Metriplectic Integrators for Dissipative Fluids

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Metriplectic Structures in Fluids and Plasmas

- many systems in fluid dynamics and plasma physics possess a metriplectic structure: their equations can be written in an abstract and general form as

$$\frac{d}{dt}\mathcal{F} = \{\mathcal{F}, \mathcal{G}\} + (\mathcal{F}, \mathcal{G}), \qquad \mathcal{G} = \mathcal{H} - \mathcal{S},$$

  consisting of a Hamiltonian anti-symmetric part $\{\cdot, \cdot\}$ and an entropy-dissipating symmetric part $(\cdot, \cdot)$

  $\mathcal{F}$ any functional of the dynamical variables
  $\mathcal{G}$ generalised free energy
  $\mathcal{H}$ total energy
  $\mathcal{S}$ entropy

- this structure implies compatibility with the laws of thermodynamics
  - conservation of energy
  - monotonic dissipation of entropy
  - existence of a unique equilibrium state
- discretisation of the brackets instead of the dynamical equation guarantees these properties at the discrete level independently of the numerical method (FEM, DG, PIC)

Outline

I. Metriplectic Dynamics

II. Dissipative Fluids

III. Metriplectic Integrators

IV. Summary and Outlook

Metriplectic Dynamics

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 $\mathcal{D}$ with coordinates x and $\mathcal{F}$ an arbitrary functional of the field variables u
- if the system is Hamiltonian the evolution of any functional $\mathcal{F}$ of u is given by

$$\frac{d\mathcal{F}}{dt} = \{\mathcal{F}, \mathcal{H}\}$$

- $\mathcal{H}$ 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

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

$$\frac{d\mathcal{F}}{dt} = \{\mathcal{F}, \mathcal{H}\}$$

- 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

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

- functionals $\mathcal{C}$ for which $\{\mathcal{F}, \mathcal{C}\} = 0$ for all functionals $\mathcal{F}$ are called Casimir invariants

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

Metriplectic Dynamics

- metriplectic dynamics describes systems that have a Hamiltonian anti-symmetric part $\{\cdot,\cdot\}$ and an entropy-dissipating symmetric part $(\cdot,\cdot)$

- the evolution of any functional $\mathcal{F}$ of the field variables u is given by

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

- the metric bracket $(\cdot,\cdot)$ is a bilinear, symmetric, positive-semidefinite operation, satisfying the Leibniz' rule

- $\mathcal{G} = \mathcal{H} - \mathcal{S}$ a generalised free energy functional with Hamiltonian $\mathcal{H}$ and entropy $\mathcal{S}$

- $\mathcal{S}$ is a Casimir invariant of the Poisson bracket and $\mathcal{H}$ is a Casimir invariant of the metric bracket

$$\{\mathcal{F},\mathcal{S}\} = 0 \qquad \text{and} \qquad (\mathcal{F},\mathcal{H}) = 0 \qquad \text{for all functionals } \mathcal{F}$$

Metriplectic Dynamics

- metriplectic dynamics reproduces the First and Second Law of Thermodynamics

$$\frac{\mathrm{d}\mathcal{H}}{\mathrm{d}t} = \{\mathcal{H}, \mathcal{G}\} + (\mathcal{H}, \mathcal{G}) = -\{\mathcal{H}, \mathcal{S}\} = 0 \qquad \text{(Conservation of Energy)}$$

$$\frac{\mathrm{d}\mathcal{S}}{\mathrm{d}t} = \{\mathcal{S}, \mathcal{G}\} + (\mathcal{S}, \mathcal{G}) = -(\mathcal{S}, \mathcal{S}) \leq 0 \qquad \text{(Monotonic Dissipation of Entropy)}$$

- the equilibrium state is reached when the evolution of any functional stalls and entropy is at minimum
- the equilibrium state u_{eq} satisfies an energy principle, according to which the first variation of the free energy vanishes, $\delta\mathcal{G}[u_{eq}] = 0$, and its second variation is strictly positive, $\delta^2\mathcal{G}[u_{eq}] > 0$
- if further Casimir invariants $\mathcal{C}_i$ exist, the equilibrium state becomes degenerate, and the energy principle must be modified to an energy--Casimir principle that accounts for these Casimirs

$$\delta\mathcal{G}[u_{eq}] + \sum_i \lambda_i \delta\mathcal{C}_i[u_{eq}] = 0$$

- λ_i act as Lagrange multipliers that are determined uniquely from the values of the Casimirs at u_0

