Geometric Discontinuous Galerkin Methods for Fluids and Plasmas

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Outline

1. Discontinuous Galerkin Methods in a Nutshell
2. Hamiltonian Dynamics and Poisson Brackets
3. Discretisation of Poisson Brackets
4. Summary and Outlook

Discontinuous Galerkin Methods in a Nutshell

The Finite Element Method in a Nutshell

- seek the solution $u \in U$ to

$$\begin{cases} -\Delta u = f & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

- formally: multiply by a test function $v \in V$ and integrate by parts

$$\int_\Omega (-\Delta u - f)\, v\, dx = \int_\Omega \nabla u \cdot \nabla v\, dx - \int_\Omega f v\, dx - \int_{\partial\Omega} n \cdot \nabla u\, v\, dx = 0$$

- requiring $v = 0$ on $\partial\Omega$, this is formally equivalent to the weak form: find $u \in U$ such that

$$\int_\Omega \nabla u \cdot \nabla v\, dx - \int_\Omega f v\, dx = 0 \qquad \text{for all} \quad v \in V$$

- U is called the *space of trial functions* and V the *space of test functions* (here: $V = U$)

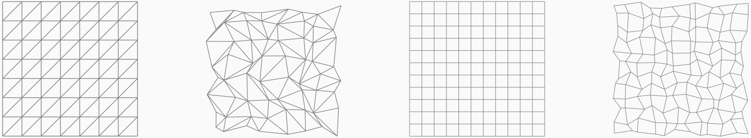
$$U = H_0^1(\Omega) = \left\{ u \in H^1(\Omega),\ u = 0 \text{ on } \partial\Omega \right\} = \left\{ u = u(x) \ :\ u,\, \nabla u \in L^2(\Omega),\ u = 0 \text{ on } \partial\Omega \right\}$$

The Finite Element Method in a Nutshell

- problem:

$$\text{Find } u \in U \text{ such that } \int_\Omega \nabla u \cdot \nabla v \, dx - \int_\Omega f v \, dx = 0 \text{ for all } v \in V.$$

- partition the domain Ω into a set Ω_h of sub-domains (elements) Ω_i (triangles, quadrilaterals, ...)



- construct finite dimensional subspaces $U_h \subset U$ by approximation of functions in U by simpler functions, defined on each sub-domain Ω_i with suitable matching conditions at interfaces

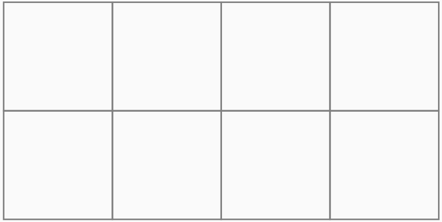
$$U_h = \left\{ u_h = u_h(x) \, : \, u_h|_{\Omega_i} \in \mathbb{P}^r(\Omega_i), \; u_h \in C^0(\Omega), \; u_h = 0 \text{ on } \partial\Omega \right\}$$

- finite element problem:

$$\text{Find } u_h \in U_h \text{ such that } \int_\Omega \nabla u_h \cdot \nabla v_h \, dx - \int_\Omega f v_h \, dx = 0 \text{ for all } v_h \in V_h.$$

Finite-dimensional Function Spaces

- consider a uniform cartesian grid



- consider a tensor-product Lagrange basis using Lobatto quadrature points as nodes

$$u_h(x)|_{\Omega_k} = \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} u_{k,ij}\, \phi_{k,i}(x^1)\, \phi_{k,j}(x^2)$$

$$\phi_{k,i}(x) = \begin{cases} l^{r,i}\big((x - x_k)/(x_{k+1} - x_k)\big), & x_k \leq x \leq x_{k+1}, \\ 0, & \text{else}, \end{cases} , \qquad l^{r,i}(\xi) = \prod_{\substack{1 \leq j \leq r, \\ j \neq i}} \frac{\xi - \xi_j}{\xi_i - \xi_j},$$

here $l^{r,i}(\xi)$ denotes the i-th Lagrange polynomial of order r

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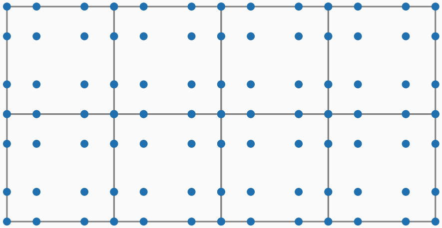

