Variational Numerical Methods in Geometric PDE

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Preserving conservation laws

- Many physical systems have conserved quantities.
 - energy, angular momentum, electric charge

Figure: Rigid body dynamics (International Space Station)

- There is no guarantee that these conservation laws will continue to hold when we numerically simulate the system.
 - energy gain or loss (numerical dissipation)
- Goal: create numerical methods that preserve conservation laws.

Figure: A simple harmonic oscillator. Video credit: Wikipedia

Equations of Motion

$$\ddot{x} = -x.$$

Conservation of energy

 $\frac{1}{2}(\dot{x}^2+x^2)$ is conserved.

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- Consider curves $q: [0, T] \to \mathbb{R}^3$ with $q(0) = q_0$ and $q(T) = q_T$.
- The critical point q of \mathfrak{S} is a solution to $\ddot{q} = 0$.

Variational formulations

Example

Geodesics in (M,g) are critical points $q \colon [0,T] \to M$ of

$$\mathfrak{S}(q) = \int_0^T \tfrac{1}{2} \left\| \dot{q} \right\|_g^2 \, dt$$

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Harmonic oscillator trajectories $\ddot{x} = -x$ are critical points $x : [0, T] \to \mathbb{R}$ of

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- See Marsden and West, Discrete Mechanics and Variational Integrators, 2001.

Variational formulations for PDEs: Poisson's equation

Standard PDE formulation

Given $f: \Omega \to \mathbb{R}$, seek a solution v to

 $\Delta v + f = 0 \text{ on } \Omega, \qquad v = 0 \text{ on } \partial \Omega.$

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$$E(\mathbf{v}) = \int_{\Omega} \left(\frac{1}{2} \| \nabla \mathbf{v} \|^2 - f \mathbf{v} \right), \qquad \mathbf{v} = 0 \text{ on } \partial \Omega.$$

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Weak formulation

Seek a v for which the equation holds for all w.

$$\int_{\Omega} \left(\langle \nabla v, \nabla w \rangle - fw \right) = 0, \qquad v = w = 0 \text{ on } \partial \Omega.$$

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- converts an infinite-dimensional variational problem to a finite-dimensional variational problem.
- approximates critical functions v with critical functions v_h coming from a finite-dimensional space.

The Galerkin method for Poisson's equation

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 - For example, $V = \{ v \in L^2(\Omega) \mid \nabla v \in L^2(\Omega), v |_{\partial \Omega} = 0 \}.$

Seek a critical point $v \in V$ of E.

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- Choose a finite-dimensional subspace V_h of V.
 - The bigger V_h is, the better our approximation.



Figure: A triangulation of a square domain.

Constructing the finite-dimensional subspace $V_h \subset V$

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 - By refining the triangulation, we get a larger V_h and a better approximation.

The finite element method: degrees of freedom

How do we specify a piecewise linear function v_h ?

The finite element method: degrees of freedom

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Figure: Degrees of freedom (blue) of piecewise linear functions (left) and piecewise quadratic functions (right).

- Specifying a value at each degree of freedom
 - uniquely determines the function on each triangle, and
 - enforces continuity between adjacent triangles.

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Understanding the degrees of freedom of vector fields with tangential continuity

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 - - Yakov Berchenko-Kogan.

Duality in finite element exterior calculus, 2018. http://arxiv.org/abs/1807.01161.

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Duality in finite element exterior calculus and the Hodge star operator on the sphere. In preparation, 2019.

Yakov Berchenko-Kogan

Variational Numerical Methods in Geometric PDE

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An alternative: hybrid methods

Standard finite element method

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Interpretation of the hybrid method

• Each triangle is now an independent system.

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- See (Brezzi and Fortin, 1991).

(optional slide) Hybrid methods for Poisson's problem

Variational formulation

Instead of
$$E(v_h) = \int_{\Omega} \left(\frac{1}{2} \|\nabla v_h\|^2 - fv_h\right)$$
, we have
 $E_h(v_h, \hat{p}_h) = \sum_{K \in \mathcal{T}_h} \int_K \left(\frac{1}{2} \|\nabla v_h\|^2 - fv_h\right) - \sum_{K \in \mathcal{T}_h} \int_{\partial K} (\hat{p}_h \cdot n) v_h.$

Weak formulation

• For all
$$K \in \mathcal{T}_h, w_h \in V_h$$
,

$$\int_{\mathcal{K}} (\langle \nabla v_h, \nabla w_h \rangle - fw_h) - \int_{\partial K} (\hat{p}_h \cdot n) w_h = 0$$
• Weakly enforces $-\Delta v_h = f$ on K and $\hat{p}_h \cdot n = \nabla v_h \cdot n$ on ∂K .

• For all
$$\hat{q}_h \in \hat{P}_h$$
,

$$\sum_{K \in \mathcal{T}_h} \int_{\partial K} (\hat{q}_h \cdot n) v_h = 0 \text{ for all } \hat{q}_h \in \hat{P}_h.$$

• Weakly enforces continuity of v_h .

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Conservation of charge in numerical methods for Maxwell's equations

Yakov Berchenko-Kogan and Ari Stern.

Constraint-preserving hybrid finite element methods for Maxwell's equations.

In preparation, 2019.

Yakov Berchenko-Kogan and Ari Stern.

Constraint-preserving hybrid finite element methods for the Yang–Mills equations.