Dissipative Fluids

Viscous Heat-conductive Flows

- state variables: mass density ρ, momentum density m, and entropy density σ
- Poisson bracket

$$\{\mathcal{A},\mathcal{B}\} = \int_{\mathcal{D}} m(x,t)\cdot\left[\frac{\delta\mathcal{B}}{\delta m}\cdot\nabla\frac{\delta\mathcal{A}}{\delta m} - \frac{\delta\mathcal{A}}{\delta m}\cdot\nabla\frac{\delta\mathcal{B}}{\delta m}\right] + \int_{\mathcal{D}} \rho(x,t)\left[\frac{\delta\mathcal{B}}{\delta m}\cdot\nabla\frac{\delta\mathcal{A}}{\delta\rho} - \frac{\delta\mathcal{A}}{\delta m}\cdot\nabla\frac{\delta\mathcal{B}}{\delta\rho}\right] + \int_{\mathcal{D}} \sigma(x,t)\left[\frac{\delta\mathcal{B}}{\delta m}\cdot\nabla\frac{\delta\mathcal{A}}{\delta\sigma} - \frac{\delta\mathcal{A}}{\delta m}\cdot\nabla\frac{\delta\mathcal{B}}{\delta\sigma}\right]$$

- Hamiltonian functional

$$\mathcal{H} = \int_{\mathcal{D}}\left[\frac{1}{\rho}\frac{|m|^2}{2} + \rho\, U(\rho,\sigma/\rho)\right]\mathrm{d}x$$

- the ideal dynamics preserves the total mass $\mathcal{M}$, momentum $\mathcal{P}$ and entropy $\mathcal{S}$

$$\mathcal{M} = \int_{\mathcal{D}} \rho(x,t)\,\mathrm{d}x, \qquad \mathcal{P} = \int_{\mathcal{D}} m(x,t)\,\mathrm{d}x, \qquad \mathcal{S} = \int_{\mathcal{D}} \sigma(x,t)\,\mathrm{d}x$$

Viscous Heat-conductive Flows

- dissipation due to viscous friction and heat conduction is modelled by the metric bracket

$$
\begin{aligned}
(\mathcal{A}, \mathcal{B}) = & \int_{\mathcal{D}} 2\mu \left[T \left\langle \nabla \frac{\delta \mathcal{A}}{\delta m} \right\rangle - \frac{\delta \mathcal{A}}{\delta \sigma} \left\langle \nabla v \right\rangle \right] : \left[T \left\langle \nabla \frac{\delta \mathcal{B}}{\delta m} \right\rangle - \frac{\delta \mathcal{B}}{\delta \sigma} \left\langle \nabla v \right\rangle \right] \mathrm{d}x \\
& + \int_{\mathcal{D}} \lambda \left[T \nabla \cdot \frac{\delta \mathcal{A}}{\delta m} - \frac{\delta \mathcal{A}}{\delta \sigma} \nabla \cdot v \right] \cdot \left[T \nabla \cdot \frac{\delta \mathcal{B}}{\delta m} - \frac{\delta \mathcal{B}}{\delta \sigma} \nabla \cdot v \right] \mathrm{d}x \\
& + \int_{\mathcal{D}} \kappa \, T^2 \, \nabla \left[\frac{1}{T} \frac{\delta \mathcal{A}}{\delta \sigma} \right] \cdot \nabla \left[\frac{1}{T} \frac{\delta \mathcal{B}}{\delta \sigma} \right] \mathrm{d}x
\end{aligned}
$$

