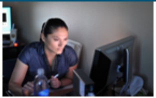
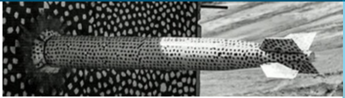
W24-09 Geometric Mechanics Formulations and Structure Preserving Discretizations: An Introductory Course





Presented by:

Chris Eldred (SNL), Artur Palha (TU Delft), Marc Gerritsma (TU Delft)

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July 22, 2024

Course Schedule

- **08:45 - 10:15** Introduction
- **10:15 - 10:30** Coffee Break
- **10:30 - 12:00** Geometric Mechanics Formulations
- **12:00 - 13:00** Lunch Break
- **13:00 - 14:30** Structure-Preserving Discretizations I
- **14:30 - 14:45** Coffee Break
- **14:45 - 16:15** Structure-Preserving Discretizations II
- **16:15 - 16:30** Break
- **16:30 - 17:00** Wrap Up

Session Outline

Introductions

Geometric Mechanics Formulations

Structure Preserving Discretizations

Spatial Discretizations

Time Discretizations

Summary

Introductions

Instructors

- Chris Eldred
  - Staff Scientist at Sandia National Laboratories since 2019
  - PhD in Atmospheric Science from Colorado State University in 2015
  - Postdocs in France from 2015-2019
  - Research Interests:
    - geometric mechanics formulations for continuum mechanics and kinetic models
    - structure-preserving spatial and temporal discretizations
    - high-productivity software frameworks
    - structure-preserving reduced-order modeling and neural networks
    - GM-aware uncertainty quantification
    - GM-aware optimal control and design

Instructors

- Artur Palha
  - Associate Professor at Delft Institute of Applied Mathematics, TU Delft
  - Senior researcher at Netherlands eScience Center
  - Researcher at ASML
  - Postdocs at TU Delft and TU Eindhoven
  - PhD in Aerospace Engineering, TU Delft
  - **Research Interests**:
    - Structure-preserving spatial and temporal discretizations
    - Spectral Finite Element Methods (including IGA)
    - Geometric mechanics formulations for continuum mechanics.
    - Finite Element software frameworks

Instructors

- Marc Gerritsma
  - Mathematics & Physics Groningen University, The Netherlands
  - Postdoc University of Wales, Aberystwyth
  - Aerospace Engineering, TU Delft, The Netherlands
  - **Research Interests**:
    - Spectral Element Methods
    - Structure-preserving discretizations
    - Differential Geometry
    - Variational Multiscale Methods

Students

- Introduce yourselves!
  - Brief History
  - Research Interests
  - What do you want to get out of this course?

Geometric Mechanics Formulations

Models of Physical Systems

How can we develop a model* for a physical system?

Force Balances (Newton's Laws ie. $F = ma$)?

- How do we determine F for general systems?
- How does this generalize to continuum mechanics and kinetic models?
- What about arbitrary manifolds and coordinate-free approaches?
- Where do conserved quantities and involution constraints enter into the picture?

Is there a "better" way?

*-model in the sense of a system of ODEs/PDEs/DAEs

Geometric Mechanics Formulations

- **variational/Lagrangian**: equations of motion for **x** come from a *variational principle* applied to an *action functional* $\mathbb{S}[\mathbf{x}]$, which is typically based on a *Lagrangian* $\mathscr{L}[\mathbf{x}]$

$$\delta\,\mathbb{S}[\mathbf{x}] = \delta \int_{t_1}^{t_2} \mathscr{L}[\mathbf{x}] = 0 \tag{1}$$

- **Hamiltonian**: equations of motion for **x** come from a *Poisson Bracket* $\{\mathbb{A}, \mathbb{B}\}$ and a **Hamiltonian** $\mathbb{H}[\mathbf{x}]$

$$\frac{\mathrm{d}\mathbb{F}}{\mathrm{d}t} = \{\mathbb{F}, \mathbb{H}\} \tag{2}$$

The two approaches can (usually) be connected through a *Legendre transform*, complications arise when $\mathscr{L}[\mathbf{x}]$ is *degenerate* or has *constraints*: requires *Dirac brackets* and *Morse families*

There are extensions of these approaches to incorporate *irreversible processes*, which conserve *energy* and generate *thermodynamic entropy*: ex. **metriplectic**, **single** and **double generator**, **GENERIC**

Variational Formulations

Variational/Lagrangian formulations consist generally of three pieces:

