$-\frac{\partial \star\mathbf{e}^1}{\partial t} + \,\mathrm{d}\star\mathbf{b}^2 = \mathbf{j}^2$$

and using that $\star\star = \mathrm{Id}$ in three dimensions

$$-\frac{\partial \mathbf{e}^1}{\partial t} + \,\mathrm{d}^*\mathbf{b}^2 = \star\mathbf{j}^2.$$

In the same way we can express (4.29) using $\mathbf{e}^1$: $\,\mathrm{d}\star\,\mathbf{e}^1 = \rho^3$ and using the expression of the codifferential for a 1-form

$$-\,\mathrm{d}^*\mathbf{e}^1 = \star\rho^3.$$

The expression of Maxwell's equations with differential forms suitable for Finite Element discretisation thus reads

$$-\frac{\partial \mathbf{e}^1}{\partial t} + \mathrm{d}^*\mathbf{b}^2 = \star\mathbf{j}^2 \tag{4.33}$$

$$\frac{\partial \mathbf{b}^2}{\partial t} + \mathrm{d}\mathbf{e}^1 = 0, \tag{4.34}$$

$$-\mathrm{d}^*\mathbf{e}^1 = \star\rho^3, \tag{4.35}$$

$$\mathrm{d}\mathbf{b}^2 = 0. \tag{4.36}$$

The two equations involving the codifferential can be expressed in weak form to replace the codifferential by the exterior derivative. Indeed taking the scalar product of (4.33) with a test 1-form $\mathbf{f}^1$ and using that d^* is the adjoint of d provided the boundary terms vanish (else they need to be added as required by (4.22))

$$-\frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{e}^1, \mathbf{f}^1) + (\mathbf{b}^2, \mathrm{d}\mathbf{f}^1) = (\star\mathbf{j}^2, \mathbf{f}^1) \quad \forall \mathbf{f}^1 \in H\Lambda^1(\mathcal{M}). \tag{4.37}$$

We recognize here the weak form of Ampère's equation and in the same way taking the inner product of (4.35) with a test 0-form yields the weak form of Gauss's law:

$$-(\mathbf{e}^1, \mathrm{d}\psi^0) = (\star\rho^3, \psi^0) \quad \forall \psi^0 \in H\Lambda^0(\mathcal{M}). \tag{4.38}$$

Chapter 5

Finite Element Exterior Calculus (FEEC)

The aim of this chapter is to introduce Finite Element spaces defining a discrete de Rham complex, each of the spaces being a subset of the corresponding continuous space. In standard vector calculus language this reads

$$\begin{array}{ccccccc} H^1(\Omega) & \xrightarrow{\text{grad}} & H(\text{curl},\Omega) & \xrightarrow{\text{curl}} & H(\text{div},\Omega) & \xrightarrow{\text{div}} & L^2(\Omega) \\ \downarrow{\scriptstyle \Pi_0} & & \downarrow{\scriptstyle \Pi_1} & & \downarrow{\scriptstyle \Pi_2} & & \downarrow{\scriptstyle \Pi_3} \\ V_0 & \xrightarrow{\text{grad}} & V_1 & \xrightarrow{\text{curl}} & V_2 & \xrightarrow{\text{div}} & V_3 \end{array} \tag{5.1}$$

The first row of (5.1) represents the exact sequence of function spaces involved in Maxwell's equations in the sense that at each node, the kernel of the next operator is the image of the previous: Im(grad) = Ker(curl), Im(curl) = Ker(div). The bottom row of (5.1) defines an exact sequence of finite dimensional function spaces. Moreover the diagram is commuting at each level, *e.g.* for $\phi \in H^1(\Omega)$:

$$\Pi_1(\text{grad}\,\phi) = \text{grad}(\Pi_0\,\phi).$$

The de Rham complex can also be expressed in the language of differential forms for an arbitrary dimension n as we have already seen in the continuous case

$$\begin{array}{ccccccc} H\Lambda^0(\mathcal{M}) & \xrightarrow{\text{d}} & H\Lambda^1(\mathcal{M}) & \xrightarrow{\text{d}} & \cdots & \xrightarrow{\text{d}} & H\Lambda^n(\mathcal{M}) \\ \downarrow{\scriptstyle \Pi_0} & & \downarrow{\scriptstyle \Pi_1} & & & & \downarrow{\scriptstyle \Pi_n} \\ V_0 & \xrightarrow{\text{grad}} & V_1 & \xrightarrow{\text{d}} & \cdots & \xrightarrow{\text{d}} & V_n \end{array} \tag{5.2}$$

Classical Finite Element methods are generally constructed element by element, which are generally triangles of quads in 2D and tetrahedra or cubes in 3D. A Finite Element approximation is defined by a finite dimensional function space with dimension N, and N degrees of freedom which characterise uniquely an element of the previous finite dimensional

function space. The simplest examples are the Lagrange Finite Elements for scalar functions schematically represented for triangles on the left where the Finite Dimensional space is

$$\mathbb{P}_k = \{\text{Span}(x^\alpha y^\beta), \quad (\alpha, \beta) \in \mathbb{N}^2, \quad 0 \leq \alpha + \beta \leq k\},$$

for $k = 3$, the degrees of freedom being point values of the function at the specified points. For quads the Finite Dimensional space is

$$\mathbb{Q}_k = \{\text{Span}(x_1^{\alpha_1} \dots x_n^{\alpha_n}), \quad (\alpha_1, \dots, \alpha_n) \in \mathbb{N}^n, \quad 0 \leq \alpha_1, \dots, \alpha_n \leq k\}$$

here for $k = 2$.

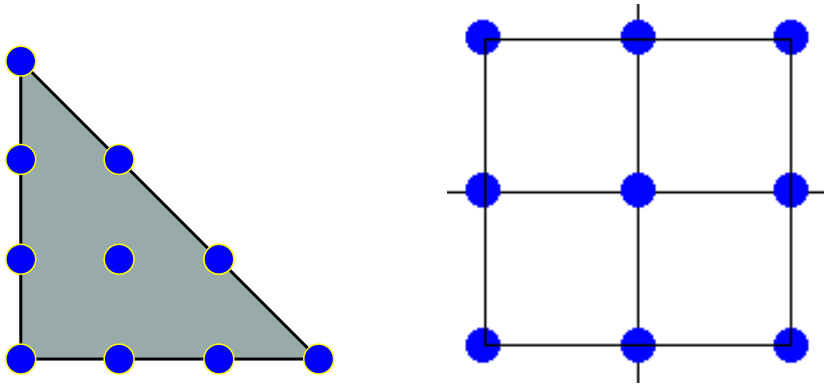

Figure 5.1: (Left) $\mathbb{P}_3$ Finite Element, (Right) $\mathbb{Q}_2$ Finite Element

From the definition of the degrees of freedom, the single elements are glued together sharing the degrees of freedom on the interface, such that the global Finite Element space, *e.g.* $\mathbb{P}_k(\Omega)$ is continuous and hence a subspace of $H^1(\Omega)$.

In order to define subspaces of $H(\text{curl}, \Omega)$ and $H(\text{div}, \Omega)$, for which only respectively the tangential and the normal components need to be continuous at the interface between two elements the degrees of freedom need to be defined accordingly. Typical spaces, which form a discrete de Rham complex, with the Lagrange Finite Element as the first space are in 2D the Nedelec space $N_k \subset H(\text{curl}, \Omega)$, the Raviart-Thomas space $RT_k \subset H(\text{div}, \Omega)$ and the discontinous Galerkin space $DG_{k-1} \subset L^2(\Omega)$, which is completely discontinuous.

The commuting diagram defined in (5.1) is the essential piece needed in the FEEC theory to ensure stability and convergence of the Finite Element approximation. These complexes are described in [2, 1]. A classical complex based on polynomials of degree k for a mesh of tetrahedra is

$$0 \to \mathbb{P}_k(\Omega) \overset{\text{grad}}{\to} N_k(\Omega) \overset{\text{curl}}{\to} RT_k(\Omega) \overset{\text{div}}{\to} DG_{k-1}(\Omega) \to 0.$$

5.1 Discrete differential forms based on B-splines

5.1.1 B-Splines

We will consider here mostly the Isogeometric Analysis point of view, where we have a physical mesh mapped from a cartesian logical mesh (see Figure 5.2). An important insight for Finite Elements is to understand what properties depend only on the connectivity of

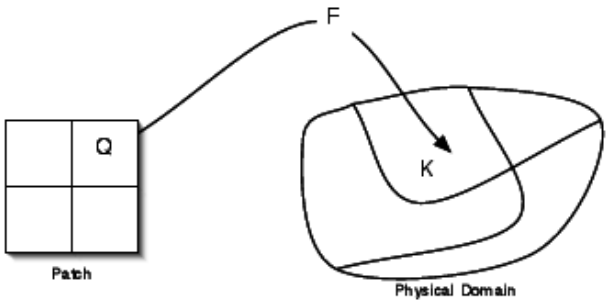

Figure 5.2: An example of a mapping from the logical to the physical mesh

the mesh (topological properties invariant by continuous deformation of the mesh) and what properties depend on the mapping (geometrical properties).