- here $v = m/\rho$ denotes the velocity, μ the coefficient of shear viscosity, λ the coefficient of bulk viscosity, κ the thermal conductivity, and $\langle \cdot \rangle$ denotes the projection

$$
\langle \nabla v \rangle = \frac{1}{2} (\nabla v + \nabla v^T) - \frac{1}{3} (\mathrm{trace} \, \nabla v) \mathbb{1}
$$

with $\mathbb{1}$ the 3×3 identity matrix

Viscous Heat-conductive Flows

- the equations of motion follow from the metriplectic bracket for $\mathcal{F} \in \{\rho, m, \sigma\}$

$$\begin{aligned}\frac{\partial \rho}{\partial t} &= \{\rho, \mathcal{G}\} + (\rho, \mathcal{G}) \\ &= -\nabla \cdot m,\end{aligned}$$

$$\begin{aligned}\frac{\partial m}{\partial t} &= \{m, \mathcal{G}\} + (m, \mathcal{G}) \\ &= -\nabla \cdot (m \otimes v) + \nabla \cdot \big[(\rho \nabla \cdot \xi - p)1 - \nabla \rho \otimes \xi + 2\mu \left\langle \nabla v \right\rangle + \lambda (\nabla \cdot v) 1\big],\end{aligned}$$

$$\begin{aligned}\frac{\partial \sigma}{\partial t} &= \{\sigma, \mathcal{G}\} + (\sigma, \mathcal{G}) \\ &= -\nabla \cdot \left[\sigma v - \frac{\kappa \nabla T}{T}\right] + \frac{1}{T}\left[2\mu \left\langle \nabla v \right\rangle \cdot \left\langle \nabla v \right\rangle + \lambda (\nabla \cdot v)^2 + \frac{\kappa}{T} \left| \nabla T \right|^2\right].\end{aligned}$$

- equations in terms of other variables are obtained via a coordinate transformation on the brackets
    - e.g. non-conservative coordinates: density ρ, velocity $v = m/\rho$ and entropy $s = \sigma/\rho$

Metriplectic Integrators

Metriplectic Integrators

- metriplectic integrators: discretise the metriplectic brackets to obtain structure-preserving integrators
- automatic preservation of important physical quantities, such as mass, energy and the laws of thermodynamics, independently of the particular discretisation framework
- spatial discretisation:
  (a) choose approximations of the function spaces of the dynamical variables
  (b) choose approximations of the inner products on these spaces
  (c) choose an approximation of functionals
  (d) choose a finite-dimensional representation of the functional derivative
- temporal discretisation: integral-preserving methods such as discrete gradients

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  $\rightarrow$ apart from these degrees of freedom, the whole construction is systematic and automatic

- temporal discretisation: integral-preserving methods such as discrete gradients

Metriplectic Integrators: Function Spaces

- let v and w be elements of $\mathbb{V} = L^2(\mathcal{D})$, the space of square integrable functions over $\mathcal{D}$ with scalar product

$$\langle v \, , \, w \rangle_{\mathcal{D}} = \int_{\mathcal{D}} v(x) \, w(x) \, \mathrm{d}x$$

- denote by $\mathbb{V}_h$ a finite dimensional subspace of $\mathbb{V}$ with basis $\{\varphi_i\}_{i=1}^N$, so that $v_h \in \mathbb{V}_h$ can be written as

$$v_h(t, x) = \sum_{i=1}^N v_i(t) \, \varphi_i(x)$$

- the discretisation of the density ρ, momentum density m and entropy density σ follows in full analogy with appropriately chosen function spaces $\mathbb{V}$

Metriplectic Integrators: Quadrature Rule

- in simple situations, we can retain the inner product $\langle \cdot \, , \, \cdot \rangle$ on $\mathbb{V}$ and work with the continuous functionals $\mathcal{F}$ evaluated on (ρ_h, m_h, σ_h)

- in many situations the resulting integrals cannot be computed easily and we need to construct approximations of the inner product $\langle \cdot \, , \, \cdot \rangle_h$ as well as functionals $\mathcal{F}_h$

→ choose some quadrature rule $\{(b_n, c_n)\}_{n=1}^{R}$ with nodes c_n and weights b_n

$$\langle v_h \, , \, w_h \rangle_h = \sum_{n=1}^{R} b_n v_h(c_n) \, w_h(c_n) = \hat{v}^T \mathbb{M} \hat{w}$$

- $\hat{v} = (v_1, v_2, ..., v_N)^T$ denotes the coefficient vector of v_h when expressed in the basis $\{\varphi_i\}_{i=1}^{N}$