- *Lagrangian* $\mathscr{L}[\mathbf{x}]$: this is usually the kinetic energy minus the potential energy, although in many cases it has some additional terms
- *Action* $\mathbb{S}[\mathbf{x}]$: this is usually $\int_{t^1}^{t^2} \mathscr{L}$, although not always
- *Variational Principle*: given $\mathscr{L}[\mathbf{x}]$, the variational principle says how to form the action $\mathbb{S}[\mathbf{x}]$, and how to obtain the equations of motion from the action $\mathbb{S}[\mathbf{x}]$ (always involving taking variations of $\mathbb{S}[\mathbf{x}]$)
- Applicability of a given variational principle depends on factors such as the configuration space, coordinate system and presence/absence of constraints

examples of variational principles: *Hamilton's principle*, ***Euler-Poincaré***, ***Lie-Poisson***, *Clebsch*, *Hamilton-Pontryagin*,...

Hamiltonian Formulations I

Hamiltonian formulations consist of two pieces:

- *Hamiltonian* $\mathbb{H}[\mathbf{x}]$: this is usually the total energy, although in some cases it has some additional terms
- *Poisson bracket* $\{\mathbb{A},\mathbb{B}\}$: this is an operator $X^* \times X^* \to \mathbb{R}$, that is
  - *bilinear*: $\{\mathbb{A}+\mathbb{B},\mathbb{F}+\mathbb{G}\} = \{\mathbb{A},\mathbb{F}\}+\{\mathbb{A},\mathbb{G}\}+\{\mathbb{B},\mathbb{F}\}+\{\mathbb{B},\mathbb{G}\}$
  - *anti-symmetric*: $\{\mathbb{A},\mathbb{B}\} = -\{\mathbb{B},\mathbb{A}\}$

  and satisfies
  - *Leibniz rule*: $\{\mathbb{A},\mathbb{B}\mathbb{F}\} = \mathbb{B}\{\mathbb{A},\mathbb{F}\}+\{\mathbb{A},\mathbb{B}\}\mathbb{F}$
  - *Jacobi identity*: $\{\mathbb{A},\{\mathbb{B},\mathbb{F}\}\}+\{\mathbb{F},\{\mathbb{A},\mathbb{B}\}\}+\{\mathbb{B},\{\mathbb{F},\mathbb{A}\}\} = 0$

Time evolution of an arbitrary functional $\mathbb{F}[\mathbf{x}]$ is

$$\frac{d\mathbb{F}}{dt} = \{\mathbb{F},\mathbb{H}\} \tag{3}$$

examples of Hamiltonian formulations: *canonical*, ***Lie-Poisson***, ***Curl-Form***, ...

Hamiltonian Formulations II

- For continuum mechanics in Eulerian coordinates, $\{\mathbb{A},\mathbb{B}\}$ is (almost always) *non-canonical*: there exist a set of functionals, termed *Casimirs*, such that

$$\{\mathbb{A},\mathbb{C}\} = 0 \qquad \forall \mathscr{A} \tag{4}$$

Can identify a symplectic operator $\mathbb{J}(\mathbf{x})$ through

$$\{\mathbb{A},\mathbb{B}\} = \left\langle \frac{\delta \mathbb{A}}{\delta \mathbf{x}}, \mathbb{J}(\mathbf{x}) \frac{\delta \mathbb{B}}{\delta \mathbf{x}} \right\rangle \tag{5}$$

Usually requires integration by parts: works in domains without boundaries or with material boundary conditions ($\mathbf{u}\cdot\hat{\mathbf{n}} = 0$), complicated when general boundary conditions are used

Why use geometric mechanics?

- Deep connections with fundamental features of physical systems
  - conservation laws = symmetries: mass, momentum, energy, potential vorticity, potential enstrophy, etc.
  - involution constraints: non-divergent magnetic field, etc.
- Generalizable: the same framework works for a wide range of physical systems, reveals commonalities
- Closely connected with structure-preserving discretizations
- The "modern" language for physics!
  - GM formulations are how models in quantum field theory, condensed matter and general relativity are developed

Where can GM formulations be used?

- Classical particle mechanics
- Fluid mechanics
- Solid mechanics
- General relativity
- Quantum mechanics and quantum field theory
- Can handle both reversible (thermodynamic entropy conserving) and irreversible (thermodynamic entropy generating) dynamics

We will focus on fluids here, specifically the *shallow water equations*

Making things more concrete: 1D Wave Equation

Consider a Hamiltonian formulation of the linear wave equation in 1st order form, ex. linearized shallow water with fluid height h and velocity $\mathbf{u}$:

Hamiltonian and Functional Derivatives

$$\mathbb{H}[\mathbf{u}, h] = \int_\Omega H\frac{\mathbf{u}\cdot\mathbf{u}}{2} + g\frac{h^2}{2}$$

$$\frac{\delta\mathbb{H}}{\delta\mathbf{u}} = H\mathbf{u} \qquad \frac{\delta\mathbb{H}}{\delta h} = gh$$

Equations of Motion

$$\begin{aligned} \frac{\partial h}{\partial t} + \nabla\cdot\frac{\delta\mathbb{H}}{\delta\mathbf{u}} &= 0 \\ \frac{\partial\mathbf{u}}{\partial t} + \nabla\frac{\delta\mathbb{H}}{\delta h} &= 0 \end{aligned}$$

Where can I learn more (very incomplete lists)?

