# 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

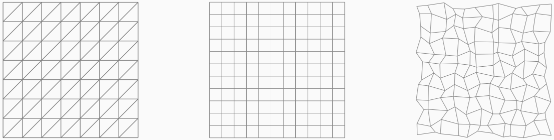
# Discontinuous Galerkin Methods in a Nutshell

# Discontinuous Galerkin Methods in a Nutshell

- fluid dynamics and plasma physics: hyperbolic conservation laws

$$\partial_t u + \nabla \cdot F(u) = 0, \qquad u \in U$$

- partition the domain $\Omega$ into a set $\Omega_h$ of sub-domains (elements) $\Omega_i$ (triangles, quadrilaterals, ...)



- approximation of functions in $U$ by simpler functions, defined on each sub-domain $\Omega_i$ 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

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

# 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 $\Omega$ with coordinates $x$
- for Hamiltonian systems the evolution of any functional $\mathcal{F}$ of the field variables $u$ is given by

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

- $\mathcal{F}$, $\mathcal{G}$ 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 a 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

- for Hamiltonian systems, the evolution of any functional $\mathcal{F}$ is given by

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

- 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 $\Phi$, i.e., $\{\mathcal{H}, \Phi\} = 0$, then $\Phi$ 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.,

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

# 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 and Hamiltonian

$$\{\mathcal{F}, \mathcal{G}\}[u] = -\int u\left(\frac{\delta\mathcal{F}}{\delta u}\frac{\partial}{\partial x}\frac{\delta\mathcal{G}}{\delta u} - \frac{\delta\mathcal{G}}{\delta u}\frac{\partial}{\partial x}\frac{\delta\mathcal{F}}{\delta u}\right)\mathrm{d}x, \qquad \mathcal{H}[u] = \frac{1}{2}\int |u|^2\,\mathrm{d}x$$

- equations of motion

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

- the Poisson bracket leads to a *split-form* of the equations that includes non-conservative terms

# 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
  - 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
- dynamical systems theory: study finite-dimensional approximations 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)
- particle-in-cell methods for kinetic and some fluid models (e.g., Vlasov–Maxwell)
- grid-based methods for non-constant Poisson structure: *hic sunt dracones*

# Discretisation of Poisson Brackets: Functionals

- choose a finite dimensional (broken) function space

$$U_h = \left\{ u_h = u_h(x) \,:\, u_h|_{\Omega_i} \in \mathbb{P}^r(\Omega_i) \right\}, \qquad u_h(x) = \sum_{i=1}^{n} u_i \, \varphi_i(x), \qquad \hat{u} = (u_1, ..., u_n)^T$$

- 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

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

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

# Discretisation of Poisson Brackets: Functional Derivatives

- 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 $\hat{u}$

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

- on each element $k$, we can write the discrete Poisson bracket of the Burgers equation as

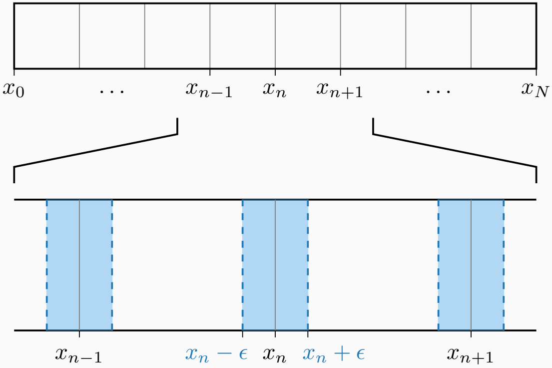
$$\{F, G\}_k = \sum_{i,l,m} c^l_{im} u_l \, \frac{\partial F}{\partial u_i} \, \frac{\partial G}{\partial u_m},$$

$$c^l_{im} = - \sum_{j,n} \mathbb{M}^{-1}_{ij} \, \mathbb{M}^{-1}_{mn} \int_{\Omega_k} \phi_l(x) \left( \phi_n(x) \frac{\partial}{\partial x} \phi_j(x) - \phi_j(x) \frac{\partial}{\partial x} \phi_n(x) \right) \mathrm{d}x$$

- Jacobi identity

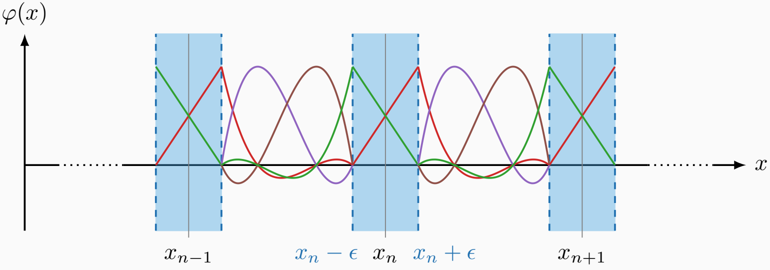
$$J^i_{klm} = \sum_j \left[ c^i_{kj} c^j_{lm} + c^i_{mj} c^j_{kl} + c^i_{lj} c^j_{mk} \right] = 0 \quad \forall \, i, k, l, m$$