- $\mathbb{M}$ denotes the mass matrix with components

$$\mathbb{M}_{ij} = \sum_{n=1}^{R} b_n \, \varphi_i(c_n) \, \varphi_j(c_n)$$

Metriplectic Integrators: Functionals

- in the same fashion, functionals of (ρ, m, σ) are approximated using the quadrature rule $\{(b_n, c_n)\}_{n=1}^{R}$

$$\mathcal{H}_h[\rho_h, m_h, \sigma_h] = \sum_{n=1}^{R} b_n \left[\frac{|m_h(c_n)|^2}{2\rho_h(c_n)} + \rho_h(c_n)\, U\big(\rho_h(c_n),\, \sigma_h(c_n)/\rho_h(c_n)\big) \right] \equiv \mathsf{H}(\hat{\rho}, \hat{m}, \hat{\sigma}),$$

$$\mathcal{M}_h[\rho_h] = \sum_{n=1}^{R} b_n\, \rho_h(c_n) = 1_N^T \mathbb{M}^\rho \hat{\rho} \equiv \mathsf{M}(\hat{\rho}),$$

$$\mathcal{P}_h[\rho_h] = \sum_{n=1}^{R} b_n\, m_h(c_n) = 1_{3N}^T \mathbb{M}^m \hat{m} \equiv \mathsf{P}(\hat{m}),$$

$$\mathcal{S}_h[\sigma_h] = \sum_{n=1}^{R} b_n\, \sigma_h(c_n) = 1_N^T \mathbb{M}^\sigma \hat{\sigma} \equiv \mathsf{S}(\hat{\sigma}),$$

- $\hat{\rho} = (\rho_1, \rho_2, ..., \rho_N)$ are the coefficients of ρ_h, and analogously $\hat{m}$ and $\hat{\sigma}$ are the coefficients of m_h and σ_h
- $1_N \in \mathbb{R}^N$ and $1_{3N} \in \mathbb{R}^{3N}$ denote the respective vectors with all components being equal to 1
- $\mathbb{M}^a$ denotes the mass matrices for $a \in \{\rho, m, \sigma\}$ corresponding to the respective basis functions φ^a

Metriplectic Integrators: Functional Derivatives

- finally, we need to construct a discrete equivalent to the functional derivative
- set $\mathsf{A}(\hat{v}) = \mathcal{A}_h[v_h]$ and require that

$$\left\langle \frac{\delta \mathcal{A}}{\delta v} [v_h] \, , \, w_h \right\rangle_h = \left\langle \frac{\partial \mathsf{A}}{\partial \hat{v}} \, , \, \hat{w} \right\rangle_N$$

- $\langle \cdot \, , \, \cdot \rangle_N$ denotes the inner product in $\mathbb{R}^N$, i.e., the scalar product
- the functional derivative $\delta \mathcal{A} / \delta v$ is an element of the dual space $\mathbb{V}^*$ of $\mathbb{V}$
- restricting $\mathcal{A}$ to elements v_h of $\mathbb{V}_h$, we can express $\delta \mathcal{A} / \delta v[v_h]$ in the basis $\{\psi_i\}_{i=1}^N$ of $\mathbb{V}_h^*$ as

$$\frac{\delta \mathcal{A}}{\delta v} [v_h] = \sum_{i=1}^{N} a_i \, \psi_i(x)$$

- by the Riesz representation theorem we can express the basis functions ψ_i in terms of the basis $\{\varphi_i\}_{i=1}^N$, and using the duality between the bases, i.e., $\langle \psi_i \, , \, \varphi_j \rangle = \delta_{ij}$, we find that

$$\frac{\delta \mathcal{A}}{\delta v} [v_h] = \sum_{i,j=1}^{N} \frac{\partial \mathsf{A}}{\partial v_i} \, \mathbb{M}_{ij}^{-1} \, \varphi_j(x)$$