Let us now construct a Finite Element discretisation using basis functions for the different spaces based on B-Splines.

In order to define a family of n B-splines of degree k, we need $(x_i)_{0\leqslant i\leqslant n+k}$ a non-decreasing sequence of points on the real line called *knots* in the spline terminology. There can be several knots at the same position. In the case when there are m knots at the same point, we say that the knot has multiplicity m.

Definition 17 (B-Spline) *Let $(x_i)_{0\leqslant i\leqslant n+k}$ be a non-decreasing sequence of knots. We then define n functions called B-Splines, where the j-th B-Spline ($0 \leq j \leq n-1$) denoted by N_j^k of degree k is defined by the recurrence relation:*

$$N_j^k(x) = w_j^k(x)N_j^{k-1}(x) + (1 - w_{j+1}^k(x))N_{j+1}^{k-1}(x)$$

where,

$$w_j^k(x) = \frac{x - x_j}{x_{j+k} - x_j}, \qquad N_j^0(x) = \chi_{[x_j, x_{j+1}[}(x).$$

We note some important properties of a B-splines basis:

- B-splines are piecewise polynomial of degree k,
- B-splines are non negative,
- Compact support; the support of N_j^k is contained in $[x_j, .., x_{j+k+1}]$,
- Partition of unity: $\sum_{i=0}^{n-1} N_i^k(x) = 1, \forall x \in \mathbb{R}$,
- Local linear independence,
- If a knot x_i has a multiplicity m then the B-spline is $\mathcal{C}^{(k-m)}$ at x_i.

A key point for constructing a complex of Finite Element spaces for p-forms comes from the recursion formula for the derivatives:

$$N_i^{k\prime}(x) = k\left(\frac{N_i^{k-1}(x)}{x_{i+k} - x_i} - \frac{N_{i+1}^{k-1}(x)}{x_{i+k+1} - x_{i+1}}\right). \tag{5.3}$$

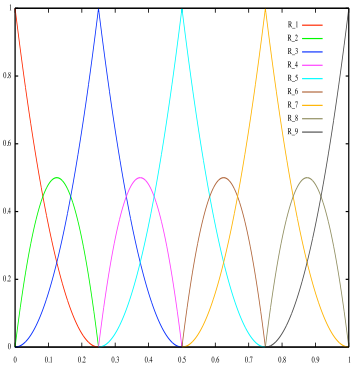

Figure 5.3: All B-splines functions associated to a knot sequence defined by $n = 9$, $k = 2$, $T = \{000, \frac{1}{4}\frac{1}{4}, \frac{1}{2}\frac{1}{2}, \frac{3}{4}\frac{3}{4}, 111\}$

It will be convenient to introduce the notation $D_i^k(x) = k\frac{N_i^{k-1}(x)}{x_{i+k}-x_i}$. Then the recursion formula for derivatives simply becomes

$$N_i^{k\prime}(x) = D_i^k(x) - D_{i+1}^k(x). \tag{5.4}$$

Remark 9 *In the case where all knots, except the boundary knots are of multiplicity 1, the set $(N_i^k)_{0\leq i\leq n-1}$ of B-splines of degree k forms a basis of the spline space ($\dim \mathcal{S}^k = n$) defined by*

$$\mathcal{S}^k = \{v \in C^{k-1}([x_0, x_n]) \; | v_{|[x_i,x_{i+1}]} \in \mathbb{P}_k([x_i, x_{i+1}]).$$

The boundary knots are chosen to have multiplicity $k+1$ so that the spline becomes interpolatory on the boundary in order to simplify the application of Dirichlet boundary conditions. This setting is called open boundary conditions for the spline.

Then due to the definitions if follows immediately that $(D_i^k)_{1\leq i\leq n-1}$ is a basis of $\mathcal{S}^{k-1}$. Note that if the first knot has multiplicity $k+1$, D_0^k will have a support restricted to one point and be identically 0.

Remark 10 *Splines can be easily defined in the case of periodic boundary conditions by taking a periodic knot sequence. The dimension of the spline space is then the number of distinct knots.*

5.1.2 Discrete differential forms in 1D

In 1D the continuous and its corresponding discrete de Rham complexes are defined by

$$\begin{array}{ccc} H^1(\Omega) & \xrightarrow{\text{grad}} & L^2(\Omega) \\ \Pi_0 \downarrow & & \downarrow \Pi_1 \\ V_0 & \xrightarrow{\text{grad}} & V_1 \end{array} \tag{5.5}$$

where in 1D, we denote by $\text{grad}\,\psi = \frac{\mathrm{d}\psi}{\mathrm{d}x} = \psi'(x)$. For the first line of the diagram, we deal with classical continuous functions, so for $\psi \in H^1$ we obviously have $\text{grad}\,\psi \in L^2$.

Let us now construct V_0 and V_1, such that for $\psi_h \in V_0$ we have $\operatorname{grad} \psi_h \in V_1$. We start with the space of discrete 0-forms as being the spline space $V_0 = \mathcal{S}^k$ and write any function $\psi_h \in V_0$ as

$$\psi_h(x) = \sum_{j=0}^{n-1} c_j^0 N_j^k(x).$$

Now for $\psi_h \in V_0$ we take its gradient (or exterior derivative), then

$$\psi_h'(x) = \sum_{j=0}^{n-1} c_j^0 (N_j^k)'(x) = \sum_{j=0}^{n-1} c_j^0 (D_j^k(x) - D_{j+1}^k(x)) = \sum_{j=1}^{n-1} (c_j^0 - c_{j-1}^0) D_j^k(x)$$

using (5.4), a change of index and the fact that $D_0^k = 0$. Then defining $V_1 = \operatorname{Span}\{(D_j^k)_{1 \leq k \leq n-1}\}$, we have that for any $\psi_h \in V_0$, $\operatorname{grad} \psi_h \in V_1$.

The commuting projectors: We first construct the Π_0 projector for 0-forms. As 0-forms are characterised by point values, the natural projector is the interpolation at a set of n distinct points for the spline space V_0 of dimension n. The classical interpolation points for B-Splines are the Greville points, which are defined from the knots $x_0 \leq x_1 \leq \cdots \leq x_{n+k}$ defining the splines of degree k by

$$\xi_i = \frac{x_{i+1} + \cdots + x_{i+k}}{k} \quad 0 \leq i \leq n-1.$$

Assuming a uniform grid of nodes for $k = 1$, $\xi_i = x_{i+1}$. For $k = 2$, $\xi_i = (x_{i+1} + x_{i+2})/2$ and for $k = 3$, $\xi_i = (x_{i+1} + x_{i+2} + x_{i+3})/3$, for points where the duplicated knots at the boundary don't interfere. As x_i denotes the point at the left of the B-Spline $N_i^k(x)$, we notice that the Greville point ξ_i is located at the maximum of this B-Spline. This remains true for higher order B-Splines.

Consider now an arbitrary function $\psi \in H^1$, then its interpolant at the Greville points $\psi_h(x) = (\Pi_0 \psi)(x)$ is defined uniquely by

$$\sigma_i^0(\psi_h) = \psi_h(x_i) = \sum_{j=0}^{n-1} c_j^0 N_j^k(x_i) = \psi(x_i) = \sigma_i^0(\psi) \quad \forall \psi \in H^1,$$

where we denote by $\sigma_i^0(\psi)$ the Finite Element degrees of freedom, which are the linear forms characterising an element of the Finite Element space V_0. The matrix $\mathcal{I}_0^k = (N_j^k(x_i))_{i,j}$ is the spline interpolation matrix of degree k at the Greville points. This is an invertible matrix which defines uniquely the spline coefficients (c_j^0) characterising $\psi_h = \Pi_0 \psi$ from the values of ψ at the Greville points.

Let us now construct the projection Π_1 in order to get the commuting diagram $\operatorname{grad} \Pi_0 = \Pi_1 \operatorname{grad}$. As this operator applies to 1-forms (in 1D), the natural degrees of freedom are cell integrals, which should be, in order to get the commuting diagram with the definition of Π_0 based on interpolation at the Greville points, the histopolation between two successive Greville points. This means that for any $\varphi \in L^2$, its histopolant $\varphi_h(x) = (\Pi_1 \varphi)(x)$ is uniquely characterised by

$$\sigma_i^1(\varphi_h) = \int_{\xi_i - 1}^{\xi_i} \varphi_h(x) \, \mathrm{d}x = \sum_{j=1}^{n-1} c_j^1 \int_{\xi_i - 1}^{\xi_i} D_j^k(x) \, \mathrm{d}x = \sigma_i^1(\varphi) \quad \text{for } 1 \leq i \leq n.$$

The matrix $\mathcal{I}_1^k = (\sum_{j=1}^{n-1} \int_{\xi_i}^{\xi_{i+1}} D_j^k(x)\,\mathrm{d}x)_{i,j}$ is the spline histopolation matrix of degree k at the Greville points. This is an invertible matrix which defines uniquely the spline coefficients (c_j^1) characterising $\varphi_h = \Pi_1\varphi$ from the values of φ at the Greville points.

