



**HELMHOLTZ**

SPITZENFORSCHUNG FÜR  
GROSSE HERAUSFORDERUNGEN

# 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

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# 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

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

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

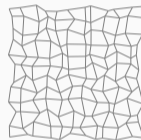
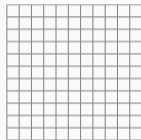
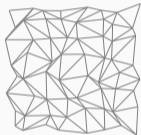
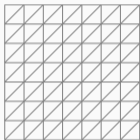
$$U = H_0^1(\Omega) = \{u \in H^1(\Omega), u = 0 \text{ on } \partial\Omega\} = \{u = u(x) : u, \nabla u \in L^2(\Omega), u = 0 \text{ on } \partial\Omega\}$$

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



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

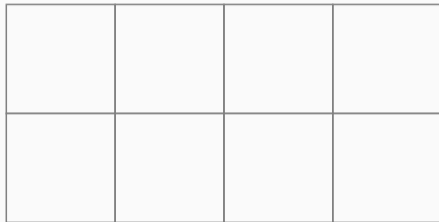
$$U_h = \{u_h = u_h(x) : u_h|_{\Omega_i} \in \mathbb{P}^r(\Omega_i), u_h \in C^0(\Omega), u_h = 0 \text{ on } \partial\Omega\}$$

- 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

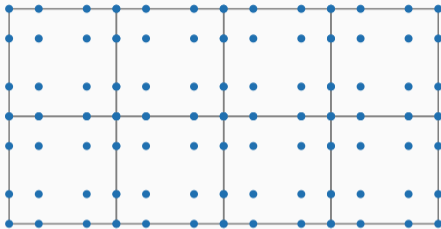
$$u_h(x)|_{\Omega_k} = \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} u_{k,ij} \phi_{k,i}(x^1) \phi_{k,j}(x^2)$$

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

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

# Finite-dimensional Function Spaces

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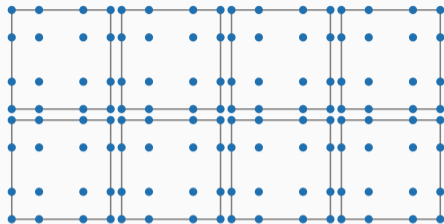
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here  $l^{r,i}(\xi)$  denotes the  $i$ -th Lagrange polynomial of order  $r$

# 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

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

- 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

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# 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

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

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

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

- 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.,

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

# Finite-dimensional Hamiltonian Systems

- consider a canonical Hamiltonian system in  $N$  dimensions

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

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

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

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

$$\omega(\xi, \eta) = \xi^T \Omega \eta, \quad \omega = -d\theta, \quad \theta = p \cdot dq$$

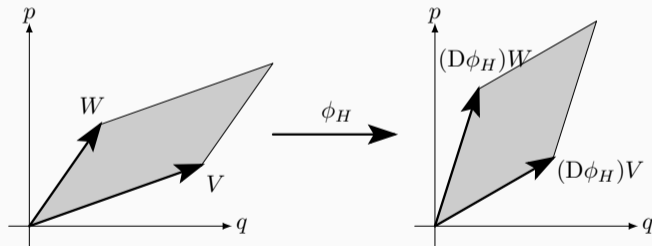
# Poincaré Integral Invariants

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

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

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

$$\frac{d}{dt} \int_{\Omega} dp \wedge dq = 0$$

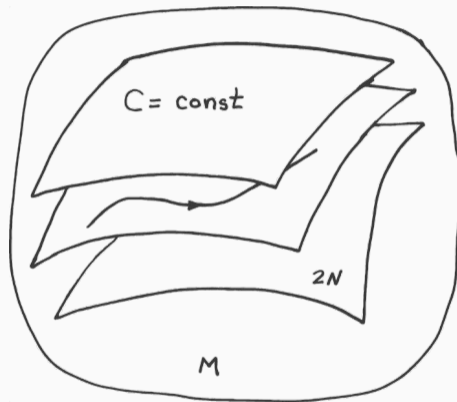


- analogously conservation of higher-order Poincaré invariants (in total  $2N$  types of invariants: loop integrals of dimension  $1, 3, 5, \dots, 2N - 1$  and surface integrals of dimension  $2, 4, 6, \dots, 2N$ )

$$\theta, \omega, \theta \wedge \omega, \omega \wedge \omega, \theta \wedge \omega \wedge \omega, \dots$$

