PRINCETON UNIVERSITY

Applied Dynamics and Geometric Mechanics Workshop
July 2008, MFO, Oberwolfach, Germany

Development of Variational Lie-Poisson Integrators

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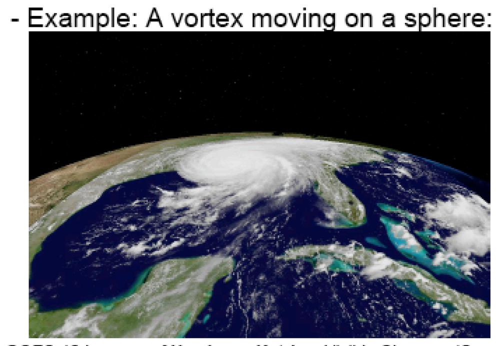
Flows on a sphere

- There exist 'large-scale atmospheric and oceanographic flows with coherent structures that persist over long periods of time' and moving over 'such large distances that the spherical geometry of the earth's surface becomes important'. (Newton2001)

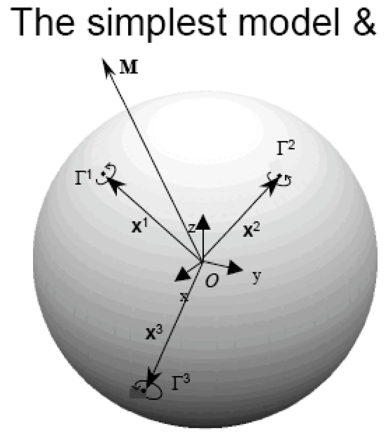
- Study of these flows will be important for understanding atmospheric weather patterns

- Example: A vortex moving on a sphere:



GOES-12 Imagery of **Hurricane Katrina**: Visible Close-up (Opaque) 2005-8-29 17:45Z (picture made in NASA World Wind)

The simplest model & **Motivating problem: N point vortices on a sphere**



A sphere with radius R, with 3 point vortices on its surface

- Equations of motion (developed in Bogomolov 1977) $\dot{\mathbf{x}}^\alpha = \frac{1}{2\pi R}\sum_{\beta\neq\alpha}^{N}\Gamma^\beta \frac{\mathbf{x}^\beta\times\mathbf{x}^\alpha}{||\mathbf{x}^\alpha-\mathbf{x}^\beta||^2}$
- It is a **Lie-Poisson Hamiltonian** system (Pekarsky & Marsden 98) , with conserved quantities:
  - Total energy (Hamiltonian): $H = -\frac{1}{4\pi R^2}\sum_{\beta<\alpha}^{N}\Gamma^\beta\Gamma^\alpha \ln(||\mathbf{x}^\beta-\mathbf{x}^\alpha||^2)$
  - All the vortices stay on the sphere (coadjoint orbits/Casimir functions): $||\mathbf{x}^\alpha||^2 \equiv R^2$
  - Moment of vorticity (momentum map): $\mathrm{M} = \sum_{i=1}^{N}\Gamma^i \mathbf{x}^i$
- **Cannot go to the Euler-Poincaré side**, as the inverse Legendre transform given in the L-P form is not analytically invertible.
- No closed form analytic solution; **geometric LP integrators** needed.

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Class I : Variational Lie-Poisson Integrators on $G\times\mathfrak{g}^*$

A Hamiltonian counterpart of the DEP on G (Moser&Veselov91, Marsden, et al. 99) at the reduced Lagrangian(Euler-Poincaré) side

Reduced Hamiltonian side

in space $\mathfrak{g}\times\mathfrak{g}^*$ ($\mathfrak{g}^*\simeq T^*G/G$)

Lie-Poisson Equations $\dot\mu = \mathrm{ad}^*_\xi\,\mu;\quad \xi = dh/d\mu$ $\qquad \mu\in\mathfrak{g}^*$, $\xi = g^{-1}\dot g \in \mathfrak{g},\ g\in G$

