Computational Mechanics and Dynamical Systems

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Joint work with many others, mentioned as we proceed
Give an overview of some topics being investigated in my group.

Overlaps to some extent with several of the other lectures (Nawaf, Oliver, Ari, Katalin, Eva, Melvin, Mark,...), but will focus on things not covered there.

Specifically, I will focus on two things:

- Variational integrators and optimal control
- Lagrangian coherent structures
A discrete version of the variational principles of mechanics (holonomic, nonholonomic, finite dimensional, infinite dimensional, forced, dissipative, controlled,...) leads to integration algorithms broadly known as variational integrators.

Bit of History: Discrete mechanics is closely related to Hamilton-Jacobi theory and has a rich history going back to Moser and Veselov, Suris, ...

In my group, it started with 1997 work with Wendlandt (finite dimensional case), 1998 paper with Patrick and Shkoller (multisymplectic field theories, as in Gotay...).

Leads to AVI methods (2003 paper with Lew, Ortiz, West)

Applies to many systems, such as nonlinear wave equations (sine-Gordon), nonlinear elasticity, E and M (Stern), etc.

The 2001 review paper with West is a nice and not yet obsolete summary; see also Gimmsy.
Basic Variational Set-Up

Lagrangian $L(q, \dot{q})$

Hamilton’s Principle

$$\delta \int_a^b L(q, \dot{q}) \, dt = 0$$

Gives the Euler-Lagrange equations

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}^i} - \frac{\partial L}{\partial q^i} = 0$$

Discrete Hamilton’s Principle

$$L_d(q_0, q_1, h) \approx \int_0^1 L(q(t), \dot{q}(t)) \, dt$$

$$\delta \sum_{k=0}^{N-1} L_d(q_k, q_{k+1}, h_k) = 0$$

Gives discrete E-L equations

$$D_2 L_d(q_{i-1}, q_i, h_{i-1}) + D_1 L_d(q_i, q_{i+1}, h_i) = 0$$
Based on above discrete variational principle of mechanics or its Lagrange-d'Alembert counterpart.

Respects the structure of mechanics (symplectic, energy, momentum).

Gets the energy budget right even for forced or dissipative systems.

People: Kane, West, Ortiz and JM
In addition, these algorithms get the statistics right—in the sense of uncertainty propagation in time (and, eventually in space, through a network). No theorem yet, but it is surely related to symplecticity.
Variational integrators compute chaotic invariant sets much more robustly than even higher order accurate algorithms.
Excellent energy behavior, even after millions of temporal updates.
Can take different time steps with different elements in the mesh.

AVI: Asynchronous Variational Integrators

People: Lew, West, Ortiz, Cirac and JM
State of the Art
What about symmetry?

☑ Examples like electromagnetism have a symmetry.

☑ Gravity too, but...

☑ Associated conservation laws, such as $\text{div } E = 0$.

☑ For discrete integrators to respect that, need the discrete action to have the same symmetry—relatively easy for translations and rotations. Not so simple for $E$ and $M$.

☑ Symmetry in $E$ and $M$ is of course the usual gauge symmetry: $A \rightarrow A + df$

☑ For $E$ and $M$, this problem is cured using DEC (Discrete Exterior Calculus)
AVIs, DEC and Computational Electromagnetism

AVI methods generalize the Yee/ Bossavit/ Kettunen scheme and allow for asynchronous time stepping (yet obey the geometry). Still multisymplectic and with good respect for the mechanics.
Discrete mechanics is great for doing optimal control problems in addition of doing time stepping in field theories.

We give a few examples of DMOC (Discrete Mechanics and Optimal Control) in action to wet your appetite.
DMOC—Discrete Mechanics and Optimal Control

- Same variational discretization methods as time stepping. Flexibility of variational methods enable hierarchical and parallelizable methodologies.

- Many problems can be parallelized.
- Applies to many sorts of problems, such as optimal walking and other robotic problems.