Books

- Classical Mechanics (Goldstein, Poole, Safko)
- Geometric Mechanics - Part I: Dynamics And Symmetry (Darryl Holm)
- Geometric Mechanics - Part II: Rotating, Translating And Rolling (Darryl Holm)
- Introduction to Mechanics and Symmetry (Marsden and Ratiu)
- Multiscale Thermo-Dynamics: Introduction to GENERIC (Pavelka, Klika, Grmela)
- Thermodynamics of Flowing Systems: with Internal Microstructure (Beris, Edwards)
- Beyond Equilibrium Thermodynamics (Öttinger)

Papers

- Morrison et. al. *Inclusive curvaturelike framework for describing dissipation: Metriplectic 4-bracket dynamics*, Physical Review E
- Gay-Balmaz et. al. *A Lagrangian variational formulation for nonequilibrium thermodynamics. Part I: Discrete systems*, Journal of Geometry and Physics
- Gay-Balmaz et. al. *A Lagrangian variational formulation for nonequilibrium thermodynamics. Part II: Continuum systems*, Journal of Geometry and Physics

Structure Preserving Discretizations

What is a structure-preserving discretization?

A numerical method that preserves some structure of the equations! Tautological definition...

What sort of structures do PDEs/ODEs have?

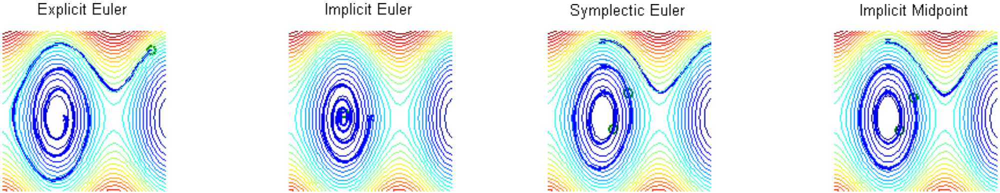
- Geometric mechanics structure!
  - Variational
  - (quasi)-Hamiltonian (unfortunately sometimes known as Poisson structure)
  - (quasi)-Metriplectic
- Exterior calculus structure
  - Calculus of differential forms
  - Hodge-deRham properties

Here we will focus on *exterior calculus structure* in space and *(quasi-)Hamiltonian/metriplectic* in time

An important class of integrators we do not discuss further is *variational integrators*

Why use structure-preserving discretizations?

Numerical methods that don't preserve structure often give misleading answers: ex. pendulum (Hamiltonian ODEs)



- Many other examples in literature: darcy flow, barotropic vorticity equations, electrostatics eigenvalue problems

Spatial Discretizations

Spatial SP Discretization

- structure-preserving (ie. mimetic) = discrete analogues of key (exterior) calculus identities such as:
  - Annihilation/Exact Sequence: $\mathrm{d}\,\mathrm{d} = 0$
    - ex. $\nabla \cdot \nabla \times = 0$, $\nabla \times \nabla = 0$
  - Integration by Parts: $\langle \alpha, \mathrm{d}\,\beta \rangle - \langle \delta\,\alpha, \beta \rangle = \langle \alpha, \beta \rangle_{d\Omega}$
    - ex. $\int_\Omega a \nabla \cdot \mathbf{b} + \int_\Omega \nabla a \cdot \mathbf{b} = \int_{\partial\Omega} a\mathbf{b} \cdot \hat{\mathbf{n}}$
  - Hodge decomposition/deRham cohomology: $\alpha = \mathrm{d}\,\psi + \delta\,\phi + h$, with $\mathrm{d}\,h = \delta\,h = 0$
    - ex. $\mathbf{a} = \nabla\psi + \nabla \times \phi + \mathbf{h}$ with $\nabla \cdot \mathbf{h} = \nabla \times \mathbf{h} = 0$
    - Spaces ψ, ϕ and h have the correct dimension (depending on topology of manifold)

What are the types of structure-preserving discretizations?