Proposition 8 *We have*

$$\sigma_i^1(\Pi_1 \mathrm{grad}\,\psi) = \sigma_i^1(\mathrm{grad}\,\Pi_0(\psi)), \quad \forall \psi \in H^1, \quad \forall i. \tag{5.6}$$

Hence the diagram (5.5) *commutes.*

Proof. As the degrees of freedom σ_i^1 characterise an element of V_1, the relation (**??**) implies that $\Pi_1 \mathrm{grad}\,\psi = \mathrm{grad}\,\Pi_0(\psi)$ for all $\psi \in H^1$.

Let us now prove (5.6):

Starting with $\psi \in H^1$, so that $\mathrm{grad}\,\psi \in L^2$, we have on the one hand

$$\mathrm{grad}\,\Pi_0\psi(x) = \sum_j c_j^0 (N_j^k)'(x) = \sum_j c_j^0 (D_j^k(x) - D_{j+1}^k(x))$$

using (5.4). Hence

$$\sigma_i^1(\mathrm{grad}\,\Pi_0\psi) = \int_{\xi_i}^{\xi_{i+1}} \psi_h'(x)\,\mathrm{d}x = \psi_h(\xi_{i+1}) - \psi_h(\xi_i).$$

And on the other hand

$$\sigma_i^1(\Pi_1 \mathrm{grad}\,\psi) = \int_{\xi_i}^{\xi_{i+1}} \psi'(x)\,\mathrm{d}x = \psi(\xi_{i+1}) - \psi(\xi_i) = \psi_h(\xi_{i+1}) - \psi_h(\xi_i),$$

as by construction ψ_h is the interpolant of ψ at the points ξ_i. Hence we have (5.6). ∎

5.1.3 Discrete differential forms in 3D

Let us construct spaces of differential forms whose coefficients are splines. In order to obtain a complex, we shall start by defining the space of 0-forms and then for $p \geq 1$ construct the space of p-forms by applying the exterior derivative to the $(p-1)$-forms. This property is needed to form a complex. Let us start with a finite dimensional space of 0-forms denoted by V_0 constructed as a tensor product of B-Splines.

We define the 3D point $\mathbf{x} = (x_1, x_2, x_3)$ and the multi-index $\mathbf{i} = (i_1, i_2, i_3)$. Then the basis functions for 0-forms will be

$$\Lambda_{\mathbf{i}}^0(\mathbf{x}) = N_{i_1}^k(x_1) N_{i_2}^k(x_2) N_{i_3}^k(x_3), \quad 1 \leq i_1 \leq n_1, 1 \leq i_2 \leq n_2, 1 \leq i_3 \leq n_3. \tag{5.7}$$

And our finite dimensional space of 0-forms base on B-splines of degree k in each direction is then $V_0 = \mathrm{Span}\{\Lambda_{\mathbf{i}}^0\}_{\mathbf{i}}$. And any discrete 0-form can be written as

$$\psi_h^0(\mathbf{x}) = \sum_{\mathbf{i}} c_{\mathbf{i}}^0 \Lambda_{\mathbf{i}}^0(\mathbf{x}).$$

Now taking the exterior derivative of ϕ_h^0 we find

$$\begin{aligned}
\mathrm{d}\psi_h^0(\mathbf{x}) &= \sum_{\mathbf{i}} c_{\mathbf{i}}^0 \,\mathrm{d}\Lambda_{\mathbf{i}}^0(\mathbf{x}) = \sum_{\mathbf{i}} c_{\mathbf{i}}^0((N_{i_1}^k)'(x_1)N_{i_2}^k(x_2)N_{i_3}^k(x_3)\,\mathrm{d}x^1 \\
&+ N_{i_1}(x_1)(N_{i_2}^k)'(x_2)N_{i_3}^k(x_3)\,\mathrm{d}x^2 + N_{i_1}^k(x_1)N_{i_2}^k(x_2)(N_{i_3}^k)'(x_3)\,\mathrm{d}x^3), \\
&= \sum_{\mathbf{i}} c_{\mathbf{i}}^0((D_{i_1}^k - D_{i_1+1}^k)(x_1)N_{i_2}^k(x_2)N_{i_3}^k(x_3)\,\mathrm{d}x^1 \\
&+ N_{i_1}(x_1)(D_{i_2}^k - D_{i_2+1}^k)(x_2)N_{i_3}^k(x_3)\,\mathrm{d}x^2 + N_{i_1}^k(x_1)N_{i_2}^k(x_2)(D_{i_3}^k - D_{i_3+1}^k)(x_3)\,\mathrm{d}x^3), \\
&= \sum_{\mathbf{i}} (c_{i_1,i_2,i_3}^0 - c_{i_1-1,i_2,i_3}^0)D_{i_1}^k(x^1)N_{i_2}^k(x_2)N_{i_3}^k(x_3)\,\mathrm{d}x^1 \\
&+ (c_{i_1,i_2,i_3}^0 - c_{i_1,i_2-1,i_3}^0)N_{i_1}^k(x^1)D_{i_2}^k(x_2)N_{i_3}^k(x_3)\,\mathrm{d}x^2 \\
&+ (c_{i_1,i_2,i_3}^0 - c_{i_1,i_2,i_3-1}^0)N_{i_1}^k(x^1)N_{i_2}^k(x_2)D_{i_3}^k(x_3)\,\mathrm{d}x^3,
\end{aligned}$$

where we used expression (5.4) for the derivative of a B-spline.

In order to form a complex the finite dimensional space of 1-forms V_1 should contain all exterior derivatives of 0-forms. This will be the case if we choose as basis functions for the 1-forms

$$\begin{aligned}
\mathbf{\Lambda}_{\mathbf{i},1}^1(\mathbf{x}) &= D_{i_1}^k(x^1)N_{i_2}^k(x_2)N_{i_3}^k(x_3)\,\mathrm{d}x^1 = \Lambda_{\mathbf{i},1}^1(\mathbf{x})\,\mathrm{d}x^1, \\
\mathbf{\Lambda}_{\mathbf{i},2}^1(\mathbf{x}) &= N_{i_1}^k(x^1)D_{i_2}^k(x_2)N_{i_3}^k(x_3)\,\mathrm{d}x^2 = \Lambda_{\mathbf{i},2}^1(\mathbf{x})\,\mathrm{d}x^2, \\
\mathbf{\Lambda}_{\mathbf{i},3}^1(\mathbf{x}) &= N_{i_1}^k(x^1)N_{i_2}^k(x_2)D_{i_3}^k(x_3)\,\mathrm{d}x^3 = \Lambda_{\mathbf{i},3}^1(\mathbf{x})\,\mathrm{d}x^3.
\end{aligned}$$

A general finite dimensional 1-form is then represented by

$$\mathbf{f}^1(\mathbf{x}) = \sum_{\mathbf{i}=1}^{\mathbf{n}} \sum_{a=1}^{3} c_{\mathbf{i},a}^1 \mathbf{\Lambda}_{\mathbf{i},a}^1(\mathbf{x}) = \sum_{\mathbf{i}=1}^{\mathbf{n}} \sum_{a=1}^{3} c_{\mathbf{i},a}^1 \Lambda_{\mathbf{i},a}^1(\mathbf{x})\,\mathrm{d}x^a.$$

In particular, if $\mathbf{f}^1 = \mathrm{d}\phi^0$, there coefficients in their respective bases are related by

$$c_{\mathbf{i},1}^1 = c_{i_1,i_2,i_3}^0 - c_{i_1-1,i_2,i_3}^0, \quad c_{\mathbf{i},2}^1 = c_{i_1,i_2,i_3}^0 - c_{i_1,i_2-1,i_3}^0, \quad c_{\mathbf{i},3}^1 = c_{i_1,i_2,i_3}^0 - c_{i_1,i_2,i_3-1}^0, \tag{5.8}$$

independently of the metric. It depends only on the neighboring splines.