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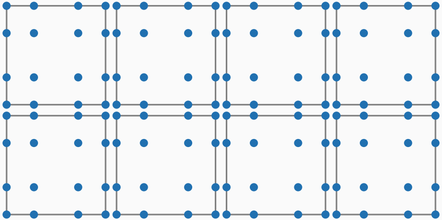
Discontinuous Galerkin Methods in a Nutshell



- fluid dynamics and plasma physics: hyperbolic conservation laws

$$\partial_t u + \nabla \cdot F(u) = 0$$

- piecewise polynomial approximation of functions with discontinuities at element boundaries

$$U_h = \left\{ u_h = u_h(x) \;:\; u_h|_{\Omega_i} \in \mathbb{P}^r(\Omega_i) \right\}$$

- discretise weak form of conservation law form of the equations

$$\sum_k \left\{ \int_{\Omega_k} v_h \, \partial_t u_h \, dx - \int_{\Omega_k} F(u_h) \cdot \nabla v_h \, dx + \int_{\partial\Omega_k} v_h \, n \cdot F(u_h) \, dx \right\} = 0$$

Hamiltonian Dynamics and Poisson Brackets

Hamiltonian Dynamics and Poisson Brackets

- let $u(t, x) = (u^1,\ u^2,\ \dots,\ u^m)^T$ be the field variables of some system of partial differential equations, defined over the space Ω with coordinates x
- for Hamiltonian systems the evolution of any functional $\mathcal{F}$ of the field variables u is given by

$$\frac{d\mathcal{F}}{dt} = \{\mathcal{F}, \mathcal{H}\} \qquad \text{with} \qquad \{\mathcal{F}, \mathcal{G}\} = \int_{\Omega} \frac{\delta \mathcal{F}}{\delta u^i}\, \mathcal{J}^{ij}(u)\, \frac{\delta \mathcal{G}}{\delta u^j}\, \mathrm{d}x$$

- $\mathcal{F}$, $\mathcal{G}$ and $\mathcal{H}$ are functionals of u and $\delta \mathcal{F} / \delta u^i$ is the functional derivative
- specifically, $\mathcal{H}$ is the Hamiltonian functional, usually the total energy of the system
- the Poisson bracket $\{\cdot, \cdot\}$ is an bilinear, anti-symmetric operation that satisfies Leibniz' rule and the Jacobi identity,

$$\{\{\mathcal{F}, \mathcal{G}\}, \mathcal{H}\} + \{\{\mathcal{G}, \mathcal{H}\}, \mathcal{F}\} + \{\{\mathcal{H}, \mathcal{F}\}, \mathcal{G}\} = 0,$$

  for arbitrary functionals $\mathcal{F}, \mathcal{G}, \mathcal{H}$ of u

Hamiltonian Dynamics and Poisson Brackets

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$$\frac{d\mathcal{F}}{dt} = \{\mathcal{F}, \mathcal{H}\} \qquad \text{with} \qquad \{\mathcal{F}, \mathcal{G}\} = \int_\Omega \frac{\delta \mathcal{F}}{\delta u^i} \, \mathcal{J}^{ij}(u) \, \frac{\delta \mathcal{G}}{\delta u^j} \, \mathrm{d}z$$

- Hamiltonian systems preserve energy due to anti-symmetry of the Poisson bracket

$$\frac{d\mathcal{H}}{dt} = \{\mathcal{H}, \mathcal{H}\} = -\{\mathcal{H}, \mathcal{H}\} = 0$$

- if the Hamiltonian is constant along the flow of some functional Φ, i.e., $\{\mathcal{H}, \Phi\} = 0$, then Φ is a momentum map that is preserved by the flow of $\mathcal{H}$ as

$$\frac{d\Phi}{dt} = \{\Phi, \mathcal{H}\} = -\{\mathcal{H}, \Phi\} = 0$$

- if $\mathcal{J}(u)$ has a non-empty nullspace, there exist so-called Casimir invariants, that is functionals $\mathcal{C}$ for which $\{\mathcal{F}, \mathcal{C}\} = 0$ for all functionals $\mathcal{F}$, i.e.,

$$\mathcal{J}^{ij}(u) \, \frac{\delta \mathcal{C}}{\delta u^j} = 0$$

Finite-dimensional Hamiltonian Systems

- consider a canonical Hamiltonian system in N dimensions

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \qquad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, \qquad i = 1, ..., N$$