Metriplectic Integrators: Discrete Brackets

- a semi-discrete metriplectic system is obtained by replacing the functional derivatives and integrals in the continuous brackets with the discrete derivatives and the quadrature rule $\{(b_n, c_n)\}_{n=1}^{R}$, e.g.,

$$\{\mathsf{A},\mathsf{B}\}_h = \sum_{i,j,k}^{3N} \mathbb{P}^{mm}_{ijk}\, m_k \left[\frac{\partial \mathsf{B}}{\partial m_i} \frac{\partial \mathsf{A}}{\partial m_j} - \frac{\partial \mathsf{A}}{\partial m_i} \frac{\partial \mathsf{B}}{\partial m_j} \right] + \sum_{i}^{3N} \sum_{j,k=1}^{N} \mathbb{P}^{m\rho}_{ijk}\, \rho_k \left[\frac{\partial \mathsf{B}}{\partial m_i} \frac{\partial \mathsf{A}}{\partial \rho_j} - \frac{\partial \mathsf{A}}{\partial m_i} \frac{\partial \mathsf{B}}{\partial \rho_j} \right] + \sum_{i}^{3N} \sum_{j,k=1}^{N} \mathbb{P}^{m\sigma}_{ijk}\, \sigma_k \left[\frac{\partial \mathsf{B}}{\partial m_i} \frac{\partial \mathsf{A}}{\partial \sigma_j} - \frac{\partial \mathsf{A}}{\partial m_i} \frac{\partial \mathsf{B}}{\partial \sigma_j} \right]$$

$$\mathsf{A}(\hat\rho, \hat m, \hat\sigma) = \mathcal{A}[\rho_h, m_h, \sigma_h], \qquad \mathsf{B}(\hat\rho, \hat m, \hat\sigma) = \mathcal{B}[\rho_h, m_h, \sigma_h],$$

$$\mathbb{P}^{mm}_{ijk} = \sum_{p,q=1}^{3N} \mathbb{L}^{mm}_{pqk} \left(\mathbb{M}^{m}\right)^{-1}_{ip} \left(\mathbb{M}^{m}\right)^{-1}_{qj}, \qquad \mathbb{L}^{mm}_{ijk} = \sum_{n=1}^{R} b_n\, \varphi^m_k(c_n)\, \varphi^m_i(c_n) \cdot \nabla \varphi^m_j(c_n),$$

$$\mathbb{P}^{m\rho}_{ijk} = \sum_{p=1}^{3N} \sum_{q=1}^{N} \mathbb{L}^{m\rho}_{pqk} \left(\mathbb{M}^{m}\right)^{-1}_{ip} \left(\mathbb{M}^{\rho}\right)^{-1}_{qj}, \qquad \mathbb{L}^{m\rho}_{ijk} = \sum_{n=1}^{R} b_n\, \varphi^\rho_k(c_n)\, \varphi^m_i(c_n) \cdot \nabla \varphi^\rho_j(c_n),$$

$$\mathbb{P}^{m\sigma}_{ijk} = \sum_{p=1}^{3N} \sum_{q=1}^{N} \mathbb{L}^{m\sigma}_{pqk} \left(\mathbb{M}^{m}\right)^{-1}_{ip} \left(\mathbb{M}^{\sigma}\right)^{-1}_{qj}, \qquad \mathbb{L}^{m\sigma}_{ijk} = \sum_{n=1}^{R} b_n\, \varphi^\sigma_k(c_n)\, \varphi^m_i(c_n) \cdot \nabla \varphi^\sigma_j(c_n).$$

Metriplectic Integrators: Conservation Properties

- the discrete Poisson bracket is anti-symmetric, but does not satisfy the Jacobi identity
- energy conservation, $\mathsf{H}(\hat{\rho}, \hat{m}, \hat{\sigma})$, follows from anti-symmetry so that $\{\mathsf{H}, \mathsf{H}\}_h = 0$
- conservation of mass $\mathsf{M}(\hat{\rho})$ and entropy $\mathsf{S}(\hat{\sigma})$ can be seen by inserting the respective expressions into the discrete bracket, e.g.,

$$\{\mathsf{M}, \mathsf{B}\}_h = \sum_{i,l}^{3N} \sum_{j,k=1}^{N} \mathbb{L}_{ijk}^{m\rho} \, \rho_k \, 1_j \, (\mathbb{M}^m)_{il}^{-1} \, \frac{\partial \mathsf{B}}{\partial m_l} = 0 \qquad \text{as} \qquad \sum_{j=1}^{N} \mathbb{L}_{ijk}^{m\rho} \, 1_j = 0$$