Single deRham complex discretizations

$$\mathbb{W}^0 \subset H^1 \underset{\nabla\cdot}{\overset{\nabla}{\rightleftarrows}} \mathbb{W}^1 \subset H(curl) \underset{\nabla\times}{\overset{\nabla\times}{\rightleftarrows}} \mathbb{W}^2 \subset H(div) \underset{\nabla}{\overset{\nabla\cdot}{\rightleftarrows}} \mathbb{W}^3 \subset L_2$$

- Discretization of standard exterior calculus = calculus of differential forms ($\mathbb{W}^k = \Lambda^k_h \subset \Lambda^k$, $\nabla, \nabla\cdot, \nabla\times = \mathrm{d}, \delta$)
- Fundamental object is inner product $\langle\rangle$ and associated integration by parts $\langle\alpha, \mathrm{d}\,\beta\rangle - \langle\delta\,\alpha, \beta\rangle = \langle\alpha, \beta\rangle_{d\Omega}$ ex. $\int_\Omega a\nabla\cdot\mathbf{b} + \int_\Omega \nabla a\cdot\mathbf{b} = \int_{\partial\Omega} a\mathbf{b}\cdot\hat{\mathbf{n}}$
- Main example is **compatible Galerkin methods**: finite element exterior calculus (FEEC), mimetic Galerkin differences (MGD), compatible isogeometric methods, spectral exterior calculus; another is mimetic finite differences (MFD); also meshfree and POU deRham complex methods

Double deRham complex discretizations

$$\begin{tikzcd}
\mathbb{W}^0 \arrow[r, "\nabla"] \arrow[d, shift left, "\star"] & \mathbb{W}^1 \arrow[r, "\nabla\times"] \arrow[d, shift left, "\star"] & \mathbb{W}^2 \arrow[r, "\nabla\cdot"] \arrow[d, shift left, "\star"] & \mathbb{W}^3 \arrow[d, shift left, "\star"] \\
\tilde{\mathbb{W}}^3 \arrow[u, shift left, "\star"] & \tilde{\mathbb{W}}^2 \arrow[l, "\nabla\cdot"] \arrow[u, shift left, "\star"] & \tilde{\mathbb{W}}^1 \arrow[l, "\nabla\times"] \arrow[u, shift left, "\star"] & \tilde{\mathbb{W}}^0 \arrow[l, "\nabla"] \arrow[u, shift left, "\star"]
\end{tikzcd}$$

- Discretization of split exterior calculus = calculus of oriented differential forms
- Fundamental object is the Hodge star $\star$, which induces the inner product $\langle\rangle$ and $\delta = (-1)^{nk+n+1} \star d \star$
- Main examples are **discrete exterior calculus** (staggered (Arakawa C) grid, Marker-And-Cell scheme, etc.), **split compatible Galerkin methods** (not well developed, only a few examples all with limitations- harmonic extension, spectral exterior calculus, algebraic dual polynomials)

Making things more concrete

Discretize linear wave equation using mixed finite elements (FEEC, single deRham complex approach), with $h \in \Lambda_h^n = L_2$, $\mathbf{u} \in \Lambda_h^{n-1} = H(div)$

$$\left\langle \hat{h}, \frac{\partial h}{\partial t} \right\rangle + \left\langle \hat{h}, \nabla \cdot \frac{\delta \mathbb{H}}{\delta \mathbf{u}} \right\rangle = 0 \quad (6)$$

$$\left\langle \hat{\mathbf{u}}, \frac{\partial \mathbf{u}}{\partial t} \right\rangle - \left\langle \nabla \cdot \hat{\mathbf{u}}, \frac{\delta \mathbb{H}}{\delta h} \right\rangle = 0 \quad (7)$$

$$\left\langle \hat{h}, \frac{\delta \mathbb{H}}{\delta h} \right\rangle = \left\langle \hat{h}, gh \right\rangle \quad (8)$$

$$\left\langle \hat{\mathbf{u}}, \frac{\delta \mathbb{H}}{\delta \mathbf{u}} \right\rangle = \langle \hat{\mathbf{u}}, H\mathbf{u} \rangle \quad (9)$$

Gives a set of Hamiltonian ODEs! Usually we get quasi-Hamiltonian ODEs (no Jacobi identity), but this is a special case.

Where do I learn more (very incomplete lists)?