- combining the dynamical variables into a vector $z = (q, p)$, we can write

$$\Omega \dot{z} = \nabla H(z) \qquad \text{with} \qquad \nabla = (\partial_q, \partial_p)$$

with Ω being a $2N \times 2N$ skew-symmetric matrix

$$\Omega = \begin{pmatrix} \mathbb{0}_{N\times N} & -\mathbb{1}_{N\times N} \\ \mathbb{1}_{N\times N} & \mathbb{0}_{N\times N} \end{pmatrix}$$

- special case of a Poisson system of ODEs with $2N$ degrees of freedom and $P = \Omega^{-1}$

$$\dot{z} = P(z) \, \nabla H(z)$$

- symplectic structure: bilinear map of vectors ξ and η in phasespace

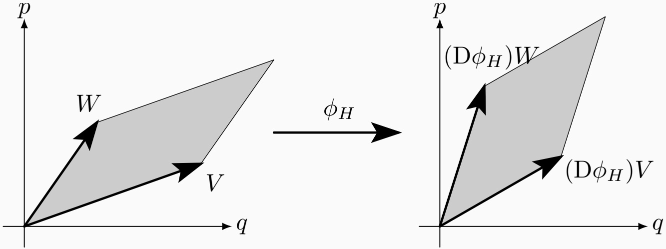
$$\omega(\xi, \eta) = \xi^T \Omega \eta, \qquad \omega = -\mathrm{d}\theta, \qquad \theta = p \cdot \mathrm{d}q$$

Poincaré Integral Invariants

- phase space circulation theorem (similar to ordinary fluids): conservation of loop integrals along any closed curve Γ in phasespace

$$\frac{d}{dt}\oint_{\Gamma} p \cdot \mathrm{d}q = 0$$

- symplecticity: conservation of phasespace area (and as consequence of phasespace volume)

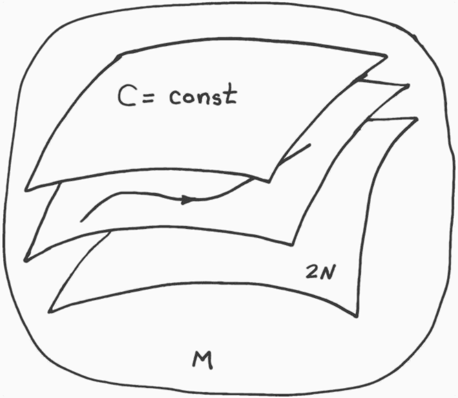


- analogously conservation of higher-order Poincaré invariants (in total 2N invariants: loop integrals of dimension $1, 3, 5, ..., 2N-1$ and surface integrals of dimension $2, 4, 6, ..., 2N$)

$$\theta,\ \omega,\ \theta\wedge\omega,\ \omega\wedge\omega,\ \theta\wedge\omega\wedge\omega,\ \ldots$$

Phasespace Structure of Poisson Systems

- local structure of a Poisson manifold



- phasespace is foliated into symplectic submanifolds by the level sets of the Casimir invariants
- every orbit remains on the surface defined by the initial values of the Casimir invariants

Some Examples

Ideal Compressible Fluids

- Euler's equations for an ideal compressible fluid

$$\begin{aligned} \rho_t + \nabla\cdot(\rho v) &= 0, \\ \rho v_t + \rho v\cdot\nabla v &= -\nabla p, \\ s_t + v\cdot\nabla s &= 0, \end{aligned} \qquad \begin{aligned} p &= \rho^2 \varepsilon_\rho(\rho, s), \\ \varepsilon &= \beta\rho^{\gamma-1}\exp\{(\gamma-1)/\alpha\, s\}, \end{aligned}$$

v velocity field

ρ fluid density

s entropy per unit mass

ε internal energy

p gas pressure

- Poisson bracket:

$$\begin{aligned} \{\mathcal{F}, G\}[v,\rho,s] = -\int \Bigg[&\frac{\delta\mathcal{F}}{\delta\rho}\nabla\cdot\frac{\delta G}{\delta v} - \frac{\delta G}{\delta\rho}\nabla\cdot\frac{\delta\mathcal{F}}{\delta v} + \frac{\delta\mathcal{F}}{\delta v}\cdot\left(\frac{\nabla\times v}{\rho}\times\frac{\delta G}{\delta v}\right) \\ &+ \frac{1}{\rho}\nabla s\cdot\left(\frac{\delta\mathcal{F}}{\delta s}\frac{\delta G}{\delta v} - \frac{\delta G}{\delta s}\frac{\delta\mathcal{F}}{\delta v}\right)\Bigg]\mathrm{d}x \end{aligned}$$

$$\mathcal{H} = \int \left[\tfrac{1}{2}\rho\,|v|^2 + \rho\varepsilon(\rho,s)\right]\mathrm{d}x$$

Ideal Compressible Fluids

- Euler's equations for an ideal compressible fluid

$$\begin{aligned} \rho_t + \nabla \cdot (\rho v) &= 0, & p &= \rho^2 \varepsilon_\rho(\rho, s), \\ \rho v_t + \rho v \cdot \nabla v &= -\nabla p, & \varepsilon &= \beta \rho^{\gamma-1} \exp\{(\gamma - 1)/\alpha\, s\}, \\ s_t + v \cdot \nabla s &= 0, \end{aligned}$$

v velocity field

s entropy per unit mass

p gas pressure

ρ fluid density

ε internal energy

- Lie-Poisson bracket in momentum variables: $m = \rho v$, $\sigma = \rho s$

$$\begin{aligned} \{\mathcal{F}, \mathcal{G}\}[\rho, m, \sigma] = -\int \Bigg[\rho \left(\frac{\delta \mathcal{F}}{\delta m} \nabla \cdot \frac{\delta \mathcal{G}}{\delta \rho} - \frac{\delta \mathcal{G}}{\delta m} \nabla \cdot \frac{\delta \mathcal{F}}{\delta \rho} \right) + m \cdot \left(\frac{\delta \mathcal{F}}{\delta m} \cdot \nabla \frac{\delta \mathcal{G}}{\delta m} - \frac{\delta \mathcal{G}}{\delta m} \cdot \nabla \frac{\delta \mathcal{F}}{\delta m} \right) \\ + \sigma \left(\frac{\delta \mathcal{F}}{\delta m} \nabla \cdot \frac{\delta \mathcal{G}}{\delta \sigma} - \frac{\delta \mathcal{G}}{\delta m} \nabla \cdot \frac{\delta \mathcal{F}}{\delta \sigma} \right) \Bigg] \mathrm{d}x \end{aligned}$$

$$\mathcal{H} = \int \left[\tfrac{1}{2} \rho^{-1} \left| m \right|^2 + \rho \varepsilon(\rho, \sigma) \right] \mathrm{d}x$$

Burgers Equation

- Burgers Equation

$$\partial_t u + 3u\partial_x u = 0$$

- conservation law form

$$\partial_t u + \frac{3}{2}\partial_x(u^2) = 0$$

- Poisson Bracket

$$\{\mathcal{F},\mathcal{G}\}[u] = -\int u\left(\frac{\delta\mathcal{F}}{\delta u}\frac{\partial}{\partial x}\frac{\delta\mathcal{G}}{\delta u} - \frac{\delta\mathcal{G}}{\delta u}\frac{\partial}{\partial x}\frac{\delta\mathcal{F}}{\delta u}\right)\mathrm{d}x$$

$$\mathcal{H} = \frac{1}{2}\int |u|^2\ \mathrm{d}x$$

Discretisation of Poisson Brackets

Discretisation of Poisson Brackets: Why and how?

Why?

- structure-preserving numerical schemes
  - preserving anti-symmetry immediately leads to energy preserving algorithms (easy!)
  - preserving Casimir invariants and momentum maps leads to conservation law preserving algorithms
  - preserving the Jacobi identity leads to phasespace structure and Poincaré invariant preserving algorithms (very hard!)
- dynamical systems theory: study finite-dimensional versions of complicated infinite-dimensional Hamiltonian systems

But how?