  (note that this holds for any B)
- conservation of momentum $\mathsf{P}(\hat{m})$ depends on the specific form of H and is not warranted for any discrete Hamiltonian, but only for specific choices of basis functions and quadrature rules

Metriplectic Integrators

- discretisation of the metric bracket and proof of its conservation properties follow along the same lines
- the semi-discrete equations of motion of the full system are obtained by

$$\frac{du}{dt} = \{u, \mathsf{G}\}_h + (u, \mathsf{G})_h \qquad \text{for} \qquad u \in \{\rho_1, ..., \rho_N,\ m_1, ..., m_{3N},\ \sigma_1, ..., \sigma_N\}$$

- $\mathsf{G} = \mathsf{H} - \mathsf{S}$ approximates the free energy $\mathcal{G}$
- fully discrete equations are obtained after a temporal discretisation with integral-preserving methods such as discrete gradients or continuous stage Runge--Kutta methods
- using the discrete gradient properties, exact conservation of mass and energy and monotonic decrease of entropy are straightforward to prove

Summary and Outlook

Summary and Outlook

- metriplectic dynamics provides a flexible framework for the construction of structure-preserving numerical algorithms for dissipative fluids and plasmas
  - preserve important invariants like mass, momentum and energy
  - preserve the laws of thermodynamics (H-theorem and unique equilibrium state)
- general framework: applicable to a large variety of systems of equations and numerical methods
  - geophysical fluid flows, magnetohydrodynamics, kinetic systems, hybrid models, ...
  - finite elements, discontinuous Galerkin, isogeometric analysis, spectral methods, ...
- in contrast to typical finite volume or discontinuous Galerkin methods, the conservation properties of the resulting schemes do not depend on the coordinate representation of the system
- not shown: temporal discretisation, discrete conservation laws, discrete H-theorem, implementation

Appendix: More on Metriplectic Systems

Metriplectic Systems: Energy Principle and Equilibrium State

- H-theorem: entropy decreases monotonically and there exists a unique equilibrium state u_{eq}

- for an equilibrium state u_{eq}, the time evolution of any functional $\mathcal{F}$ stalls, the free-energy functional $\mathcal{G}$ reaches its maximum, and the entropy functional $\mathcal{S}$ reaches its minimum

$$\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t}[u_{eq}] = 0, \qquad \frac{\mathrm{d}\mathcal{G}}{\mathrm{d}t}[u_{eq}] = 0, \qquad \frac{\mathrm{d}\mathcal{S}}{\mathrm{d}t}[u_{eq}] = 0, \qquad \mathcal{G}[u_{eq}] = \mathcal{G}_{\max}, \qquad \mathcal{S}[u_{eq}] = \mathcal{S}_{\min}$$

- the equilibrium state satisfies an energy principle
  - the first variation of the free energy vanishes

$$\delta\mathcal{G}[u_{eq}] = 0$$

  - the second variation of the free energy is strictly positive

$$\delta^2\mathcal{G}[u_{eq}] > 0$$

Metriplectic Systems: Energy--Casimir Principle and Equilibrium State

- if Casimir invariants $\mathcal{C}_i$ exist, the equilibrium state becomes degenerate, and the energy principle must be modified to account for the Casimirs (typically mass, momentum and energy)

- energy--Casimir principle: the equilibrium state satisfies

$$\delta\mathcal{G}[u_{eq}] + \sum_i \lambda_i \, \delta\mathcal{C}_i[u_{eq}] = 0,$$

  where λ_i act as Lagrange multipliers that are determined uniquely from the values of the Casimirs $\mathcal{C}_i[u_0]$ at the initial conditions u_0

- uniqueness: for each $z \in \Omega$ the equilibrium state of the free-energy functional $\mathcal{G}$ is unique

$$\delta^2 (\mathcal{G}[u_{eq}] + \sum_i \lambda_i \mathcal{C}_i[u_{eq}]) > 0$$

  (convexity argument: if Ω is a convex domain and $\mathcal{G}$ is strictly convex, then $\mathcal{G}$ has at most one critical point [Giaquinta and Hildebrandt, Calculus of Variations I, 2004])

Appendix: Phasespace Structure of Poisson 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 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