⇕

Lie-Poisson Variational Principle (Cendra *et al.* 2003) $\delta\int_0^T(\langle\mu,\xi\rangle - h(\mu))\,dt = 0$ $\qquad \delta\mu$ arbitrary, $\delta\xi = \dot\eta + [\xi,\eta],\ \eta = g^{-1}\delta g$, δg arbitrary except at endpoints

continuous
⇕
discrete

Discrete L-P Variational Principle $\delta\sum_{k=0}^{N-1}\bar\Theta_k(\mu_k, f_{k+1k}) = 0$

w/ $\eta_k = g_k^{-1}\delta g_k$; $\delta\mu_k, \delta g_k$ arbitrary, except for $\delta g_0 = \delta g_N = 0$.

approximate $\xi_k = \xi_k(f_{k+1k})$ w/ $f_{k+1k} = g_{k+1}^{-1}g_k$

e.g. $\xi_k = g_{k+1}^{-1}\frac{g_{k+1}-g_k}{\Delta t} = \frac{1}{\Delta t}(Id - f_{k+1k})$

in space $G\times\mathfrak{g}^*$

⇕

Variational Lie-Poisson Equations

$$\left\langle\frac{\partial\bar\Theta_k}{\partial f_{k+1k}}, f_{k+1k}\eta_k\right\rangle - \left\langle\frac{\partial\bar\Theta_{k-1}}{\partial f_{kk-1}}, \eta_k f_{kk-1}\right\rangle = 0,\quad \xi_k - \frac{dh_k}{d\mu_k} = 0$$

i.e.

$$\left\langle\mu_k\frac{d\xi_k}{df_{k+1k}}, f_{k+1k}\eta_k\right\rangle - \left\langle\mu_{k-1}\frac{d\xi_{k-1}}{df_{kk-1}}, \eta_k f_{kk-1}\right\rangle = 0,\quad \xi_k(f_{k+1k}) = \frac{dh(\mu_k)}{d\mu_k}$$

$(f_{k+1k},\mu_k)\mapsto(f_{k+2k+1},\mu_{k+1})$ (in $G\times\mathfrak{g}^*$)

- By defining a discrete reduced Legendre transformation, this VLP on $G\times\mathfrak{g}^*$ is equivalent to the DEP on G (Marsden, et al. 99). It thus preserves an induced Poisson structure.
- Problem: Computation of Lie group elements is ('unnecessarily') needed, and usually complicated.

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Class II: VLP on $\mathfrak{g}\times\mathfrak{g}^*$

A Hamiltonian counterpart of the VEP on $\mathfrak{g}$ (Bou-Rabee & Marsden B-RM06) at the reduced Lagrangian (Euler-Poincaré) side.

in space $\mathfrak{g}\times\mathfrak{g}^*$ *Lie-Poisson Variational Principle*

$$\delta\int_{t_1}^{t_2}(\langle\mu(t),\xi(t)\rangle - h(\mu(t))\,dt = 0 \qquad \xi = g^{-1}\dot g,\ \delta\xi = \dot\eta + [\xi,\eta],\ \eta = g^{-1}\delta g$$

w/ $\delta\eta(t_1) = \delta\eta(t_2) = 0$ $\quad\delta\mu$ arbitrary

continuous
⇕
discrete

Discrete L-P Variational Principle

$$0 = \delta\sum_{k=0}^{N-1}(\langle\mu_{k+\beta},\xi_{k+\gamma}\rangle - h(\mu_{k+\beta}))$$

$\delta\mu_k$ arbitrary, η_k arbitrary except for $k = 0, N$.

with $\gamma,\beta\in[0,1]$
$\mu_{k+\beta} := (1-\beta)\mu_k + \beta\mu_{k+1}$;
$\xi_{k+\gamma} := (1-\gamma)\xi_k + \gamma\xi_{k+1}$
$\delta\mu_k$ arbitrary
$\delta\xi_{k+\gamma} := \frac{\eta_{k+1}-\eta_k}{\Delta t} + (1-\gamma)\,\mathrm{ad}_{\xi_k}\eta_k + \gamma\,\mathrm{ad}_{\xi_{k+1}}\eta_{k+1}$
where $\eta_k = g_k^{-1}\delta g_k$