In the same way, to construct a basis for V_2 we take the exterior derivative of an element of V_1. This yields

$$\begin{aligned}
\mathrm{d}\mathbf{f}^1(\mathbf{x}) &= \sum_{\mathbf{i}=1}^{\mathbf{n}} \sum_{a=1}^{3} c_{\mathbf{i},a}^1 \,\mathrm{d}\mathbf{\Lambda}_{\mathbf{i},a}^1(\mathbf{x}) && (5.9) \\
&= \sum_{\mathbf{i}=1}^{\mathbf{n}} \big((c_{i_1,i_2,i_3,3}^1 - c_{i_1,i_2-1,i_3,3}^1) - (c_{i_1,i_2,i_3,2}^1 - c_{i_1,i_2,i_3-1,2}^1)\big) \\
&\qquad N_{i_1}^k(x^1)D_{i_2}^k(x_2)D_{i_3}^k(x_3)\,\mathrm{d}x^2 \wedge \mathrm{d}x^3 && (5.10) \\
&+ \big((c_{i_1,i_2,i_3,1}^1 - c_{i_1,i_2,i_3-1,1}^1) - (c_{i_1,i_2,i_3,3}^1 - c_{i_1-1,i_2,i_3,3}^1)\big) \\
&\qquad D_{i_1}^k(x^1)N_{i_2}^k(x_2)D_{i_3}^k(x_3)\,\mathrm{d}x^3 \wedge \mathrm{d}x^1 && (5.11) \\
&+ \big((c_{i_1,i_2,i_3,2}^1 - c_{i_1-1,i_2,i_3,2}^1) - (c_{i_1,i_2,i_3,1}^1 - c_{i_1,i_2-1,i_3,1}^1)\big) \\
&\qquad D_{i_1}^k(x^1)D_{i_2}^k(x_2)N_{i_3}^k(x_3)\,\mathrm{d}x^1 \wedge \mathrm{d}x^2 && (5.12)
\end{aligned}$$

In order to form a complex the space of finite dimensional 2-forms should contain all exterior derivatives of 1-forms. This will be the case if we choose as basis functions for the 2-forms

$$\begin{aligned}
\mathbf{\Lambda}^2_{\mathbf{i},1}(\mathbf{x}) &= N^k_{i_1}(x^1) D^k_{i_2}(x_2) D^k_{i_3}(x_3)\, \mathrm{d}x^2 \wedge \mathrm{d}x^3 = \Lambda^2_{\mathbf{i},1}(\mathbf{x})\, \mathrm{d}x^2 \wedge \mathrm{d}x^3, \\
\mathbf{\Lambda}^2_{\mathbf{i},2}(\mathbf{x}) &= D^k_{i_1}(x^1) N^k_{i_2}(x_2) D^k_{i_3}(x_3)\, \mathrm{d}x^3 \wedge \mathrm{d}x^1 = \Lambda^2_{\mathbf{i},2}(\mathbf{x})\, \mathrm{d}x^3 \wedge \mathrm{d}x^1, \\
\mathbf{\Lambda}^1_{\mathbf{i},3}(\mathbf{x}) &= D^k_{i_1}(x^1) D^k_{i_2}(x_2) N^k_{i_3}(x_3)\, \mathrm{d}x^1 \wedge \mathrm{d}x^2 = \Lambda^2_{\mathbf{i},3}(\mathbf{x})\, \mathrm{d}x^1 \wedge \mathrm{d}x^2.
\end{aligned}$$

A general discrete 2-form is then represented by

$$\mathbf{b}^2(\mathbf{x}) = \sum_{\mathbf{i}=1}^{\mathbf{n}} \sum_{a=1}^{3} c^2_{\mathbf{i},a} \mathbf{\Lambda}^2_{\mathbf{i},a}(\mathbf{x}).$$

In particular, if $\mathbf{b}^2 = \mathrm{d}\mathbf{f}^1$, their coefficients in their respective bases are related by

$$c^2_{\mathbf{i},1} = (c^1_{i_1,i_2,i_3,3} - c^1_{i_1,i_2-1,i_3,3}) - (c^1_{i_1,i_2,i_3,2} - c^1_{i_1,i_2,i_3-1,2}), \tag{5.13}$$

$$c^2_{\mathbf{i},2} = (c^1_{i_1,i_2,i_3,1} - c^1_{i_1,i_2,i_3-1,1}) - (c^1_{i_1,i_2,i_3,3} - c^1_{i_1-1,i_2,i_3,3}), \tag{5.14}$$

$$c^2_{\mathbf{i},3} = (c^1_{i_1,i_2,i_3,2} - c^1_{i_1-1,i_2,i_3,2}) - (c^1_{i_1,i_2,i_3,1} - c^1_{i_1,i_2-1,i_3,1}), \tag{5.15}$$

independently of the metric. It depends only on the neighboring splines.

We finally come to the last space V_3 of discrete 3-forms. These are constructed such that the exterior derivative of an element of V_2 is in V_3. Taking the exterior derivative of a generic element $\mathbf{b}^2 \in V_2$ yields

$$\begin{aligned}
\mathbf{b}^2(\mathbf{x}) &= \sum_{\mathbf{i}=1}^{\mathbf{n}} \sum_{a=1}^{3} c^2_{\mathbf{i},a}\, \mathrm{d}\mathbf{\Lambda}^2_{\mathbf{i},a}(\mathbf{x}) \\
&= \big((c^2_{i_1,i_2,i_3,1} - c^2_{i_1-1,i_2,i_3,1}) + (c^2_{i_1,i_2,i_3,2} - c^2_{i_1,i_2-1,i_3,2}) + (c^2_{i_1,i_2,i_3,3} - c^2_{i_1,i_2,i_3-1,3})\big) \\
&\qquad\qquad D^k_{i_1}(x^1) D^k_{i_2}(x_2) D^k_{i_3}(x_3)\, \mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \mathrm{d}x^3.
\end{aligned}$$

So the basis functions for the three forms are of the form

$$\Lambda^3_{\mathbf{i}}(\mathbf{x}) = D^k_{i_1}(x_1) D^k_{i_2}(x_2) D^k_{i_3}(x_3)\, \mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \mathrm{d}x^3,$$

and a general 3-form writes

$$\rho^3(\mathbf{x}) = \sum_{\mathbf{i}=1}^{\mathbf{n}} c^3_{\mathbf{i}} \Lambda^3_{\mathbf{i}}(\mathbf{x}). \tag{5.16}$$

And the coefficients in V_3 of the exterior derivative of an element of V_2 are given by

$$c^3_{\mathbf{i}} = (c^2_{i_1,i_2,i_3,1} - c^2_{i_1-1,i_2,i_3,1}) + (c^2_{i_1,i_2,i_3,2} - c^2_{i_1,i_2-1,i_3,2}) + (c^2_{i_1,i_2,i_3,3} - c^2_{i_1,i_2,i_3-1,3}). \tag{5.17}$$

Here again this is independent of the metric an only involves neighbouring spline coefficients.

Commuting projectors The projectors are naturally based on spline integration and histopolation at the Greville points in each direction: $\boldsymbol{\xi}_{\mathbf{j}} = (\xi_{1j_1}, \xi_{2j_2}, \xi_{3j_3})$. On a tensor product periodic grid, these are defined to be the grid points for odd degree splines and the grid midpoints for even degree splines, so that the interpolation and histopolation problems

are always well-posed and that the tensor product spline interpolation matrix of degree p, denoted by $\mathcal{I}^p = ((N^p_{i_1}(\xi_{1j_1})N^p_{i_2}(\xi_{2j_2})N^p_{i_3}(\xi_{3j_3}))_{\mathbf{i},\mathbf{j}}$ is square and symmetric.

For any function $\psi \in H^1(\Omega)$ we define $\Pi_0\psi = \sum_{\mathbf{i}} \psi_{\mathbf{i}}\Lambda^0_{\mathbf{i}} \in V_0$, where the $\psi_{\mathbf{i}}$ are the unique solution of the interpolation problem

$$\psi(\boldsymbol{\xi}_{\mathbf{j}}) = \psi(\xi_{1j_1}, \xi_{2j_2}, \xi_{3j_3}) = \sum_{\mathbf{i}} \psi_{\mathbf{i}}\Lambda^0_{\mathbf{i}}(\mathbf{x}_{\mathbf{j}}) = \sum_{i_1,i_2,i_3} \psi_{i_1,i_2,i_3} N^p_{i_1}(\xi_{1j_1})N^p_{i_2}(\xi_{2j_2})N^p_{i_3}(\xi_{3j_3}).$$

As is usual for Kronecker products, we denote by $\mathrm{vec}(\psi(\boldsymbol{\xi}_{\mathbf{j}}))$ the vector with the stacked entries $(\psi(\boldsymbol{\xi}_{\mathbf{j}})$, so that the interpolation problem can be written in matrix form

$$\mathrm{vec}(\psi(\boldsymbol{\xi}_{\mathbf{j}})) = K^p \mathrm{vec}(\psi_{\mathbf{i}}). \tag{5.18}$$

The projection of a function ψ onto V_0 is then uniquely defined by the coefficients $\psi_{\mathbf{i}}$ solution of (5.18). As those correspond to classical Finite Element degrees of freedom, we shall denote by $\sigma^0_{\mathbf{i}}(\psi) = \psi_{\mathbf{i}}$ and the vector of all degrees of freedom by

$$\sigma^0(\psi) = \mathrm{vec}(\psi_{\mathbf{i}}) = (K^p)^{-1}\mathrm{vec}(\psi(\boldsymbol{\xi}_{\mathbf{j}})). \tag{5.19}$$

Now in order to get the commuting diagram $\mathrm{grad}\,\Pi_0 = \Pi_1 \mathrm{grad}$, we define for any $\mathbf{E} = (E_1, E_2, E_3)^\top \in H(\mathbf{curl}, \Omega)$,

$$\Pi_1 \mathbf{E} = \sum_{\mathbf{i}} \sum_{\alpha=1}^{3} e_{\mathbf{i},\alpha}\Lambda^1_{\mathbf{i},\alpha} \in V_1.$$

