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.
Toy example: the harmonic oscillator

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.
The harmonic oscillator: numerical conservation

\[ \ddot{x} = \dot{y} = -x. \]

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

**Figure:** Phase space diagram for the harmonic oscillator. \( \ddot{x} = \dot{y} = -x \). The energy \( \frac{1}{2}(x^2 + \dot{x}^2) \) is conserved.
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  \[ S(q) = \int_0^T \frac{1}{2} \| \dot{q} \|^2 \, dt. \]
- Fix endpoints $q_0$ and $q_T$.
- Consider curves $q: [0, T] \rightarrow \mathbb{R}^3$ with $q(0) = q_0$ and $q(T) = q_T$. 
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- The critical point $q$ of $S$ is a solution to $\ddot{q} = 0$. 
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Geodesics in $(M, g)$ are critical points $q: [0, T] \rightarrow M$ of

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Variational formulations

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

\[
\mathcal{G}(x) = \int_0^T \frac{1}{2} \left( |\dot{x}|^2 - |x|^2 \right) \, dt
\]

with fixed endpoints.
Numerically solving ODEs using a variational formulation

Say we seek curves $q: [0, T] \rightarrow M$ that are critical points of a functional $S(q)$. Consider points $q_0, q_1, \ldots, q_N$ on $q$. We call such a sequence of points a discrete curve.

Figure: A discrete curve (red) on a continuous curve (blue).

Construct a functional $S_d: \{\text{discrete curves}\} \rightarrow \mathbb{R}$ such that $S_d(q_0, \ldots, q_N) \approx S(q)$.
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Numerically solve a finite system of equations to find the critical discrete curves for $S_d$.

The discrete curves that are critical points of $S_d$ are numerical approximations for the continuous curves that are critical points of $S$.

This numerical method preserves conservation laws.

### Variational Numerical Methods in Geometric PDE

**Variational integrators for ODEs**

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This numerical method preserves conservation laws. See Marsden and West, Discrete Mechanics and Variational Integrators, 2001.
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Variational formulations for PDEs: Poisson’s equation

Standard PDE formulation

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

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Seek a critical point $v$ of $E$.

$$E(v) = \int_{\Omega} \left( \frac{1}{2} \|\nabla v\|^2 - fv \right), \quad v = 0 \text{ on } \partial \Omega.$$
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**Weak formulation**

Seek a \( v \) for which the equation holds for all \( w \).

\[
\int_\Omega \left( \langle \nabla v, \nabla w \rangle - fw \right) = 0, \quad v = w = 0 \text{ on } \partial \Omega.
\]
The Galerkin method

Variational integrator for ODEs

converts an infinite-dimensional variational problem to a finite-dimensional variational problem.

approximates critical curves of $S(q)$ with critical discrete curves of $S_d(q_0, \ldots, q_N)$.

The Galerkin method for PDEs

can be used to convert 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.
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Let $V$ denote the space of functions $v : \Omega \to \mathbb{R}$.
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Variational formulation
Seek a critical point $v_h \in V_h$ of $E|_{V_h}$.

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**Figure:** A triangulation of a square domain.

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- The Galerkin method gives us the \( v_h \in V_h \) that is the “best” approximation of the true solution.
  - By refining the triangulation, we get a larger \( V_h \) and a better approximation.
How do we specify a piecewise linear function $v_h$?
The finite element method: degrees of freedom

How do we specify a piecewise linear function $v_h$?

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.
The finite element method for vector fields

What if we wanted to solve \( \Delta v + f = 0 \) where \( v \) and \( f \) are vector fields (with appropriate boundary conditions)?
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Understanding the degrees of freedom of vector fields with tangential continuity
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Understanding the degrees of freedom of vector fields with tangential continuity

- Two dimensions (Raviart, Thomas, 1977; Brezzi, Douglas, Marini, 1985).
- Three dimensions (Nédélec, 1980; Nédélec, 1986).
- Finite element exterior calculus (Arnold, Falk, Winther, 2006).
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An alternative: hybrid methods

Standard finite element method

Seek a continuous piecewise linear function \( v_h \) that best approximates the true solution.