⇕

in space $\mathfrak{g}\times\mathfrak{g}^*$ *Variational L-P integrator* $((\xi_k,\mu_k)\mapsto(\xi_{k+1},\mu_{k+1}))$

$$\begin{cases}\xi_{k+\gamma} = \left.\frac{dh}{d\mu}\right|_{k+\beta};\\ \frac{1}{\Delta t}(\mu_{k+\beta}-\mu_{k-1+\beta}) = \mathrm{ad}^*_{\xi_k}\left[(1-\gamma)\mu_{k+\beta}+\gamma\mu_{k-1+\beta}\right].\end{cases}$$

- By defining a discrete reduced Legendre transformation, this VLP on $\mathfrak{g}\times\mathfrak{g}^*$ is equivalent to the VEP on $\mathfrak{g}$ (B-RM06).
- A discrete symplecticity perserved when $\gamma = 1/2$. When $\gamma = 1/2, \beta = 0$, the scheme is semi-implicit. Specially, In free R.B. / N-point vortex on the sphere cases, it is explicit.
- Problem: Computation of Lie algebra elements is ('unnecessarily') needed.

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A special case of Class II: VLP purely on $\mathfrak{g}^*$

in space $\mathfrak{g}\times\mathfrak{g}^*$ *Lie-Poisson Variational Principle*

$$\delta\int_{t_1}^{t_2}(\langle\mu(t),\xi(t)\rangle - h(\mu(t))\,dt = 0 \qquad \xi = g^{-1}\dot g,\ \delta\xi = \dot\eta + [\xi,\eta],\ \eta = g^{-1}\delta g$$

w/ $\delta\eta(t_1) = \delta\eta(t_2) = 0$

continuous
⇕
discrete

Discrete L-P Variational Principle

$$0 = \delta\sum_{k=0}^{N-1}(\langle\mu_{k+\beta},\xi_{k+\gamma}\rangle - h(\mu_{k+\beta}))$$

$\delta\mu_k$ arbitrary, η_k arbitrary except for $k = 0, N$.

with $\gamma,\beta,\alpha\in[0,1]$
$\mu_{k+\beta} := (1-\beta)\mu_k + \beta\mu_{k+1}$;
$\xi_{k+\gamma} := (1-\gamma)\xi_k + \gamma\xi_{k+1}$
$\delta\mu_k$ arbitrary
$\delta\xi_{k+\gamma} := \frac{\eta_{k+1}-\eta_k}{\Delta t} + (1-\gamma)\,\mathrm{ad}_{\xi_{k+\alpha}}\eta_k + \gamma\,\mathrm{ad}_{\xi_{k+\alpha}}\eta_{k+1}$
where $\eta_k = g_k^{-1}\delta g_k$ arbitrary except at endpoints

⇕

in space $\mathfrak{g}\times\mathfrak{g}^*$ *Variational L-P integrator* $((\xi_k,\mu_k)\mapsto(\xi_{k+1},\mu_{k+1}))$

$$\begin{cases}\xi_{k+\gamma} = \left.\frac{dh}{d\mu}\right|_{k+\beta};\\ \frac{1}{\Delta t}(\mu_{k+\beta}-\mu_{k-1+\beta}) = (1-\gamma)\,\mathrm{ad}^*_{\xi_{k+\alpha}}\mu_{k+\beta} + \gamma\,\mathrm{ad}^*_{\xi_{k-1+\alpha}}\mu_{k-1+\beta}.\end{cases}$$

in space $\mathfrak{g}^*$ when $\alpha = \gamma$, this integrator is purely in $\mathfrak{g}^*$ (Fo $\beta = 0, \alpha = \gamma = \frac{1}{2}$, it is the trapezoidal rule.)

$$\frac{1}{\Delta t}(\mu_{k+\beta}-\mu_{k-1+\beta}) = (1-\gamma)\,\mathrm{ad}^*_{\left.\frac{dh}{d\mu}\right|_{k+\beta}}\mu_{k+\beta} + \gamma\,\mathrm{ad}^*_{\left.\frac{dh}{d\mu}\right|_{k+\beta}}\mu_{k-1+\beta}.$$

However, it is not symplectic for any $\gamma\in[0,1]$.