On a cartesian mesh the three components decouple, and there is a separate interpolation-histopolation problem to solve for each component: the first components $e_{\mathbf{i},1}$ are the unique solutions of the interpolation-histopolation problem

$$\begin{aligned}\int_{\xi_{1j_1-1}}^{\xi_{1j_1}} E_1(x_1, \xi_{2j_2}, \xi_{3j_3})\,\mathrm{d}x_1 &= \sum_{\mathbf{i}} \int_{\xi 1_{j_1-1}}^{\xi_{1j_1}} e_{\mathbf{i},1}\Lambda^1_{\mathbf{i},1}(x_1, \xi_{2j_2}, \xi_{3j_3})\,\mathrm{d}x_1 \\ &= \sum_{i_1,i_2,i_3} e_{\mathbf{i},1} \int_{\xi_{1j_1-1}}^{\xi_{1j_1}} D^p_{i_1}(x_1)\,\mathrm{d}x_1 N^p_{i_2}(\xi_{2j_2})N^p_{i_3}(\xi_{3j_3}).\end{aligned}$$

We denote by $\mathcal{I}^p_{1,1}$ the corresponding tensor product interpolation-histopolation matrix for the first component and the right hand side $\mathrm{vec}(\int_{\xi_{1j_1-1}}^{\xi_{1j_1}} E_1(x_1, \xi_{2j_2}, \xi_{3j_3})\,\mathrm{d}x_1)$ by $\mathcal{E}_1(E_1)$, $\mathcal{E}_1$ standing for edges in the first direction. So introducing the linear operator $\sigma^1_{\mathbf{i},\alpha}(\mathbf{E}) = e_{\mathbf{i},\alpha}$, we have

$$\sigma^1_1(\mathbf{E}) = \mathrm{vec}(e_{\mathbf{i},1}) = (\mathcal{I}^p_{1,1})^{-1}\mathrm{vec}(\int_{\xi_{1j_1-1}}^{\xi_{1j_1}} E_1(x_1, \xi_{2j_2}, \xi_{3j_3})\,\mathrm{d}x_1) = (\mathcal{I}^p_{1,1})^{-1}\mathcal{E}_1(E_1). \tag{5.20}$$

Similarly, the two other components of the projection $\Pi_1(E)$ are defined by

$$\sigma^1_2(\mathbf{E}) = \mathrm{vec}(e_{\mathbf{i},2}) = (\mathcal{I}^p_{1,2})^{-1}\mathrm{vec}(\int_{\xi_{2j_2-1}}^{\xi_{2j_2}} E_2(\xi_{1j_1}, x_2, \xi_{3j_3})\,\mathrm{d}x_2) = (\mathcal{I}^p_{1,2})^{-1}\mathcal{E}_2(E_2), \tag{5.21}$$

$$\sigma_3^1(\mathbf{E}) = \mathrm{vec}(e_{\mathbf{i},3}) = (\mathcal{I}_{1,3}^p)^{-1}\mathrm{vec}(\int_{\xi_{3_{j_3-1}}}^{\xi_{3_{j_3}}} E_3(\xi_{1j_1}, \xi_{2j_2}, x_3)\,\mathrm{d}x_3) = (\mathcal{I}_{1,3}^p)^{-1}\mathcal{E}_3(E_3). \tag{5.22}$$

We can now continue in the same way, with the definition of $\Pi_2\mathbf{B}$ for $\mathbf{B} \in H(\mathrm{div}\,, \Omega)$.

$$\Pi_2\mathbf{B} = \sum_{\mathbf{i}}\sum_{\alpha=1}^{3} b_{\mathbf{i},\alpha}\mathbf{\Lambda}_{\mathbf{i},\alpha}^2 \in V_2.$$

And, introducing the linear operators $\sigma_{\mathbf{i},\alpha}^2(\mathbf{B}) = b_{\mathbf{i},\alpha}$, is $1 \leq \alpha \leq 3$, we have

$$\sigma_1^2(\mathbf{B}) = \mathrm{vec}(b_{\mathbf{i},1}) = (\mathcal{I}_{2,1}^p)^{-1}\mathrm{vec}(\int_{\xi_{2_{j_2-1}}}^{\xi_{2_{j_2}}}\int_{\xi_{3_{j_3-1}}}^{\xi_{3_{j_3}}} B_1(\xi_{1_{j_1}}, x_2, x_3)\,\mathrm{d}x_2\,\mathrm{d}x_3) = \mathcal{F}_1(B_1), \tag{5.23}$$

$$\sigma_2^2(\mathbf{B}) = \mathrm{vec}(b_{\mathbf{i},2}) = (\mathcal{I}_{2,2}^p)^{-1}\mathrm{vec}(\int_{\xi_{1_{j_1-1}}}^{\xi_{1_{j_1}}}\int_{\xi_{3_{j_3-1}}}^{\xi_{3_{j_3}}} B_2(x_1, \xi_{2_{j_2}}, x_3)\,\mathrm{d}x_1\,\mathrm{d}x_3) = \mathcal{F}_2(B_2), \tag{5.24}$$

$$\sigma_3^2(\mathbf{B}) = \mathrm{vec}(b_{\mathbf{i},3}) = (\mathcal{I}_{2,3}^p)^{-1}\mathrm{vec}(\int_{\xi_{1_{j_1-1}}}^{\xi_{1_{j_1}}}\int_{\xi_{2_{j_2-1}}}^{\xi_{2_{j_2}}} B_3(x_1, x_2, \xi_{3_{j_3}})\,\mathrm{d}x_1\,\mathrm{d}x_2) = \mathcal{F}_3(B_3). \tag{5.25}$$

Here $\mathcal{F}_\alpha$ stands for an integral on a face perpendicular the the α^{th} direction. And finally for $\rho \in L^2(\Omega)$, we can define $\Pi_3\rho = \sum_{\mathbf{i}} \rho_{\mathbf{i}}\Lambda_{\mathbf{i}}^3 \in V_3$ as the solution of the tensor product histopolation problem

$$\sigma^3(\rho) = \mathrm{vec}(\rho_{\mathbf{i}}) = (\mathcal{I}_3^p)^{-1}\mathrm{vec}(\int_{\xi_{1_{j_1-1}}}^{\xi_{1_{j_1}}}\int_{\xi_{2_{j_2-1}}}^{\xi_{2_{j_2}}}\int_{\xi_{3_{j_3-1}}}^{\xi_{3_{j_3}}} \rho(x_1, x_2, x_3)\,\mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}x_3). \tag{5.26}$$

5.2 Discretisation of Maxwell's equations with spline differential forms

Having constructed the spline differential forms, we have already obtained relations between the basis coefficients defining the exterior derivatives. All equations expressed in the strong sense (not involving the co-derivative) can be expressed using only these at the discrete level. This can be written in a convenient matrix form by introducing the discrete gradient $\mathbb{G}$ defined by (5.8), the discrete curl matrix $\mathbb{C}$ defined by (5.13)-(5.15), and the discrete divergence $\mathbb{D}$ by (5.17). Note that these matrices are incidence matrices containing only 0, 1, -1 coefficients.

Expanding $\mathbf{e}_h^1$ in the basis of V_1 and $\mathbf{b}_h^2$ in the basis of V_2 we get

$$\mathbf{e}_h^1(t, \mathbf{x}) = \sum_{\mathbf{i}=1}^{\mathbf{n}}\sum_{a=1}^{3} e_{\mathbf{i},a}^1(t)\mathbf{\Lambda}_{\mathbf{i},a}^1(\mathbf{x}), \qquad \mathbf{b}_h^2(\mathbf{x}) = \sum_{\mathbf{j}=1}^{\mathbf{n}}\sum_{b=1}^{3} b_{\mathbf{j},b}^2\mathbf{\Lambda}_{\mathbf{j},b}^2(\mathbf{x}).$$

Denoting respectively by $\mathbf{E}_1$ the vector of coefficients $e_{\mathbf{i},a}^1(t)$ and by $\mathbf{B}_2$ the vector of coefficients $b_{\mathbf{j},b}^2(t)$, the discrete version of Faraday's law (4.34) simply becomes

$$\frac{\mathrm{d}\mathbf{B}_1}{\mathrm{d}t} + \mathbb{C}\mathbf{E}_1 = 0,$$

and the discrete version of $\mathrm{d}\mathbf{b}^2 = 0$ (4.36) becomes

$$\mathbb{D}\mathbf{B}_2 = 0.$$

Let us now consider the discretisation of the weak formulations in this setting. For Maxwell's equations this is needed for the Ampere equation and the Gauss law. Let us start with the weak form of the Ampere equation. We first need to build the mass matrix corresponding to $(\mathbf{e}_h^1, \mathbf{f}_h^1)$ for $\mathbf{e}_h^1, \mathbf{f}_h^1 \in V_1$. Expanding $\mathbf{e}_h^1, \mathbf{f}_h^1$ in the basis of V_1 we get

$$\mathbf{e}_h^1(t, \mathbf{x}) = \sum_{\mathbf{i}=1}^{\mathbf{n}} \sum_{a=1}^{3} e_{\mathbf{i},a}^1(t) \mathbf{\Lambda}_{\mathbf{i},a}^1(\mathbf{x}), \qquad \mathbf{f}_h^1(\mathbf{x}) = \sum_{\mathbf{j}=1}^{\mathbf{n}} \sum_{b=1}^{3} f_{\mathbf{j},b}^1 \mathbf{\Lambda}_{\mathbf{j},b}^1(\mathbf{x}).$$