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

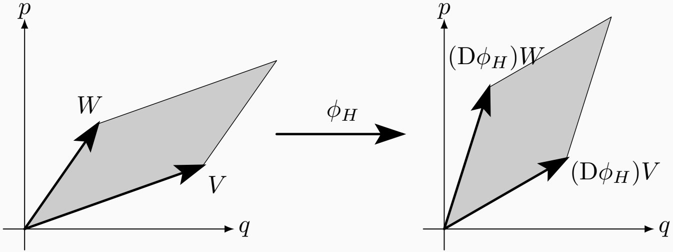
Poincaré Integral Invariants

- 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)

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

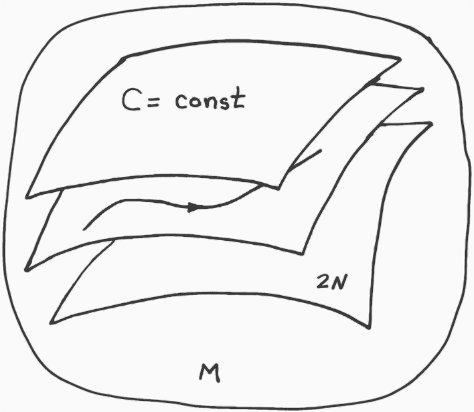


- analogously conservation of higher-order Poincaré invariants (in total 2N types of invariants: loop integrals of dimension $1, 3, 5, ..., 2N-1$ and surface integrals of dimension $2, 4, 6, ..., 2N$)

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

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

Appendix: Discrete Functional Derivatives

Discretisation of Functional Derivatives

- the functional derivative of a functional $\mathcal{F}[u]$ with respect to u is defined by

$$\frac{d}{d\epsilon}\mathcal{F}\big[u+\epsilon v\big]\Big|_{\epsilon=0} = \left\langle \frac{\delta \mathcal{F}}{\delta u} \, , \, v \right\rangle_{L^2} = \int_{\mathcal{D}} \frac{\delta u}{\delta u} \, v(z) \, \mathrm{d}x,$$

where v is an element of the same space as u, e.g., $u, v \in L^2(\mathcal{D})$, while the functional derivative $\delta \mathcal{F} / \delta u$ is an element of the dual space and $\langle \cdot \, , \, \cdot \rangle$ denotes the appropriate pairing

- require that the pairing be equal to some finite-dimensional equivalent

$$\left\langle \frac{\delta \mathcal{F}[u_h]}{\delta u} \, , \, v_h \right\rangle_{L^2} = \left\langle \frac{\partial F}{\partial \vec{u}} \, , \, \vec{v} \right\rangle_{\mathbb{R}^N} = \sum_{i=1}^{N} \frac{\partial F}{\partial u_i} \, v_i$$

where $\vec{v}(t) = \big(v_1(t), \dots, v_N(t)\big)^T \in \mathbb{R}^N$ denotes the degrees of freedom of v_h

$$v_h(t,x) = \sum_{i=1}^{N} v_i(t) \, \varphi_i(x)$$

Discretisation of Functional Derivatives

- denote the dual basis to $\varphi = (\varphi_1, \dots, \varphi_N)^T$ by $\psi = (\psi_1, \dots, \psi_N)^T$

$$\langle \psi_i \,,\, \varphi_j \rangle_{L^2} = \int_{\mathcal{D}} \psi_i(x)\, \varphi_j(x)\, \mathrm{d}x = \delta_{ij} \qquad \text{for} \qquad 1 \leq i, j \leq N$$

- in the dual basis, the functional derivative can be written as

$$\frac{\delta \mathcal{F}[u_h]}{\delta u} = \sum_{i=1}^{N} a_i\, \psi_i(x)$$

- choose $\vec{v} = (0,\, \dots,\, 0,\, 1,\, 0,\, \dots,\, 0)^\top$ with 1 at the i-th position and 0 else, s.th. $v_h = \varphi_i$ and

$$\left\langle \frac{\delta \mathcal{F}[u_h]}{\delta u} \,,\, v_h \right\rangle_{L^2} = \int_{\mathcal{D}} \sum_{j=1}^{N} a_j\, \psi_j(x)\, \varphi_i(x)\, \mathrm{d}x = \frac{\partial F}{\partial u_i} = \left\langle \frac{\partial F}{\partial \vec{u}} \,,\, \vec{v} \right\rangle_{\mathbb{R}^N}$$