A positive result: The scheme is 'almost symplectic' when $\gamma = 1/2$. E.g., trapezoidal rule.

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Class III: VLP on $\mathfrak{g}^*$ using Modified Lie-Poisson Variational Principle

in space $\mathfrak{g}^*$ *Lie-Poisson Equations* $\dot\mu = \mathrm{ad}^*_{\delta h/\delta\mu}\,\mu$

⇕

Modified Lie-Poisson Variational Principle

$$\delta\int_0^T\left(\left\langle\mu(t),\frac{dh}{d\mu}(t)\right\rangle - h(\mu(t))\right)dt = 0 \qquad \frac{d^2h}{d\mu^2}\delta\mu = \delta\left(\frac{dh}{d\mu}\right) = \dot\eta + \left[\frac{dh}{d\mu},\eta\right] \text{ where } \eta = g^{-1}\delta g,$$

δg arbitrary except $\delta g(t_1) = \delta g(t_2) = 0$.

continuous
⇕
discrete

Discrete Modified L-P Variational Principle

$$\delta\sum_{k=0}^{K-1}\left(\left\langle\mu_{k+\beta},\left.\frac{dh}{d\mu}\right|_{\mu_{k+\beta}}\right\rangle - h(\mu_{k+\beta})\right)\Delta t = 0.$$

with

$$\delta\left.\frac{dh}{d\mu}\right|_{\mu_{k+\beta}} = \frac{\eta_{k+1}-\eta_k}{\Delta t} + (1-\beta)\,\mathrm{ad}_{\left.\frac{dh}{d\mu}\right|_{\mu_k}}\eta_k + \beta\,\mathrm{ad}_{\left.\frac{dh}{d\mu}\right|_{\mu_{k+1}}}\eta_{k+1}$$

where $\eta_k = g_k^{-1}\delta g_k$ arbitrary except at endpoints

⇕

in space $\mathfrak{g}^*$ *Modified Variational L-P integrator (MVLP)*

$$\frac{1}{\Delta t}(\mu_{k+\beta}-\mu_{k-1+\beta}) = \mathrm{ad}^*_{\left.\frac{dh}{d\mu}\right|_{\mu_k}}((1-\beta)\mu_{k+\beta}+\beta\mu_{k-1+\beta})$$

- **A positive result**:
  When the Hamiltonian is quadratic, the MVLP integrator is symplectic foı $\beta = 1/2$.

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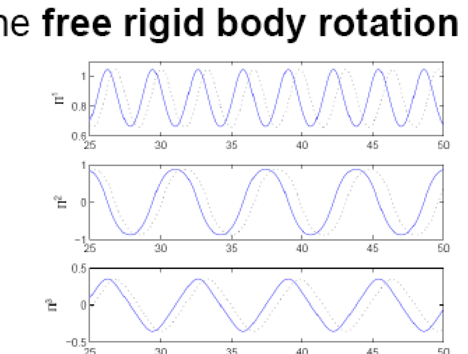
Example 1: VLP integrators applied to the **free rigid body rotation** case

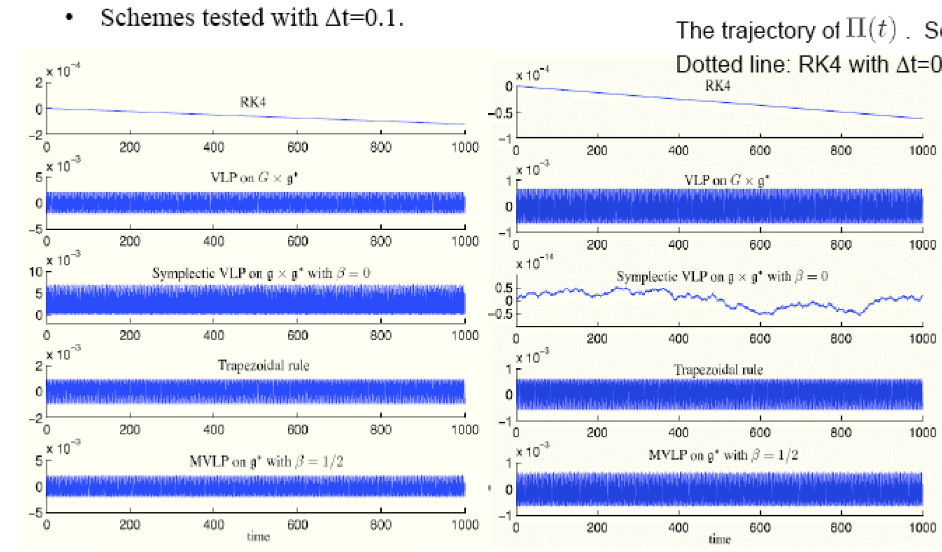
$$\dot{\mathbf{\Pi}} = \mathbf{\Pi}\times\mathbf{\Omega} = \mathbf{\Pi}\times\frac{dh(\mathbf{\Pi})}{d\mathbf{\Pi}}$$