Using the bilinearity of the scalar product we find

$$(\mathbf{e}_h^1, \mathbf{f}_h^1) = \sum_{\mathbf{i}=1}^{\mathbf{n}} \sum_{a=1}^{3} \sum_{\mathbf{j}=1}^{\mathbf{n}} \sum_{b=1}^{3} e_{\mathbf{i},a}^1(t) f_{\mathbf{j},b}^1 (\mathbf{\Lambda}_{\mathbf{i},a}^1, \mathbf{\Lambda}_{\mathbf{j},b}^1). \tag{5.27}$$

Then, using the definition of the scalar product of 1-forms (4.16) we get

$$(\mathbf{\Lambda}_{\mathbf{i},a}^1, \mathbf{\Lambda}_{\mathbf{j},b}^1) = \int \Lambda_{\mathbf{i},a}^1 \Lambda_{\mathbf{i},b}^1 g^{ab} \sqrt{g} \, \mathrm{d}\mathbf{x}. \tag{5.28}$$

We denote by M_1 this mass matrix, stacking the multi-index (i_1, i_2, i_3, a) into one index to define the matrix lines, and similarly with (j_1, j_2, j_3, b) for the columns. Denoting respectively by $\mathbf{E}_1$ the corresponding vector of coefficients $e_{\mathbf{i},a}^1(t)$ and by $\mathbf{F}_1$ the vector of coefficients $f_{\mathbf{j},b}^1(t)$ we get that

$$(\mathbf{e}_h^1, \mathbf{f}_h^1) = \mathbf{F}_1^\top M_1 \mathbf{E}_1.$$

Now, expanding $\mathbf{b}_h^2$ in the basis of V_2, we have

$$\mathbf{b}_h^2(t, \mathbf{x}) = \sum_{\mathbf{i}=1}^{\mathbf{n}} \sum_{a=1}^{3} b_{\mathbf{i},a}^2(t) \Lambda_{\mathbf{i},a}^2(\mathbf{x}).$$

On the other hand

$$\mathrm{d}\mathbf{f}_h^1 = \sum_{\mathbf{j}=1}^{\mathbf{n}} \sum_{b=1}^{3} f_{\mathbf{j},b}^1 \, \mathrm{d}\Lambda_{\mathbf{j},b}^1(\mathbf{x}) = \sum_{\mathbf{j}=1}^{\mathbf{n}} \sum_{b=1}^{3} \tilde{f}_{\mathbf{j},b}^2 \Lambda_{\mathbf{j},b}^2(\mathbf{x}) = \tilde{\mathbf{f}}_h^2.$$

And the coefficients $\tilde{f}_{\mathbf{j},b}^2$ are related to $f_{\mathbf{j},b}^1$ by (5.13)-(5.15). Using the discrete curl matrix $\mathbb{C}$ and denoting by $\tilde{\mathbf{F}}_2$ the vector containing the coefficients $\tilde{f}_{\mathbf{j},b}^2$, expression (5.13)-(5.15) can be written in matrix form

$$\tilde{\mathbf{F}}_2 = \mathbb{C}\mathbf{F}_1.$$

Now,

$$(\mathbf{b}_h^2, \, \mathrm{d}\mathbf{f}_h^1) = (\mathbf{b}_h^2, \tilde{\mathbf{f}}_h^2) = \sum_{\mathbf{i}=1}^{\mathbf{n}} \sum_{a=1}^{3} \sum_{\mathbf{j}=1}^{\mathbf{n}} \sum_{b=1}^{3} b_{\mathbf{i},a}^2(t) \tilde{f}_{\mathbf{j},b}^2 (\Lambda_{\mathbf{i},a}^2, \Lambda_{\mathbf{j},b}^2).$$

We now need to find the expression of the scalar product of 2-forms yielding the 2-forms mass matrix. Using the formula of the scalar product (4.16) for 2-forms together with (4.12), we get

$$(\mathbf{\Lambda}_{\mathbf{i},a}^2, \mathbf{\Lambda}_{\mathbf{j},d}^2) = \int \Lambda_{\mathbf{i},a}^2 \Lambda_{\mathbf{j},d}^2 \det(g^{ab}) \sqrt{g} \, \mathrm{d}\mathbf{x}, \tag{5.29}$$

where b and c are chosen such that (a, b, c) is an even permutation of $(1, 2, 3)$ and e and f are chosen such that (d, e, f) is an even permutation of $(1, 2, 3)$. Then $\det(g^{bc}g^{ef})$ is composed of the inverse metric matrix with the line a and the column d removed. Also by checking the ordering for the different cases, also taking into account that the matrix G and its inverse are symmetric, we have that $\det(g^{bc}g^{ef}) = (-1)^{a+d}\mathrm{cof}(G^{-1})$, where cof denotes the cofactor. Hence using the computation of the inverse of a matrix based on the adjugate matrix $A^{-1} = (1/\det A)C^\top$, C being the cofactor matrix, we have that

$$g_{ad} = \frac{1}{|g|}\det(g^{bc}g^{ef}).$$

Whence

$$(\mathbf{\Lambda}^2_{\mathbf{i},a}, \mathbf{\Lambda}^2_{\mathbf{j},d}) = \int \Lambda^2_{\mathbf{i},a}\Lambda^2_{\mathbf{j},d}\frac{g_{ad}}{\sqrt{g}}\,\mathrm{d}\mathbf{x}. \tag{5.30}$$

Let us denote by M_2 this matrix. Then we can write, denoting by $\mathbf{B}_2$ the vector of coefficients of b^2_h

$$(\mathbf{b}^2_h,\, \mathrm{d}\mathbf{f}^1_h) = (\mathbf{b}^2_h, \tilde{\mathbf{f}}^2_h) = \tilde{\mathbf{F}}_2^\top M_2\mathbf{B}_2 = \mathbf{F}_1^\top\mathbb{C}^\top M_2\mathbf{B}_2.$$

In the FEEC setting, the mass matrices are the only matrices involving the metric that need to be assembled. Indeed the exterior derivative can be computed, as we saw with an explicit formula independent of the metric.

The same procedure can then be used for the weak divergence needed in the discrete version of Gauss's law (4.38)

$$-(\mathbf{e}^1_h,\, \mathrm{d}\psi^0_h) = \mathbf{\Psi}_0^\top\mathbb{G}^\top M_1\mathbf{E}_1.$$

Taking the sources ρ^0_h in V_0 and denoting by $\mathbf{\Upsilon}_0$ the corresponding vector of coefficients, and $\mathbf{j}^1_h \in V_1$ and denoting by $\mathbf{J}_1$ the corresponding vector of coefficients, we find that

$$(\mathbf{j}^1_h, \mathbf{f}^1_h) = \mathbf{F}_1^\top M_1\mathbf{J}_1, \qquad (\rho^0_h, \psi^0_h) = \mathbf{\Psi}_0^\top M_0\mathbf{\Upsilon}_0.$$

We are now ready to write the matrix form of the discrete Maxwell equations:

$$M_1\frac{\mathrm{d}\mathbf{E}_1}{\mathrm{d}t} - \mathbb{C}^\top M_2\mathbf{B}_2 = -M_1\mathbf{J}_1, \tag{5.31}$$

$$\frac{\mathrm{d}\mathbf{B}_2}{\mathrm{d}t} + \mathbb{C}\mathbf{E}_1 = 0, \tag{5.32}$$

$$\mathbb{G}^\top M_1\mathbf{E}_1 = M_0\mathbf{\Upsilon}_0, \tag{5.33}$$

$$\mathbb{D}\mathbf{B}_2 = 0. \tag{5.34}$$

5.3 Classical Finite Element approximation of Maxwell's equations

In a classical derivation of a Finite Element method for Maxwell's equations, one starts by choosing the spaces in which the fields are defined and derive a variational formulation. For Maxwell's equations the natural spaces are $H(\mathbf{curl}\,, \Omega)$ for one of the fields and $H(\mathrm{div}\,, \Omega)$ for the others. As the Ampère and Faraday equations have the same structure, we have the choice of choosing either $\mathbf{E}$ or $\mathbf{B}$ in $H(\mathbf{curl}\,, \Omega)$. Let us choose here $\mathbf{E} \in H(\mathbf{curl}\,, \Omega)$ and