Hybrid method do not require \( v_h \) to be continuous. Enforce continuity using Lagrange multipliers.

Interpretation of the hybrid method: Each triangle is now an independent system. The Lagrange multipliers describe how adjacent systems interact. For Poisson's equation: heat transfer between adjacent triangles.

See (Brezzi and Fortin, 1991).
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See (Brezzi and Fortin, 1991).
### An alternative: hybrid methods

#### Standard finite element method
- Seek a continuous piecewise linear function $v_h$ that best approximates the true solution.

#### Hybrid method
- Do not require $v_h$ to be continuous.
- Enforce continuity using Lagrange multipliers.

#### Interpretation of the hybrid method
- Each triangle is now an independent system.
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- Each triangle is now an independent system.
- The Lagrange multipliers describe how adjacent systems interact.
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- See (Brezzi and Fortin, 1991).
Variational formulation

Instead of $E(v_h) = \int_\Omega \left( \frac{1}{2} \| \nabla v_h \|^2 - f v_h \right)$, we have

$$E_h(v_h, \hat{p}_h) = \sum_{K \in T_h} \int_K \left( \frac{1}{2} \| \nabla v_h \|^2 - f v_h \right) - \sum_{K \in T_h} \int_{\partial K} (\hat{p}_h \cdot n) v_h.$$

Weak formulation

- For all $K \in T_h$, $w_h \in V_h$,

$$\int_K \left( \langle \nabla v_h, \nabla w_h \rangle - f w_h \right) - \int_{\partial K} (\hat{p}_h \cdot n) w_h = 0$$

  - Weakly enforces $-\Delta v_h = f$ on $K$ and $\hat{p}_h \cdot n = \nabla v_h \cdot n$ on $\partial K$.

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

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

  - Weakly enforces continuity of $v_h$. 
Conservation of charge in numerical methods for Maxwell’s equations


Maxwell’s equations

\[ \mathbf{E} \text{ divergence free} \]
\[ \mathbf{B} \text{ evolution equations} \]
\[ \dot{\mathbf{E}} = \text{curl} \mathbf{B} \]
\[ \dot{\mathbf{B}} = -\text{curl} \mathbf{E} \]

For purposes of exposition, we have set \( \epsilon = \mu = 1 \) and assumed there is no current.

Charge conservation:
\[ \text{div} \mathbf{E} \text{ is a conserved quantity.} \]
\[ \frac{d}{dt}(\text{div} \mathbf{E}) = \text{div} \dot{\mathbf{E}} = \text{div} \text{curl} \mathbf{B} = 0 \]

\( \text{div} \mathbf{E} \) represents the charge density, denoted \( \rho \), so this conservation law is the conservation of charge.

Yakov Berchenko-Kogan
Variational Numerical Methods in Geometric PDE
Maxwell’s equations

- Electric vector field $E$. 

\[ \dot{E} = \text{curl} \, B, \quad \dot{B} = -\text{curl} \, E. \]

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Charge conservation:

$$\text{div} \, E \text{ is a conserved quantity.}$$

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- Electric vector field $E$.
- Divergence free magnetic vector field $B$. 

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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

\[ \ddot{\mathbf{A}} = -\text{curl}\ \text{curl}\ \mathbf{A} \]

Equivalence to \( \dot{\mathbf{E}} = \text{curl}\ \mathbf{B} \) and \( \dot{\mathbf{B}} = -\text{curl}\ \mathbf{E} \)

Set \( \mathbf{E} := -\dot{\mathbf{A}} \), \( \mathbf{B} := \text{curl}\ \mathbf{A} \).

The evolution equation \( \dot{\mathbf{B}} = -\text{curl}\ \mathbf{E} \) is automatically satisfied.

\( \ddot{\mathbf{A}} = -\text{curl}\ \text{curl}\ \mathbf{A} \) implies \( \dot{\mathbf{E}} = \text{curl}\ \mathbf{B} \).
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- A vector field $A$ called the vector potential.
Maxwell’s equations: the vector potential

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- $\dddot{\mathbf{A}} = - \text{curl} \text{curl} \mathbf{A}$ implies $\dot{\mathbf{E}} = \text{curl} \mathbf{B}$. 
Maxwell’s equations: numerical charge conservation

- Yee scheme (Yee, 1966).