$$h(\mathbf{\Pi}) = \frac{1}{2}\left(\frac{(\Pi^1)^2}{\mathbb{I}^1}+\frac{(\Pi^2)^2}{\mathbb{I}^2}+\frac{(\Pi^3)^2}{\mathbb{I}^3}\right) \quad \text{(quadratic)}$$

- $\mathbb{I}^1 = 7/8, \mathbb{I}^2 = 5/8, \mathbb{I}^3 = 1/4.$
- Initial conditions: $\mathbf{\Pi}(0) = (7/8, 5/8, 1/4)^T$.
- Schemes tested with Δt=0.1.

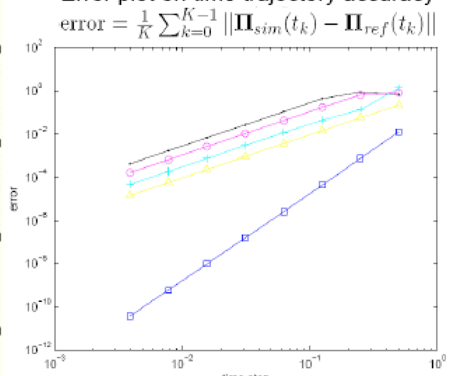


The trajectory of $\Pi(t)$. Solid line: VLP on $G\times\mathfrak{g}^*$ with Δt=0.1. Dotted line: RK4 with Δt=0.001as reference.



(I) Hamiltonian $h - h(0)$ vs time (II) Casimir $||\Pi||^2/2 - ||\Pi(0)||^2/2$ vs time

Error plot on time trajectory accuracy
$\mathrm{error} = \frac{1}{K}\sum_{k=0}^{K-1}||\mathbf{\Pi}_{sim}(t_k) - \mathbf{\Pi}_{ref}(t_k)||$



RK4 (□), VLP on $G\times\mathfrak{g}^*$ (·) symplectic VLP on $\mathfrak{g}\times\mathfrak{g}^*$ (+) Trapezoidal rule (△) symplectic MVLP on $\mathfrak{g}^*$ (○)