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Maxwell's equations

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Charge conservation

• div E is a conserved quantity.

$$\frac{d}{dt}(\operatorname{div} E) = \operatorname{div} \dot{E} = \operatorname{div} \operatorname{curl} B = 0.$$

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$$\frac{d}{dt}(\operatorname{div} E) = \operatorname{div} \dot{E} = \operatorname{div} \operatorname{curl} B = 0.$$

• div *E* represents the charge density, denoted *ρ*, so this conservation law is the conservation of charge.

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Maxwell's equations: examples



Figure: Stationary and dynamic solutions to Maxwell's equations. Image credit: Wikipedia. Video credit: Electrical Exclusive.

An equivalent formulation of Maxwell's equations

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Equivalence to
$$\dot{E} = \operatorname{curl} B$$
 and $\dot{B} = -\operatorname{curl} E$
Set

$$E := -\dot{A}, \qquad B := \operatorname{curl} A.$$

• The evolution equation $\dot{B} = -\operatorname{curl} E$ is automatically satisfied.

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Set

$$E := -\dot{A},$$
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- The evolution equation $\dot{B} = -\operatorname{curl} E$ is automatically satisfied.
- $\ddot{A} = -\operatorname{curl}\operatorname{curl} A$ implies $\dot{E} = \operatorname{curl} B$.

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 - Weak charge conservation.
- Hybrid method (BK, Stern, 2019).
 - Strong charge conservation.
 - Improved rate of convergence.

The Galerkin method for Maxwell's equations (Nédélec)

Weak formulation

 $\ddot{A} = -\operatorname{curl}\operatorname{curl} A$ is equivalent to

$$\int_{\Omega} \langle \ddot{\mathcal{A}}, \mathcal{A}'
angle = - \int_{\Omega} \langle \operatorname{curl} \mathcal{A}, \operatorname{curl} \mathcal{A}'
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for all vector fields A' whose tangential components vanish on $\partial \Omega$.

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• We only have charge conservation in a weighted average sense.

Joint work with Ari Stern.

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Theorem (BK, Stern)

Solutions to our hybrid formulation of Maxwell's equations satisfy

$$rac{d}{dt}$$
 div $\hat{E}_h = 0.$

That is, we have a strong charge conservation law for our numerical method.



Figure: Total charge using E_h (Nédélec, solid line) vs. \hat{E}_h (our method, dashed line), simulating on a cube domain.

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 - We want numerical methods to conserve charge as well.

Maxwell's equations

Yakov Berchenko-Kogan Variational Numerical Methods in Geometric PDE

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- See (Christiansen and Winther, 2006).

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Yakov Berchenko-Kogan.

The entropy of the Angenent torus is approximately 1.85122. Journal of Experimental Mathematics, accepted for publication, 2019. http://arxiv.org/abs/1808.08163.

Curve shortening flow



Figure: Curve shortening flow. Image credit: Treibergs. Video credit: Angenent.
Mean curvature flow

Figure: Mean curvature flow. Video credit: Kovács.

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 - Yes, a torus (Angenent, 1989).
 - Many others (Kapouleas, Kleene, Møller, 2011).

Rotationally symmetric self-shrinkers



Figure: Cross-sections of three self-shrinkers: the sphere (green), the cylinder (orange), and the Angenent torus (blue).

Theorem (Huisken, 1990)

A hypersurface $\Sigma \subset \mathbb{R}^{n+1}$ is a self-shrinker that becomes extinct at the origin after one unit of time if and only if it is a critical point of the weighted area functional called the *F*-functional.

$$F(\Sigma) = (4\pi)^{-n/2} \int_{\Sigma} e^{-|x|^2/4} \, dA$$
rea.

Entropy of self-shrinkers

The critical value of the *F*-functional, called the entropy of the self-shrinker, is helpful in understanding what kinds of singularities can occur.



Figure: Entropies of self-shrinking surfaces

Earlier work (Drugan and Nguyen, 2018): the entropy of the Angenent torus is less than 2.

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Yakov Berchenko-Kogan

Variational Numerical Methods in Geometric PDE

A rotationally symmetric surface $\Sigma \subset \mathbb{R}^3$ with cross-sectional curve q is a self-shrinker if:

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- Compute a critical point of the finite-dimensional functional $\mathfrak{S}_d.$
 - This discrete curve approximates the cross-section of the Angenent torus.

Numerical estimates of the entropy of the Angenent torus



Figure: The entropy of the Angenent torus as computed using 128, 256, 512, 1024, and 2048 points. The values (orange) appear to lie on an exponential curve (blue) converging to 1.8512167 (green).

The convergence rate suggests that the computed value is within 2×10^{-6} of the true value.

Future directions

The index of the Angenent torus

- Critical points of a functional have an index.
 - How many independent perturbations decrease the value of the functional?
 - The number of negative eigenvalues of the Hessian.
- The index of the Angenent torus is at least 3 (Liu, 2016) but is otherwise unknown even conjecturally.
 - Computing the index of the Angenent torus would give insight into how "generic" Angenent torus singularities are.
- We can easily compute the Hessian of \mathfrak{S}_d .

Higher dimensions

- Angenent described a self-shrinking doughnut $S^1 \times S^{n-1}$ in any dimension.
- My code can compute its entropy.
- What is the limiting behavior as *n* becomes large?

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Thank you

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