- constant Poisson structure (e.g. Maxwell equations, linearised fluid models): anything goes (only antisymmetry required!)
- Fourier discretisation of sine-Euler equations (Zeitlin'91, McLachlan'93)
- finite element particle-in-cell methods for kinetic and some fluid models
- grid-based methods for non-constant Poisson structure: *hic sunt dracones*

Discretisation of Poisson Brackets: Discrete Functionals

- choose a finite dimensional (broken) function space

$$U_h = \left\{ u_h = u_h(x) \ : \ u_h|_{\Omega_i} \in \mathbb{P}^r(\Omega_i) \right\}$$

- when evaluated on the discrete field variable u_h, any linear functional $\mathcal{F}[u]$ turns into a function $F(\hat{u})$ of the degrees of freedom $\hat{u}$

$$F(\hat{u}) = \mathcal{F}[u_h]$$

- example: Hamiltonian of the Burgers equation

$$H(\hat{u}) = \mathcal{H}[u_h] = \frac{1}{2} \int\limits_{\Omega} u_h^2 \, dx = \frac{1}{2} \, \hat{u}^T M \, \hat{u}, \qquad M_{ij} = \int\limits_{\Omega} \phi_i(x) \, \phi_j(x) \, dx$$

- the functional derivates of $\mathcal{F}$, when restricted to discrete solutions u_h, can be approximated by partial derivatives of F with respect to the degrees of freedom $\hat{u}$

Discretisation of Poisson Brackets: Discrete Functional Derivatives

- let the functional derivative be defined as the L^2-representative of the Fréchet derivative

$$\langle D\mathcal{F}[u] \, , \, v \rangle_{L^2} = \int_\Omega \frac{\delta \mathcal{F}}{\delta u} \cdot v \, dx$$

- let $\{\phi_i\}_{i=1}^N$ denote a basis in U_h and $\{\psi_i\}_{i=1}^N$ the dual basis in U_h^*, such that $\langle \psi_i \, , \, \varphi_j \rangle_{L^2} = \delta_{ij}$
- the functional derivative can be expressed in the dual basis as

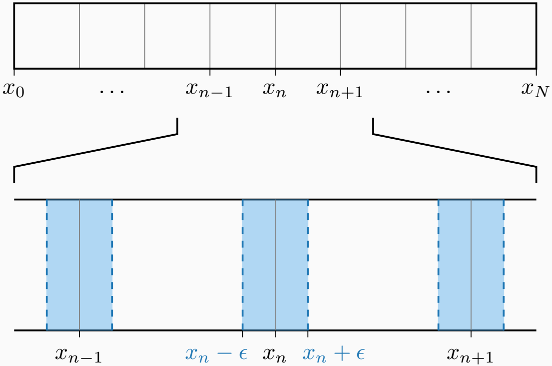
$$\frac{\delta \mathcal{F}}{\delta u}[u_h](x) = \sum_i \frac{\partial F}{\partial u_i} \, \psi_i(x) = \sum_{i,j} \frac{\partial F}{\partial u_i} \mathbb{M}_{ij}^{-1} \, \varphi_j(x)$$

- on each element k, we can write the discrete Poisson bracket as

$$\{F, G\}_k = \sum_{i,l,m} c_{im}^l u_l \, \frac{\partial F}{\partial u_i} \, \frac{\partial G}{\partial u_m},$$

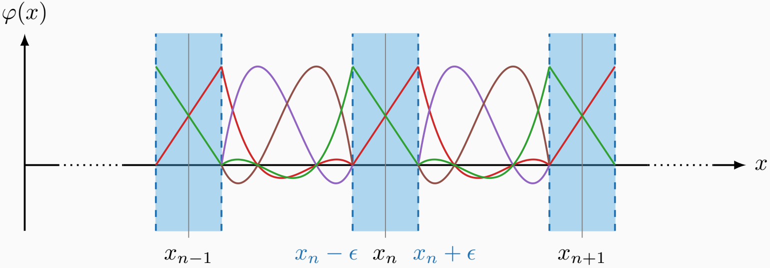
$$c_{im}^l = - \sum_{j,n} \mathbb{M}_{ij}^{-1} \, \mathbb{M}_{mn}^{-1} \int_{\Omega_k} \varphi_l(x) \left(\varphi_n(x) \frac{\partial}{\partial x} \varphi_j(x) - \varphi_j(x) \frac{\partial}{\partial x} \varphi_n(x) \right) \mathrm{d}x$$