$\mathbf{B} \in H(\mathrm{div}\,, \Omega)$. This corresponds to a strong Faraday and weak Ampère formulation. Indeed multiplying Ampère by a test function $\mathbf{F} \in H(\mathbf{curl}\,, \Omega)$ and integrating by parts the **curl** term and assuming that $\mathbf{F} \times \mathbf{n}$ vanishes on the boundary, which corresponds to essential perfectly conducting boundary conditions.

$$-\int_\Omega \frac{\partial \mathbf{E}}{\partial t} \cdot \mathbf{F}\, \mathrm{d}\mathbf{x} + c^2 \int_\Omega \mathbf{B} \cdot \nabla \times\, \mathbf{F}\, \mathrm{d}\mathbf{x} = \frac{1}{\varepsilon_0} \int_\Omega \mathbf{J} \cdot \mathbf{F}\, \mathrm{d}\mathbf{x}, \quad \forall \mathbf{F} \in H(\mathbf{curl}\,, \Omega)$$

We notice that for $\psi \in H^1(\Omega)$, taking $\mathbf{F} = \nabla\psi \in H(\mathbf{curl}\,, \Omega)$. Hence we can use it as a test function in the previous equation which yields

$$-\int_\Omega \frac{\partial \mathbf{E}}{\partial t} \cdot \nabla\psi\, \mathrm{d}\mathbf{x} = \frac{1}{\varepsilon_0} \int_\Omega \mathbf{J} \cdot \nabla\psi\, \mathrm{d}\mathbf{x} = \int_\Omega \frac{\partial \rho}{\partial t} \psi\, \mathrm{d}\mathbf{x} \quad \forall \psi \in H^1(\Omega)$$

using the weak form of the continuity equation

$$\int_\Omega \frac{\partial \rho}{\partial t} \psi\, \mathrm{d}\mathbf{x} - \int_\Omega \mathbf{J} \cdot \nabla\psi\, \mathrm{d}\mathbf{x} = 0 \quad \forall \psi \in H^1(\Omega).$$

And integrating this equation in time between 0 and t, we find the weak Poisson equation at any time t

$$-\int_\Omega \mathbf{E} \cdot \nabla\psi\, \mathrm{d}\mathbf{x} = \int_\Omega \rho\psi\, \mathrm{d}\mathbf{x} \quad \forall \psi \in H^1(\Omega).$$

Replacing the continuous spaces by their FEEC counterparts, we have similarly

$$-\int_\Omega \frac{\partial \mathbf{E}_h}{\partial t} \cdot \mathbf{F}_h\, \mathrm{d}\mathbf{x} + c^2 \int_\Omega \mathbf{B}_h \cdot \nabla \times\, \mathbf{F}_h\, \mathrm{d}\mathbf{x} = \frac{1}{\varepsilon_0} \langle \mathbf{J}_h, \mathbf{F}_h \rangle, \quad \forall \mathbf{F}_h \in V_1, \tag{5.35}$$

$$-\int_\Omega \mathbf{E}_h \cdot \nabla\psi_h\, \mathrm{d}\mathbf{x} = \frac{1}{\varepsilon_0} \langle \rho_h, \psi_h \rangle, \quad \forall \psi_h \in V_0 \tag{5.36}$$

For the Faraday equation, not integration by parts is necessary, so that the weak formulation

$$\int_\Omega \frac{\partial \mathbf{B}}{\partial t} \cdot \mathbf{C}\, \mathrm{d}\mathbf{x} + \int_\Omega \nabla \times\, \mathbf{E} \cdot \mathbf{C}\, \mathrm{d}\mathbf{x} = 0, \quad \forall \mathbf{C} \in H(\mathrm{div}\,, \Omega)$$

is equivalent to the strong form

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times\, \mathbf{E} = 0.$$

This property remains true at the discrete level thanks to our choice of discrete spaces.

5.4 Derivation of PIC model from discrete action principle

Maxwell's equations can be discretized in the spaces defined above keeping time continuous. The discrete scalar potential is $\phi_h \in V_0$, the discrete vector potential $\mathbf{A}_h \in V_1$, the discrete electric field $\mathbf{E}_h \in V_1$ and the discrete magnetic field $\mathbf{B}_h \in V_2$. Because of the discrete de Rham sequence satisfied by the Finite Element spaces, the fields are defined pointwise from the potentials

$$\mathbf{E}_h = -\nabla\phi_h - \frac{\partial \mathbf{A}_h}{\partial t}, \tag{5.37}$$

$$\mathbf{B}_h = \nabla \times\, \mathbf{A}_h. \tag{5.38}$$

These definitions directly imply the Faraday equation by adding the curl of (5.37) and the time derivative of (5.38)

$$\frac{\partial \mathbf{B}_h}{\partial t} + \nabla \times \mathbf{E}_h = 0, \tag{5.39}$$

and

$$\nabla \cdot \mathbf{B}_h = \nabla \cdot (\nabla \times \mathbf{A}_h) = 0.$$

As in the continuous case these equations follow directly from the definition of the fields from the potentials.

Let us recall the continuous action principle propose by Low (2.37):

$$\mathcal{A}[\mathbf{X}_s, \mathbf{V}_s, \phi, \mathbf{A}] = \sum_{\mathrm{s}} \int f_{s,0}(\mathbf{x}_0, \mathbf{v}_0) L_s(\mathbf{X}_s(t; \mathbf{x}_0, \mathbf{v}_0), \mathbf{V}_s(t; \mathbf{x}_0, \mathbf{v}_0), \frac{\mathrm{d}\mathbf{X}_s}{\mathrm{d}t}(t; \mathbf{x}_0, \mathbf{v}_0)) \,\mathrm{d}\mathbf{x}_0 \,\mathrm{d}\mathbf{v}_0 \,\mathrm{d}t$$
$$+ \frac{\epsilon_0}{2} \int |\nabla\phi + \frac{\partial \mathbf{A}}{\partial t}|^2 \,\mathrm{d}\mathbf{x} \,\mathrm{d}t - \frac{1}{2\mu_0} \int |\nabla \times \mathbf{A}|^2 \,\mathrm{d}\mathbf{x} \,\mathrm{d}t. \tag{5.40}$$

Now in this action principle we replace the continuous potentials by their discrete FEEC approximations, $\phi_h \in V_0$, and $\mathbf{A}_h \in V_1$. Moreover, instead of a continuum distribution function, we consider a discrete distribution defined a the sum of Dirac masses:

$$f_{s,h}(t, \mathbf{x}, \mathbf{v}) = \sum_{k=1}^{N_{p,s}} w_k \delta(\mathbf{x} - \mathbf{x}_k(t)) \delta(\mathbf{v} - \mathbf{v}_k(t)). \tag{5.41}$$

First considering only the first term of (5.40) involving f_0 and the particle Lagrangian, we observe that by replacing f_0, by $f_{s,h}(t = 0)$, we get

$$\sum_{\mathrm{s}} \sum_{k=1}^{N_{p,s}} w_k L_s(\mathbf{X}_s(t; \mathbf{x}_k(0), \mathbf{v}_k(0)), \mathbf{V}_s(t; \mathbf{x}_k(0), \mathbf{v}_k(0)), \frac{\mathrm{d}\mathbf{X}_s}{\mathrm{d}t}(t; \mathbf{x}_k(0), \mathbf{v}_k(0)) \,\mathrm{d}t$$

and as $(\mathbf{X}_s(t; \mathbf{x}_k(0), \mathbf{v}_k(0)), \mathbf{V}_s(t; \mathbf{x}_k(0), \mathbf{v}_k(0)))$ is the position at time t of the macro-particle starting at $(\mathbf{x}_k(0), \mathbf{v}_k(0))$, it is $(\mathbf{x}_k(t), \mathbf{v}_k(t))$, so that

$$L_s(\mathbf{X}_s(t; \mathbf{x}_k(0), \mathbf{v}_k(0)), \mathbf{V}_s(t; \mathbf{x}_k(0), \mathbf{v}_k(0)), \frac{\mathrm{d}\mathbf{X}_s}{\mathrm{d}t}(t; \mathbf{x}_k(0), \mathbf{v}_k(0)))$$
$$= (m_s \mathbf{v}_k + q_s \mathbf{A}(t, \mathbf{x}_k)) \cdot \frac{\mathrm{d}\mathbf{x}_k}{\mathrm{d}t} - \left(\frac{1}{2} m_s |\mathbf{v}_k|^2 + q_s \phi_h(t, \mathbf{x}_k) \right).$$