# Discretisation of Poisson Brackets: Discontinuities




- at each interface $x_n$, insert an infinitesimal mortar element, 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

$$\{\cdot,\cdot\}_d = \{\cdot,\cdot\}_\circ + \{\cdot,\cdot\}_b \qquad \rightarrow \qquad \frac{du_i}{dt} = \{u_i, H\}_d$$

# Summary and Outlook

# Summary and Outlook

- the discretisation of Poisson brackets automatically leads to energy- and often other invariant-preserving methods
- skew-symmetric or split forms with non-conservative terms automatically arise from the brackets
- treatment of dissipative terms by addition of a metric bracket with suitable compatibility properties that guarantee the laws of thermodynamics
- open problem: Jacobi-identity-preserving truncation

# Appendix: Phasespace Structure of Hamiltonian Systems

# 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 $\Omega$ 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 $\xi$ and $\eta$ in phasespace

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

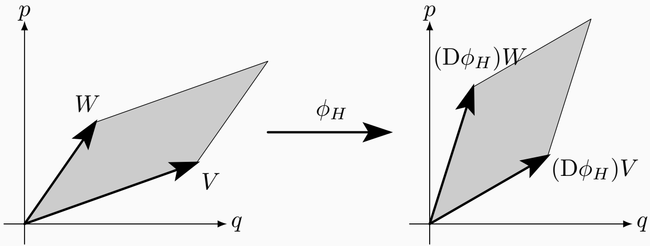
# Poincaré Integral Invariants

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

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

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

$$\frac{d}{dt}\int_{\Omega} \mathrm{d}p \wedge \mathrm{d}q = 0$$

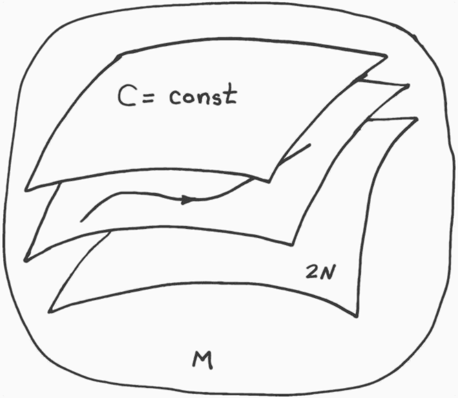



- analogously conservation of higher-order Poincaré invariants (in total 2N types of invariants: loop integrals of dimension $1, 3, 5, ..., 2N-1$ and surface integrals of dimension $2, 4, 6, ..., 2N$)

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

# 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 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 $\alpha = 1/3$ !

$$u_t(x) = \{u, \mathcal{H}\} = -\int_\Omega u(x') \left( \delta(x - x') \frac{\partial}{\partial x'} u(x') - u(x') \frac{\partial}{\partial x'} \delta(x - x') \right) \mathrm{d}x'$$
$$= -\int_\Omega \left( u(x') \frac{\partial}{\partial x'} u(x') + \frac{\partial}{\partial x'} u(x')^2 \right) \delta(x - x') \, dx' + \int_{\partial\Omega} u(x')^2 \delta(x - x') \, \mathrm{d}x'$$
$$0 = u_t(x) + u(x) \, u_x(x) + (u(x)^2)_x - \left[ u(x)^2 \right]_{\partial\Omega}$$

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

# Some Words on Dissipation

# Metriplectic Dynamics

- metriplectic dynamics describes systems that have a Hamiltonian part $\{\cdot,\cdot\}$ and a Casimir (entropy) dissipating symmetric part $(\cdot,\cdot)$
- the evolution of some functional $\mathcal{F}$ of the field variables $u$ is given by

$$\frac{d\mathcal{F}}{dt} = \{\mathcal{F},\mathcal{G}\} + (\mathcal{F},\mathcal{G})$$

- $\mathcal{G} = \mathcal{H} - \mathcal{S}$ a generalised free energy functional with Hamiltonian $\mathcal{H}$ and entropy functional $\mathcal{S}$, which is a Casimir invariant of the Poisson bracket $\{\cdot,\cdot\}$
- the metriplectic bracket $(\cdot,\cdot)$ is a bilinear, symmetric operator, satisfying Leibniz' rule,

$$(\mathcal{F},\mathcal{G}) = \int_\Omega \frac{\delta\mathcal{F}}{\delta u^i}\,\mathcal{K}^{ij}(u)\,\frac{\delta\mathcal{G}}{\delta u^j}\,dz$$

- $\mathcal{K}(u)$ is a self-adjoint operator with appropriate nullspace s.th. $(\mathcal{H},\mathcal{G}) = 0$
- metriplectic dynamics preserves energy and monotonically increases entropy

$$\frac{d\mathcal{H}}{dt} = 0, \qquad \frac{d\mathcal{S}}{dt} \geq 0$$