*People:* Ober-Bloebaum, Junge, Kobilarov and JM
Falling Cats, Optimal Swimming

People: Kanso, Martin, Ober-Bloebaum, Leyendecker and JM
Optimal Walking and Spacecraft Reorientation

\[ l = a + b \]

\[ \theta_s \]

\[ -\theta_{ns} \]

\[ M \]

People: Ober-Bloebaum, Leyendecker, Ortiz, Pekarek and JM
LCS Collaborators

• Francois Lekien, University of Brussels
• Shawn Shadden, Stanford
• Philip DuToit, Caltech
• Ben Bastide, Caltech & École des Mines
• John Dabiri, Caltech ...
What is LCS?

• Ridges in finite time Liapunov exponent fields---a measure of the separation rate of fluid particles (or more generally in a dynamical system).

• Provide barriers to particle motions

• Particles on either side of an LCS typically have different dynamical fates

• Also provides key mechanisms for mixing

• What LCS computations do: get velocity field data and spit out dynamically evolving LCS curves (2d) or surfaces (3d)
Invariant Manifolds: Standard View

- Start with the simple pendulum—a swing!
  \[ \ddot{x} + \sin x = 0 \]

- Phase portrait—showing the invariant manifolds (separatrices attached to fixed points.)
Homoclinic Chaos: Standard View

- Periodically perturb the simple pendulum with forcing

\[ \ddot{x} + \sin x + \epsilon \dot{x} \sin t = 0 \]

- Velocity field—hard to tell what is going on:
Standard way around this

- Use of the Poincaré map (1880) to get a homoclinic tangle: excellent way to view for periodic systems.
Transient Chaos

- Poincaré’s homoclinic tangle corresponds to transient chaos—dynamic events over intermediate time scales.
- Infinite time notions like strange attractors, inertial manifolds, etc are not relevant in this context.
- First, a bit more about the tangle.
Smale Horseshoe

- Smale abstracted what was going on in the tangle

- Proved lots of nice things—e.g., an invariant Cantor set.
Smale Horseshoe in the Tangle
Lagrangian Coherent Structures

- Generalizes invariant manifolds to the case of time dependent dynamical systems
- For time varying systems, LCS move in time
Look at lobes, mixing, dynamically
LCS as Separatrices
Review Some Objectives

• Understand mixing, transport and barriers in fluid flows (eg, ocean and atmosphere) and other dynamical systems

• Use LCS to help with drifter deployment, pollution dispersion, oil spills, etc.
Monterey Bay ROMS Real-Time Forecast

The Monterey Bay (MB) ocean forecasting system is based on the Regional Ocean Modeling System (ROMS). The ROMS configuration includes three level nested domains covering the U.S. West coast, central California and Monterey Bay at 15-km, 5-km and 1.6-km, respectively.

Three Level Nested Monterey Bay ROMS Model
SST shaded Relief with SSH
Two Types of LCS: Attracting and Repelling
LCS and Vortex Boundaries

LCS gives much sharper boundaries than vorticity
Lobes, Mixing, Transport
Drifter Deployment
Salinity and LCS

time=104.000000

- attracting
- repelling

Salt levels:
- 34
- 33.9286
- 33.8571
- 33.7857
- 33.7143
- 33.6429
- 33.5714
- 33.5
- 33.4286
- 33.3571
- 33.2857
- 33.2143
- 33.1429
- 33.0714
- 33
3D LCS-Meddies

Ellipsoid of vorticity

Particle trajectories
3D LCS

• Mediterranean Salt Lenses in the Atlantic
Optimization; ocean and spacecraft
LCS in the 3 Body Problem

Figure 1: (a) Intersection of the stable (green) and unstable (red) manifold tubes with the plane $y = 0$, within a constant energy surface in the CR3BP. Here $\mu = 0.1$ and $E = E(L_1) + 0.03715$. Subscripts denote the order of intersection of the manifolds with the plane. Image borrowed from Koon et al. [2]. (b) FTLE field contour plot (i.e., generated using a “three adjacent subgrids” calculation) at the plane $y = 0$ within a constant energy surface of the CR3BP. Energy and mass parameters are identical to those in the adjacent figure. Observe that this particular integration time reveals the first intersection $\Gamma_{1}^{s,s}$ of the stable manifold of the $L_1$ Lyapunov orbit with the plane $y = 0$. 
Hurricanes
Jellyfish
Lobes and Jellyfish

Lobes determine which fluid is entrained

LCS
Further information available on the projects page at:
www.cds.caltech.edu/~marsden

The End