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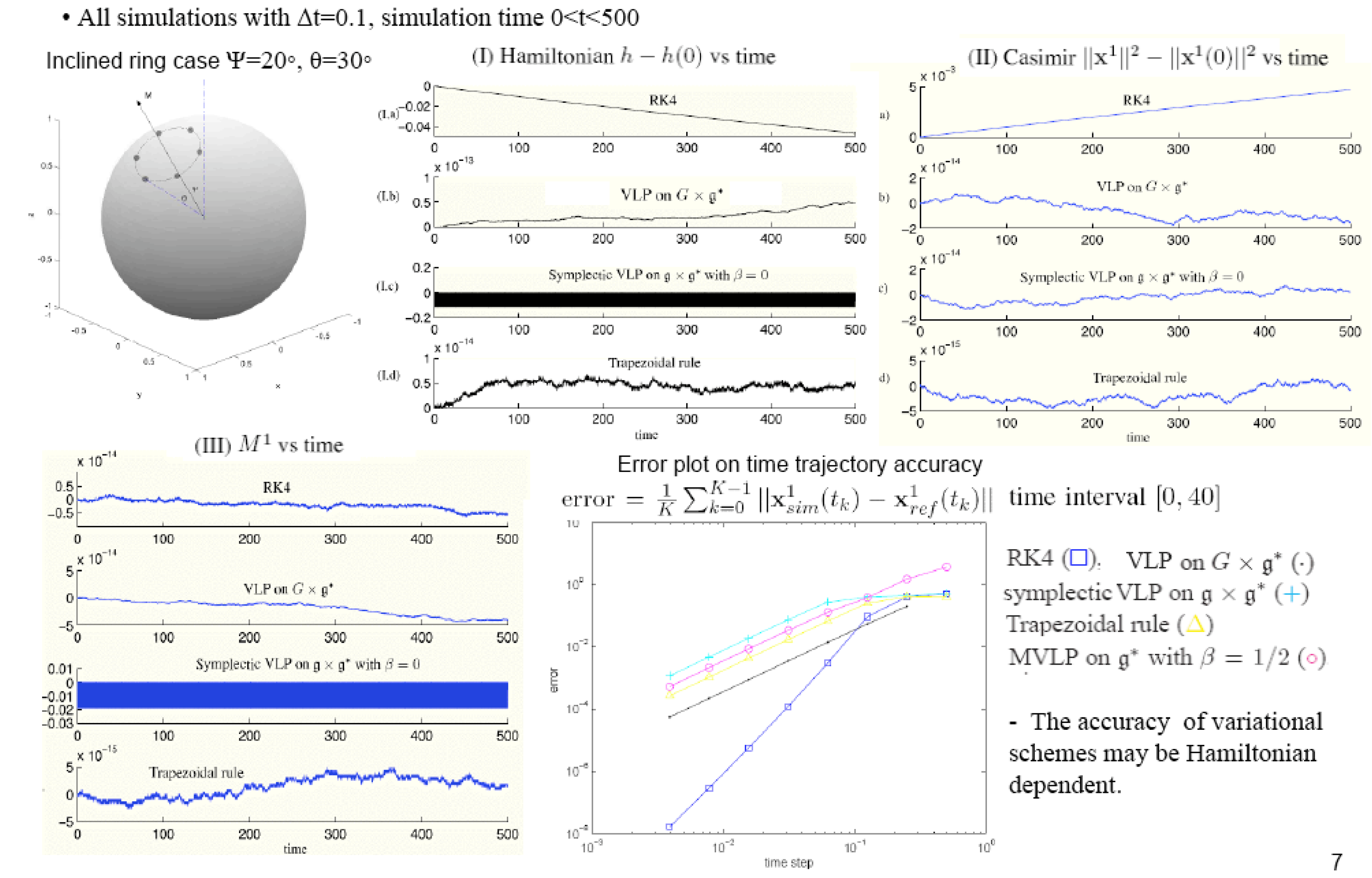
Example 2: VLP integrators applied to the **N-point vortex case**

- N=6 ring case: 6 identical p. v.s with unit strength - Stable relative equilibrium (ref: Polvani & Dritschel 1993) Period: T=1.9658;
- All simulations with Δt=0.1, simulation time 0<t<500



Error plot on time trajectory accuracy
$\mathrm{error} = \frac{1}{K}\sum_{k=0}^{K-1}||\mathbf{x}^1_{sim}(t_k) - \mathbf{x}^1_{ref}(t_k)||$ time interval $[0, 40]$

RK4 (□), VLP on $G\times\mathfrak{g}^*$ (·) symplectic VLP on $\mathfrak{g}\times\mathfrak{g}^*$ (+) Trapezoidal rule (△) MVLP on $\mathfrak{g}^*$ with $\beta = 1/2$ (○)

- The accuracy of variational schemes may be Hamiltonian dependent.