- we thus find that

$$a_i = \frac{\partial F}{\partial u_i} \qquad \text{and therefore} \qquad \frac{\delta \mathcal{F}[u_h]}{\delta u} = \sum_{i=1}^{N} \frac{\partial F}{\partial u_i}\, \psi_i(x)$$

Discretisation of Functional Derivatives

- express the dual basis ψ in terms of the primal basis φ as

$$\psi_i(x) = \sum_{j=1}^{N} \mathsf{A}_{ij}\, \varphi_j(x) \qquad \text{so that} \qquad \frac{\delta \mathcal{F}[u_h]}{\delta u} = \sum_{i,j=1}^{N} \frac{\partial F}{\partial u_i}\, \mathsf{A}_{ij}\, \varphi_j(x)$$

- determine the unknown coefficients A_{ij} by the L_2 inner product

$$\langle \psi_i \,,\, \varphi_k \rangle_{L^2} = \int_{\mathcal{D}} \sum_{j=1}^{N} \mathsf{A}_{ij}\, \varphi_j(x)\, \varphi_k(x)\, \mathrm{d}x = \sum_{j=1}^{N} \mathbb{A}_{ij} \int_{\mathcal{D}} \varphi_j(x)\, \varphi_k(x)\, \mathrm{d}x$$

- denoting by $\mathbb{M}$ the mass matrix of the basis functions φ

$$\mathbb{M}_{jk} = \int_{\mathcal{D}} \varphi_j(x)\, \varphi_k(x)\, \mathrm{d}x,$$

and using $\langle \psi_i \,,\, \varphi_k \rangle_{L^2} = \delta_{ik}$, we obtain the relation

$$\mathbb{1} = \mathsf{A}\mathbb{M} \qquad \text{and thus} \qquad \mathsf{A} = \mathbb{M}^{-1} \qquad \text{so that} \qquad \frac{\delta \mathcal{F}[u_h]}{\delta u} = \sum_{i,j=1}^{N} \frac{\partial F}{\partial u_i}\, (\mathbb{M}^{-1})_{ij}\, \varphi_j(x)$$

Appendix: Time Integration

Integral Preserving Time Integration

- consider a system of ordinary differential equations in the form

$$\frac{du}{dt} = \mathsf{S}(u)\, \nabla I(u)$$

where $\mathsf{S}(u)$ can be an anti-symmetric matrix for conservative systems, a symmetric matrix for dissipative systems, or a combination thereof for metriplectic systems, and $I : \mathbb{R}^N \to \mathbb{R}$ is a differentiable function

- discrete gradients: discrete analogues of the gradient of a function

$$\frac{u_{n+1} - u_n}{\Delta t} = \bar{\mathsf{S}}(u_n, u_{n+1})\, \bar{\nabla} I(u_n, u_{n+1})$$

- example: average discrete gradient

$$\bar{\nabla} I(u_n, u_{n+1}) = \int_0^1 \nabla I\big((1-\xi) u_n + \xi u_{n+1}\big)\, d\xi$$

Integral Preserving Time Integration

- discrete gradients: discrete analogues of the gradient of a function

$$\frac{u_{n+1} - u_n}{\Delta t} = \bar{\mathsf{S}}(u_n, u_{n+1})\,\bar{\nabla} I(u_n, u_{n+1})$$

- $\bar{\mathsf{S}}(u_n, u_{n+1})$ is any symmetric, anti-symmetric or metriplectic matrix that approaches $\mathsf{S}(u)$ in the limit of $u_{n+1} \to u_n$ and $\Delta t \to 0$

- $\bar{\nabla} I(u_n, u_{n+1})$ is a discrete gradient, that is a vector valued continuous function of (u_n, u_{n+1}), satisfying

$$(u_{n+1} - u_n) \cdot \bar{\nabla} I(u_n, u_{n+1}) = I(u_{n+1}) - I(u_n), \qquad \bar{\nabla} I(u_n, u_n) = \nabla I(u_n)$$

- using discrete gradients for the temporal discretisation leads to algorithms that preserve mass, momentum and energy exactly and exhibit the correct monotonic behaviour of the entropy