- Galerkin method (Nédélec, 1980).
  - Allows unstructured meshes.
  - Allows higher-degree piecewise polynomial fields.

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

\[ \ddot{A} = - \text{curl} \text{curl} \ A \text{ is equivalent to} \]

\[ \int_{\Omega} \langle \ddot{A}, A' \rangle = - \int_{\Omega} \langle \text{curl} \ A, \text{curl} \ A' \rangle \]

for all vector fields \( A' \) whose tangential components vanish on \( \partial \Omega \).
The Galerkin method for Maxwell’s equations (Nédélec)

Weak formulation

\[ \ddot{\mathbf{A}} = - \nabla \times \nabla \times \mathbf{A} \] is equivalent to

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for all vector fields \( \mathbf{A}' \) whose tangential components vanish on \( \partial \Omega \).

The Galerkin method

Let \( V_h \) be a finite-dimensional subspace of vector fields. Given \( \mathbf{A}_h \in V_h \), solve

\[ \int_{\Omega} \langle \ddot{\mathbf{A}}_h, \mathbf{A}'_h \rangle = - \int_{\Omega} \langle \nabla \times \mathbf{A}_h, \nabla \times \mathbf{A}'_h \rangle \]

for all \( \mathbf{A}'_h \in V_h \) for \( \ddot{\mathbf{A}}_h \in V_h \).

We now have finite system of second-order ODEs.
The Galerkin method for Maxwell’s equations (Nédélec)

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\[ \text{We want conservation of } \rho_h := \text{div } E_h = - \text{div } \dot{A}_h. \]

Let \( \phi'_h \) be a scalar field such that \( \text{grad } \phi'_h \in V_h \). Then

\[ \int_{\Omega} \langle \ddot{A}_h, \text{grad } \phi'_h \rangle = - \int_{\Omega} \langle \text{curl } A_h, \text{curl } \text{grad } \phi'_h \rangle = 0. \]

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Joint work with Ari Stern.

- We construct an appropriate version of hybrid methods for vector equations.

\[ \text{Theorem (BK, Stern)} \]

Solutions to our hybrid formulation of Maxwell’s equations satisfy
\[ \frac{d}{dt} \text{div} \hat{E}_h = 0. \]

That is, we have a strong charge conservation law for our numerical method.
Joint work with Ari Stern.

- We construct an appropriate version of hybrid methods for vector equations.
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The physical interpretation of these Lagrange multipliers are the electric and magnetic fields, so we denote them $\hat{E}_h$ and $\hat{B}_h$.

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Hybrid methods for Maxwell’s equations (BK, Stern)

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**Figure:** Total charge using $E_h$ (Nédélec, solid line) vs. $\hat{E}_h$ (our method, dashed line), simulating on a cube domain.
The Yang–Mills equations are a generalization of Maxwell’s equations.
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  - We want numerical methods to conserve charge as well.
Nédélec’s method applied to the Yang–Mills equations

Maxwell’s equations

\[ \int_{\Omega} \rho \, h \, \phi^{\prime} \, h \text{ is conserved for any scalar field } \phi^{\prime} \, h \text{ such that } \nabla \phi^{\prime} \, h \in V \, h. \]

Nédélec’s method for the Yang–Mills equations

\[ \nabla \phi^{\prime} \, h \text{ is replaced by a nonlinear operator. Consequently, the condition corresponding to } \nabla \phi^{\prime} \, h \in V \, h \text{ is much harder to satisfy. Only works if } \phi^{\prime} \, h \text{ is constant.} \]

Get conservation of \[ \int_{\Omega} \rho \, h, \] i.e. global conservation of total charge.

See (Christiansen and Winther, 2006).
Maxwell’s equations

- Nédélec’s method gave us conservation of weighted average charge.

\[ \int_{\Omega} \rho_h \phi' h \]

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Charge conservation

From before: conservation of
\[
\int_\Omega \rho_h \phi' h
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for constant functions \(\phi' h\).