Plugging the approximations of f_h, ϕ_h and $\mathbf{A}_h$ into (5.40), we find

$$\mathcal{A}_h[\mathbf{X}_s, \mathbf{V}_s, \phi, \mathbf{A}_h] = \sum_{\mathrm{s}} \int f_{s,0}(\mathbf{x}_0, \mathbf{v}_0) L_s(\mathbf{X}_s(t; \mathbf{x}_0, \mathbf{v}_0), \mathbf{V}_s(t; \mathbf{x}_0, \mathbf{v}_0), \frac{\mathrm{d}\mathbf{X}_s}{\mathrm{d}t}(t; \mathbf{x}_0, \mathbf{v}_0)) \,\mathrm{d}\mathbf{x}_0 \,\mathrm{d}\mathbf{v}_0 \,\mathrm{d}t$$
$$+ \frac{\epsilon_0}{2} \int |\nabla\phi + \frac{\partial \mathbf{A}}{\partial t}|^2 \,\mathrm{d}\mathbf{x} \,\mathrm{d}t - \frac{1}{2\mu_0} \int |\nabla \times \mathbf{A}|^2 \,\mathrm{d}\mathbf{x} \,\mathrm{d}t. \tag{5.42}$$

Finally, we separate in the above Lagrangian, the particle part, the interaction term, involving both particles and fields. This yields:

$$\mathcal{A} = \sum_k \int_{t_1}^{t_2} (m_k \mathbf{v}_k \cdot \frac{\mathrm{d}\mathbf{x}_k}{\mathrm{d}t} - \frac{1}{2} m_k \mathbf{v}_k^2)\,\mathrm{d}t \\ + q_k \int_{t_1}^{t_2} \left(\mathbf{A}_h(t, \mathbf{x}_k) \cdot \frac{\mathrm{d}\mathbf{x}_k}{\mathrm{d}t} - \phi_h(t, \mathbf{x}_k) \right) \mathrm{d}t \\ + \frac{\epsilon_0}{2} \int |\nabla \phi_h + \frac{\partial \mathbf{A}_h}{\partial t}|^2 \,\mathrm{d}\mathbf{x}\,\mathrm{d}t - \frac{1}{2\mu_0} \int |\nabla \times \mathbf{A}_h|^2 \,\mathrm{d}\mathbf{x}\,\mathrm{d}t. \quad (5.43)$$

The action now depends on the dependent variables $\mathbf{x}_k, \mathbf{v}_k$ for all k and on the discrete fields $\phi_h \in V_0$ and $\mathbf{A}_h \in V_1$.

The variations of $\mathcal{A}$ with respect to $\mathbf{v}_k$ yield directly:

$$\frac{\mathrm{d}\mathbf{x}_k}{\mathrm{d}t} - \mathbf{v}_k = 0.$$

The variations (or functional differential) of $\mathcal{A}$ with respect to $\mathbf{x}_k$ yield

$$\begin{aligned} \delta\mathcal{A}[\mathbf{x}_k; \mathbf{y}_k] &= m_k \int_{t_1}^{t_2} \mathbf{v}_k \cdot \frac{\mathrm{d}\mathbf{y}_k}{\mathrm{d}t}\,\mathrm{d}t \\ &\quad + q_k \int_{t_1}^{t_2} \left(\mathbf{y}_k \cdot \nabla \mathbf{A}_h(t, \mathbf{x}_k) \cdot \frac{\mathrm{d}\mathbf{x}_k}{\mathrm{d}t} + \mathbf{A}_h(t, \mathbf{x}_k) \cdot \frac{\mathrm{d}\mathbf{y}_k}{\mathrm{d}t} - \mathbf{y}_k \cdot \nabla \phi_h(t, \mathbf{x}_k) \right) \mathrm{d}t \\ &= -m_k \int_{t_1}^{t_2} \mathbf{y}_k \cdot \frac{\mathrm{d}\mathbf{v}_k}{\mathrm{d}t}\,\mathrm{d}t + q_k \int_{t_1}^{t_2} \left(\mathbf{y}_k \cdot \nabla \mathbf{A}_h(t, \mathbf{x}_k) \cdot \frac{\mathrm{d}\mathbf{x}_k}{\mathrm{d}t} - \mathbf{y}_k \cdot \nabla \phi_h(t, \mathbf{x}_k) \right) \mathrm{d}t \\ &\quad - q_k \int_{t_1}^{t_2} \left(\frac{\partial \mathbf{A}_h}{\partial t}(t, \mathbf{x}_k) + \frac{\mathrm{d}\mathbf{x}_k}{\mathrm{d}t} \cdot \nabla \mathbf{A}_h(t, \mathbf{x}_k) \right) \cdot \mathbf{y}_k \,\mathrm{d}t \end{aligned}$$

where we have integrated by parts the terms involving a time derivative in $\mathbf{y}_k$ using that $\mathbf{y}_k$ vanishes on the boundaries. Then as this is true for all $\mathbf{y}_k$ and as

$$\frac{\mathrm{d}\mathbf{x}_k}{\mathrm{d}t} \cdot \nabla \mathbf{A}_k - \nabla \mathbf{A}_h \cdot \frac{\mathrm{d}\mathbf{x}_k}{\mathrm{d}t} = (\nabla \times \mathbf{A}_h) \times \frac{\mathrm{d}\mathbf{x}_k}{\mathrm{d}t},$$

we find that $\delta\mathcal{A}[\mathbf{x}_k; \mathbf{y}_k] = 0$ yields

$$\frac{\mathrm{d}\mathbf{v}_k}{\mathrm{d}t} = \frac{q_k}{m_k} \left(-\frac{\partial \mathbf{A}_h}{\partial t} - \nabla \phi_h + \mathbf{v}_k \times (\nabla \times \mathbf{A}_h) \right) = \frac{q_k}{m_k} (\mathbf{E}_h + \mathbf{v} \times \mathbf{B}_h).$$

Hence we got the standard equations of motion for each particle.

On the other hand, the variations with respect to $\mathbf{A}_h$ and ϕ_h can be performed exactly as in the continuous case except that the variations are now restricted to the finite dimensional function spaces V_1 and V_0. From these we get the weak form of Ampère's law and Gauss' law that were already expressed in (5.35) and (5.36).

Expanding the fields $\mathbf{E}_h$ in the basis of V_1 and $\mathbf{B}_h$ in the basis of V_2 and denoting by $\mathbf{e}$ and $\mathbf{b}$ the respective coefficients vectors, and stacking all the particle positions in a vector $\mathbf{X}$ and all the particle velocities in a vector $\mathbf{V}$, we have the discrete form of the Vlasov-Maxwell system on the left and to see the correspondence the continuous form on the right:

$$
\begin{aligned}
\dot{\mathbf{X}} &= \mathbf{V} & \dot{\mathbf{x}} &= \mathbf{v}, \\
\dot{\mathbf{V}} &= \mathbb{M}_p^{-1}\mathbb{M}_q\big(\mathbb{\Lambda}^1(\mathbf{X})\mathbf{e} + \mathbb{B}(\mathbf{X},\mathbf{b})\mathbf{V}\big) & \dot{\mathbf{v}} &= \frac{q_s}{m_s}\left(\mathbf{E} + \mathbf{v}\times\mathbf{B}\right), \\
\dot{\mathbf{e}} &= M_1^{-1}\big(\mathbb{C}^\top M_2\mathbf{b}(t) - \mathbb{\Lambda}^1(\mathbf{X})^\top\mathbb{M}_q\mathbf{V}\big) & \frac{\partial \mathbf{E}}{\partial t} &= \nabla\times\,\mathbf{B} - \mathbf{J}, \\
\dot{\mathbf{b}} &= -\mathbb{C}\mathbf{e}(t) & \frac{\partial \mathbf{B}}{\partial t} &= -\nabla\times\,\mathbf{E}.
\end{aligned}
$$

where we introduced the notations $\mathbb{B}(\mathbf{X},\mathbf{b})$ to represent the discrete $\mathbf{v}\times\mathbf{B}$, and $\mathbb{\Lambda}^1(\mathbf{X})$ for the matrix containing all the basis functions in V_1 evaluated at all the particle positions. Moreover $\mathbb{M}_p$ is the diagonal matrix containing the mass m_k of all the particles and $\mathbb{M}_q$ is the diagonal matrix containing the charge q_k of all the particles.

It is possible to check that this defines a non canonical Hamiltonian system with hamiltonian

$$
\hat{\mathcal{H}} = \frac{1}{2}\,\mathbf{V}^\top\mathbb{M}_p\mathbf{V} + \frac{1}{2}\,\mathbf{e}^\top M_1\mathbf{e} + \frac{1}{2}\,\mathbf{b}^\top M_2\mathbf{b}
$$

such that

$$
\nabla\hat{\mathcal{H}} = (0, \mathbb{M}_p\mathbf{V}, \mathbb{M}_1\mathbf{e}, \mathbb{M}_2\mathbf{b})^\top
$$

and with the Poisson matrix

$$
\hat{\mathcal{J}} = \begin{pmatrix}
0 & \mathbb{M}_p^{-1} & 0 & 0 \\
-\mathbb{M}_p^{-1} & \mathbb{B}(\mathbf{X},\mathbf{b}) & \mathbb{\Lambda}^1(\mathbf{X})M_1^{-1} & 0 \\
0 & -M_1^{-1}\mathbb{\Lambda}^1(\mathbf{X})^\top & 0 & M_1^{-1}\mathbb{C}^\top \\
0 & 0 & -\mathbb{C}M_1^{-1} & 0
\end{pmatrix}.
$$

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