Books

- Finite Element Exterior Calculus (Arnold)

Papers

- Tonti. *Why starting from differential equations for computational physics?*, Journal of Computational Physics
- Perot et. al. *Differential forms for scientists and engineers*, Journal of Computational Physics
- Bochev and Hyman, *Principles of Mimetic Discretizations of Differential Operators*, Compatible Spatial Discretizations
- Kreeft et. al. *Mimetic framework on curvilinear quadrilaterals of arbitrary order*, arxiv
- Buffa et. al. *Isogeometric Discrete Differential Forms in Three Dimensions*. SIAM JNA
- Palha et. al. *Physics-compatible discretization techniques on single and dual grids, with application to the Poisson equation of volume forms*, Journal of Computational Physics
- Hiemstra et. al. *High order geometric methods with exact conservation properties*, Journal of Computational Physics

Time Discretizations

Geometric Integrators

Geometric integrators preserve the *geometric features* of ODEs: symplecticity, Casimirs, etc.

- Symplectic integrators: applicable to canonical Hamiltonian systems, generate a *symplectic flow*, conserve a *shadow Hamiltonian*
  - Well developed and generally applicable to arbitrary canonical systems
- (Lie)-Poisson integrators: applicable to noncanonical Hamiltonian systems (Lie-Poisson), generate a *Poisson flow*, conserve a *shadow Hamiltonian*
  - Well developed but specific to a particular type of LP system
- Metriplectic integrators: combine a symplectic or Poisson integrator with a metric/gradient flow integrator
  - Almost no examples

All of these are specific to Hamiltonian or Metriplectic ODEs

Energy-Conserving Integrators

Energy-Conserving integrators preserve *1st integrals* of ODEs, and usually some subset of *Casimirs*

- Applicable to quasi-Hamiltonian or quasi-metriplectic ODEs: lack the Jacobi identity
  - important because often spatial discretizations of Hamiltonian (metripletic) PDEs yields quasi-Hamiltonian (metriplectic) ODEs
- All known examples (to me) are *discrete gradient methods*

$$\frac{\widetilde{\delta \mathscr{A}_h}}{\delta \mathbf{x}}(\mathbf{x}^{n+1} - \mathbf{x}^n) = \mathscr{A}_h^{n+1} - \mathscr{A}_h^n \tag{10}$$

  - Many exist in the literature: average vector field, Itoh, Gonzalez
- Unfortunately, energy-conserving integration are often referred to as *Poisson* integrators, not to be confused with *geometric* Poisson integrators

Making things more concrete

Implicit midpoint method

$$\left\langle \hat{h}, \frac{h^{n+1} - h^n}{\Delta t} \right\rangle + \left\langle \hat{h}, \nabla \cdot \frac{\delta \mathbb{H}}{\delta \mathbf{u}} \right\rangle = 0 \quad (11)$$

$$\left\langle \hat{\mathbf{u}}, \frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} \right\rangle - \left\langle \nabla \cdot \hat{\mathbf{u}}, \frac{\delta \mathbb{H}}{\delta h} \right\rangle = 0 \quad (12)$$

$$\left\langle \hat{h}, \frac{\delta \mathbb{H}}{\delta h} \right\rangle = \left\langle \hat{h}, g\frac{h^{n+1} + h^n}{2} \right\rangle \quad (13)$$

$$\left\langle \hat{\mathbf{u}}, \frac{\delta \mathbb{H}}{\delta \mathbf{u}} \right\rangle = \left\langle \hat{\mathbf{u}}, H\frac{\mathbf{u}^{n+1} + \mathbf{u}^n}{2} \right\rangle \quad (14)$$

- 2nd order AVF energy-conserving integrator: conserves total energy
- Symplectic integrator: conserves symplecticity

This is a very special case since ODEs in this case are Hamiltonian with quadratic Hamiltonian, energy-conserving != symplectic in general

Where do I learn more (very incomplete lists)?

Books

- Geometric Numerical Integration (Hairer, Wanner, Lubich)
- A Concise Introduction to Geometric Numerical Integration (Blanes, Casas)
- Line Integral Methods for Conservative Problems (Brugnano, Iavernaro)

Papers

- Brugnano et. al. *Energy-preserving methods for Poisson systems*, JCAM
- Amodio et. al. *Arbitrarily high-order energy-conserving methods for Poisson problems*, Numerical Algorithms

Heavily slanted towards methods for quasi-Hamiltonian systems (also sometimes know as Poisson)

Summary

Summary

A powerful framework for developing numerical models of physical systems is:
GM Formulation + SP Discretization

For example:
Hamiltonian PDEs + single deRham complex = quasi-Hamiltonian ODEs
quasi-Hamiltonian ODEs + EC integrator = quasi-Hamiltonian numerical model

The remainder of the class will consist of studying this process in detail for the **non-rotating shallow water equations without topography**

Many other approaches not discussed: variational integrators, symplectic/Lie-Poisson integrators, double deRham complex methods, etc.