Discretisation of Poisson Brackets: Discontinuities



- at each interface x_n, insert a mortar element of size 2ϵ, spanning the interval $[x_n - \epsilon, x_n + \epsilon]$

Discretisation of Poisson Brackets: Discontinuities



- in the elements choose an arbitrary-degree polynomial basis
- in the mortar use a linear basis, interpolating between the left and right solution
- split discrete bracket into element and mortar/boundary contributions

$$\{\cdot,\cdot\}_d = \{\cdot,\cdot\}_\circ + \{\cdot,\cdot\}_b$$

- while both $\{\cdot,\cdot\}_\circ$ and $\{\cdot,\cdot\}_b$ satisfy the Jacobi identity, their sum does not

Some Words on Skew-symmetric and Split Forms

Skew-symmetric and Split Forms

- “classical approach”: discretise weak form of conservation law form of the equations
- “modern approach”: discretise skew-symmetric or split forms of equations with non-conservative terms
- while conservation law forms preserve integrals of the prognostic variables (e.g., mass, momentum, internal energy), split-forms are particularly well suited as a starting point for the construction of invariant-preserving schemes (e.g., total energy, entropy)
- usually a convex combination of advective and conservative form, e.g., for Burgers equation

$$\partial_t u + 3\left(\alpha\, u u_x + \tfrac{1}{2}(1-\alpha)\,(u^2)_x\right) = 0, \qquad \alpha \in [0,1]$$

- the FD, FV and DG literature is full of papers describing the quest for skew-symmetric or split forms especially of fluid equations (for Euler see e.g. Morinishi’98, Gassner’14, Palha’17)

→ Poisson brackets can do that job for you!

Skew-symmetric and Split Forms: Burgers Equation

- Poisson bracket and Hamiltonian

$$\{\mathcal{F}, \mathcal{G}\}[u] = -\int_\Omega u(x') \left(\frac{\delta \mathcal{F}}{\delta u} \frac{\partial}{\partial x'} \frac{\delta \mathcal{G}}{\delta u} - \frac{\delta \mathcal{G}}{\delta u} \frac{\partial}{\partial x'} \frac{\delta \mathcal{F}}{\delta u} \right) \mathrm{d}x',$$

$$\mathcal{H} = \frac{1}{2} \int_\Omega |u(x)|^2 \, \mathrm{d}x$$

- equations of motion: split form with $\alpha = 1/3$!

$$u_t(x) = \{u, \mathcal{H}\} = -\int\limits_\Omega u(x') \left(\delta(x - x') \frac{\partial}{\partial x'} u(x') - u(x') \frac{\partial}{\partial x'} \delta(x - x') \right) \mathrm{d}x'$$

$$= -\int\limits_\Omega \left(u(x') \, \frac{\partial}{\partial x'} u(x') + \frac{\partial}{\partial x'} u(x')^2 \right) \delta(x - x') \, dx' + \int\limits_{\partial\Omega} u(x')^2 \delta(x - x') \, \mathrm{d}x'$$

$$0 = u_t(x) + u(x) \, u_x(x) + (u(x)^2)_x - \left[u(x)^2 \right]_{\partial\Omega}$$

→ energy-conservation is achieved by *any* anti-symmetry preserving discretisation of the bracket

Summary and Outlook

Summary and Outlook

- the discretisation of Poisson brackets automatically leads to energy- and often other invariant-preserving methods
- open problem: Jacobi-identity-preserving truncation
- deficit in the literature: boundary conditions for Poisson brackets
- complementary approach: discretise the Lie algebra on which the constrained Eulerian action principles are based (Euler–Poincaré theory; same problems!)
- outlook
  - appropriate time integration schemes (Hamiltonian splitting often not feasible)
  - implementation for Euler and magnetohydrodynamics equations in 2d (will soon be available at `https://github.com/ddmgni/GDGSEM.jl`)
  - adaptation to the Vlasov–Maxwell–Landau system