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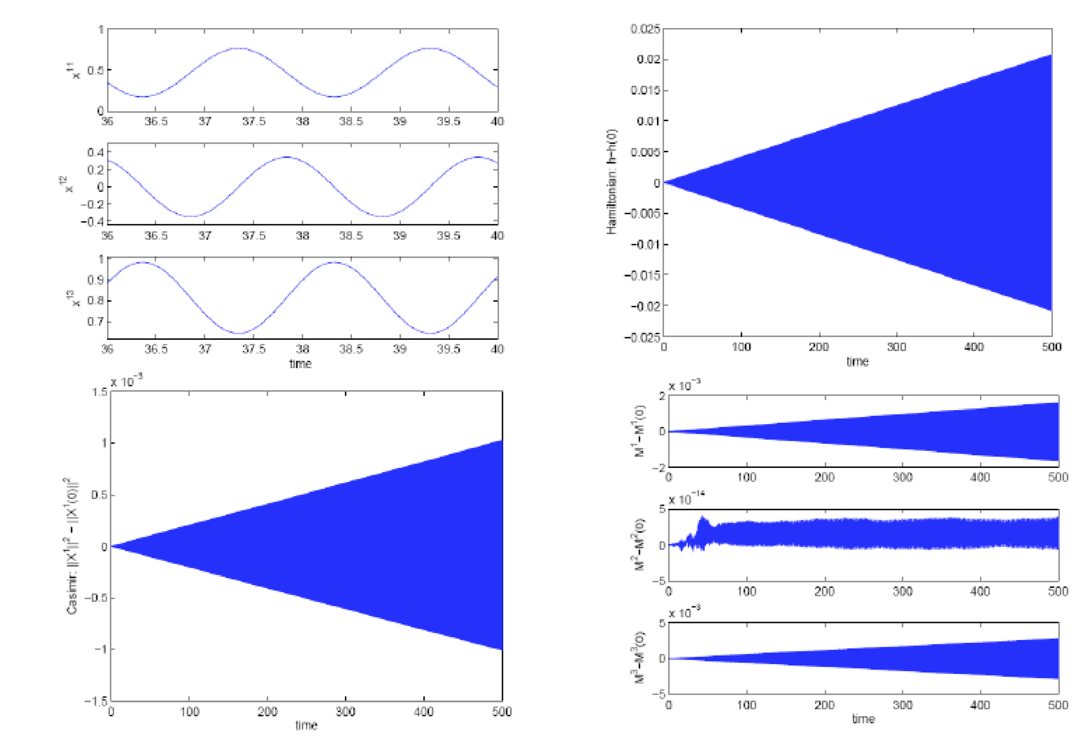
MVLP integrator applied to the N-point vortex case:

Simulation results of the MVLP on $\mathfrak{g}^*$ with $\beta = 1/2$. Time step $\Delta t = 0.01$.



- Not symplectic. Recall the Hamiltonian is not quadratic $H = -\frac{1}{4\pi R^2}\sum_{\beta<\alpha}^{N}\Gamma^\beta\Gamma^\alpha\ln(||\mathbf{x}^\beta-\mathbf{x}^\alpha||^2)$.

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Summary: Variational integrators for L-P Ham systems

Methods	Advantages	Drawbacks
Variational Lie-Poisson integrators on $G\times\mathfrak{g}^*$	• Preserve a Poisson structure • applicable to general finite dimensional L-P systems	• Implicit • computation of Lie group elements needed
Variational Lie-Poisson integrators on $\mathfrak{g}\times\mathfrak{g}^*$	• semi-explicit symplectic schemes exist in this family	• computation of Lie algebra elements needed
Variational Lie-Poisson integrators on $\mathfrak{g}^*$	• Computations involves only elements on $\mathfrak{g}^*$ • Easy to use • 'Almost symplectic' schemes, such as trapezoidal rules, work well	• Not symplectic – but there are 'almost symplectic' schemes.
Modified Variational Lie-Poisson integrators on $\mathfrak{g}^*$	• Computations involve only elements on $\mathfrak{g}^*$ • Easy to use • Exist symplectic schemes for quadratic Hamiltonians	• For non-quadratic Hamiltonians the scheme maybe not symplectic (indicated by numerical results: Conservative quantities blow up in the N-point vortex case).

Future work:

- Fast (explicit), accurate and symplectic/Lie-Poisson VLPs on $\mathfrak{g}^*$ that are easy to construct/use
- Generalization to non-conservative systems

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