# 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

# 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

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

$$\mathcal{H}[u] = \frac{1}{2} \int |u|^2 dx$$

- equations of motion

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

- the Poisson bracket leads to a so-called split-form of the equations

# Discretisation of Poisson Brackets

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# 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 phase space 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: Functionals

- choose a finite dimensional (broken) function space

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

- 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

$$H(\hat{u}) = \mathcal{H}[u_h] = \frac{1}{2} \int_{\Omega} u_h^2 dx = \frac{1}{2} \hat{u}^T M \hat{u},$$

$$M_{ij} = \int_{\Omega} \phi_i(x) \phi_j(x) dx$$

# Discretisation of Poisson Brackets: Functional Derivatives

- the functional derivatives 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  $\hat{u}$

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

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

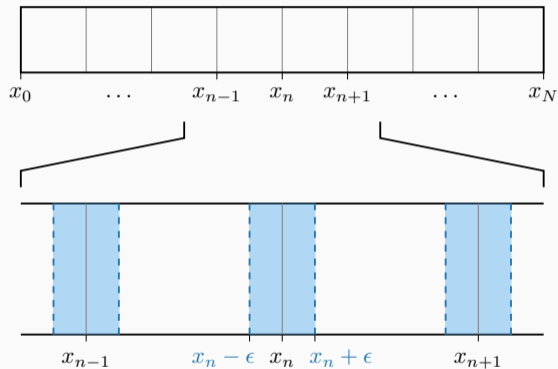
$$\{F, G\}_k = \sum_{i,l,m} c_{im}^l u_l \frac{\partial F}{\partial u_i} \frac{\partial G}{\partial u_m},$$

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

- Jacobi identity

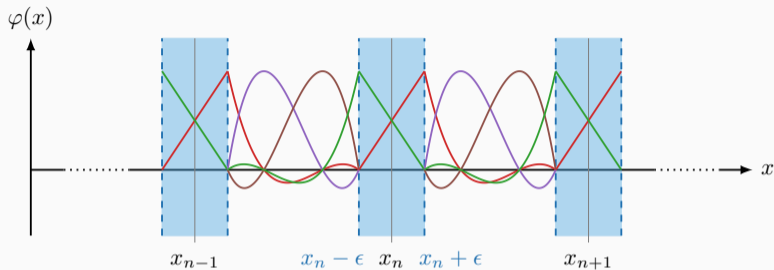
$$J_{klm}^i = \sum_j [c_{kj}^i c_{lm}^j + c_{mj}^i c_{kl}^j + c_{lj}^i c_{mk}^j] = 0 \quad \forall i, k, l, m$$

# 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

$$\{\cdot, \cdot\}_d = \{\cdot, \cdot\}_o + \{\cdot, \cdot\}_b$$

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

## Some Words on Skew-symmetric and Split Forms

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# 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

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

- 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

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

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

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

$$\begin{aligned} u_t(x) = \{u, \mathcal{H}\} &= - \int_{\Omega} u(x') \left( \delta(x-x') \frac{\partial}{\partial x'} u(x') - u(x') \frac{\partial}{\partial x'} \delta(x-x') \right) dx' \\ &= - \int_{\Omega} \left( u(x') \frac{\partial}{\partial x'} u(x') + \frac{\partial}{\partial x'} u(x')^2 \right) \delta(x-x') dx' + \int_{\partial\Omega} u(x')^2 \delta(x-x') dx' \end{aligned}$$

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

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



## Some Words on Dissipation

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# 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

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

## Summary and Outlook

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## 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 and 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