The hybrid method allows discontinuous \(\phi' h\), so we can use \(\phi' h\) that are piecewise constant with respect to a triangulation \(T_h\).

In particular, consider a \(\phi' h\) that is zero outside of a single element \(K \in T_h\).

Theorem (BK, Stern)
For our hybrid formulation of the Yang–Mills equations, the quantity \(\rho_h\) representing the charge is conserved locally:
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\int_K \rho_h \text{ is conserved in each element } K \in T_h.
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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.
Figure: Curve shortening flow. Image credit: Treibergs. Video credit: Angenent.
**Figure:** Mean curvature flow. Video credit: Kovács.
Categorize singularities by zooming in at the singular point just before the singular time.
Mean curvature flow singularities

- Categorize singularities by zooming in at the singular point just before the singular time.
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...
Categorize singularities by zooming in at the singular point just before the singular time.

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- round cylinder
Mean curvature flow singularities

- Categorize singularities by zooming in at the singular point just before the singular time.
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  - others?

Such a limiting surface must be a self-shrinker. A self-shrinker is a surface that evolves under mean curvature flow by dilations. Are there other self-shrinkers? Yes, a torus (Angenent, 1989). Many others (Kapouleas, Kleene, Møller, 2011).
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Rotationally symmetric self-shrinkers

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

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.

\[
F(\Sigma) = (4\pi)^{-n/2} \int_{\Sigma} e^{-|x|^2/4} \, d\text{Area}.
\]
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.
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.

\[
\begin{align*}
2 & \quad \text{two planes} \\
1.85 & \quad \text{Angenent torus (BK)} \\
\sqrt{\frac{2\pi}{e}} & \quad \text{cylinder} \\
\frac{4}{e} & \quad \text{sphere} \\
1 & \quad \text{plane}
\end{align*}
\]

**Figure:** Entropies of self-shrinking surfaces

Earlier work (Drugan and Nguyen, 2018): the entropy of the Angenent torus is less than 2.
Variational formulations for rotationally-symmetric self-shrinkers

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

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$$\frac{1}{2} \int_{q} r e^{-(r^2+z^2)/4} \, d\text{Arclength}.$$ 

- $q$ is a geodesic in the $(r,z)$-plane with Riemannian metric

$$g = \frac{1}{4} r^2 e^{-(r^2+z^2)/4} (dr^2 + dz^2).$$
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- $q$ is a critical point of
  \[ \mathcal{G}(q) = \int \frac{1}{4} r^2 e^{-(r^2+z^2)/2} \|\dot{q}\|^2 \, dt. \]
Computing the Angenent torus numerically

The cross-section of the Angenent torus is a closed curve $q$ in the $(r,z)$-plane that is a critical point of

$$\mathcal{S}(q) = \int 1/4 r^2 e^{-(r^2+z^2)/2} \| \dot{q} \|^2 \, dt.$$ 

- Approximate $q$ with a discrete curve $q_0, q_1, \ldots, q_N = q_0$
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- Approximate $\mathcal{S}$ with a functional $\mathcal{S}_d$ on discrete curves.

$$\mathcal{S}(q) \approx \mathcal{S}_d(q_1, \ldots, q_N).$$
Computing the Angenent torus numerically

The cross-section of the Angenent torus is a closed curve \( q \) in the \((r, z)\)-plane that is a critical point of

\[
\mathcal{S}(q) = \int 4 r^2 e^{-\left(r^2+z^2\right)/2} \| \dot{q} \|^2 \, dt.
\]

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- Compute a critical point of the finite-dimensional functional \( \mathcal{S}_d \).
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The cross-section of the Angenent torus is a closed curve $q$ in the $(r, z)$-plane that is a critical point of

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$$\mathcal{S}(q) \approx \mathcal{S}_d(q_1, \ldots, q_N).$$

- Compute a critical point of the finite-dimensional functional $\mathcal{S}_d$.
  - This discrete curve approximates the cross-section 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 $2 \times 10^{-6}$ 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 $S_d$.

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?
Thank you