Variational Integrators with Applications to Celestial Mechanics

AME-599 Final Project

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Introduction

- When one models a physical system numerical integrations is usually not part of the design process

- For example, when modeling a particle one can
  - Come up with the Lagrangian of the system, then
  - Derive the equations of motion using the Euler-Lagrange equations (via Hamilton's Principle)
  - Then, if we cannot describe the dynamics in any close form, the system is numerically integrated using some ODE solver

Introduction

- Question: What happens to this new **discretize** EOM, does it behave as the “true” solution?
- Answer: Not always!

- Because arbitrary numerical schemes know nothing of the problem one is solving
  - It does not understand the “geometry” of the problem
  - It does not understand any conservation laws (energy and momentum)
  - This may lead to incorrect solutions (e.g., energy drifts for conserved systems)

Introduction

- Solution: Use “Geometric” (structure preserving or symplectic) integrators which captures important structures and maintain certain conservation laws or other important features to the problem.

- For example: Numerical integration of initial value problems (IVP) for ODEs is done by discretizing the derivatives via finite differences, for example

$$\frac{dq}{dt} = f(q,t) \xrightarrow{\text{LHS}} \frac{q_{k+1} - q_k}{h}$$

- How do discretize the RHS?

Introduction

- For an Hamiltonian system $$\dot{q} = \frac{\partial H}{\partial p} \qquad \dot{p} = -\frac{\partial H}{\partial q}$$
- It can be shown that for the above system, *H* is constant along solutions (at all time), but
- How does one discretize the equations such that this is guaranteed, and
- It is known that for Hamiltonian systems the flow is symplectic, but will the discrete integrator maintain this?
- Symplectic integrators preserve these properties while arbitrary integrators may not

Introduction

- This does not mean that we should stop using all off-the-shelf integrators, but is useful for applications when local accuracy is not necessary desired but instead on global behavior of a system, e.g.,
  - Statistical results
  - Monte-Carlo analyses
  - Long-term propagations

- With the emergence of “geometric” integrators numerical schemes can now be part of the design process.

Aim of this Presentation

- This presentation will discuss about discrete variational mechanics and deriving variational integrators for problems in celestial dynamics

- Examples will be given for
  - Planar Circular Restricted Three Body Problem (PCR3BP)
  - Simplified 4-Body Solar System Problem (Sun, Jupiter, Saturn, and Uranus)

Aim of this Presentation

- An in-depth study of variational integrators requires the understanding of geometric mechanics and differential geometry
- To **NOT** complicate the subject matter any further this talk will try to exclude discussion regarding manifolds, tangent bundles, forms, flow, etc.
- Instead focus on applications and practical examples

Variational Integrators

- **Variational integrators** (VI) are symplectic integrators derived using the Lagrangian based on discrete variational principles (where previous work focused on the Hamiltonian, e.g., using generating functions or the Hamilton-Jacobi equation).

- More to follow . . .

Lagrange Mechanics

- Given a Lagrangian of the form $L(q,\dot{q}) = \frac{1}{2}\dot{q}^T M \dot{q} - V(q)$
- And a correspond action $S[q(t)] = \int_{t_0}^{t_1} L(q,\dot{q})dt$
- **Hamilton's Principle** states that the actual physical path taken is a stationary point of *S*, i.e., $\delta S = 0$

$$\delta S = \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} \right) \delta q = 0$$

- This gives the **Euler-Lagrange equation** and Newton's equation

$$\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = 0 \longrightarrow M\ddot{q} = -\nabla V(q)$$

Discrete Lagrange Mechanics

- Instead of considering q and $\dot{q}$ lets consider two position q_k , q_{k+1} and a Δt

- Now consider a discrete Lagrangian approximating the action integral along the segment between the two position by quadrature rule of interpolating functions (more later)

$$L_d\left(q_k, q_{k+1}\right) \approx \int_{t_k}^{t_{k+1}} L\left(q, \dot{q}\right) dt$$

- Now instead of an action integral we have an **action sum**

$$S_d\left[q_k\right] = \sum_{k=0}^{N-1} L_d\left(q_k, q_{k+1}\right)$$

Discrete Lagrange Mechanics

- Analogous to the continuous derivation we compute the variations of the action sum with the boundary points held fixed (Hamilton's Principle)

$$\delta S_d[q_k] = \delta \sum_{k=0}^{N-1} L_d(q_k, q_{k+1}) = \sum_{k=0}^{N-1} \left[\frac{\partial L_d(q_k, q_{k+1})}{\partial q_k} \delta q_k + \frac{\partial L_d(q_k, q_{k+1})}{\partial q_{k+1}} \delta q_{k+1} \right] = 0$$

- This results in the **discrete Euler-Lagrange equations**

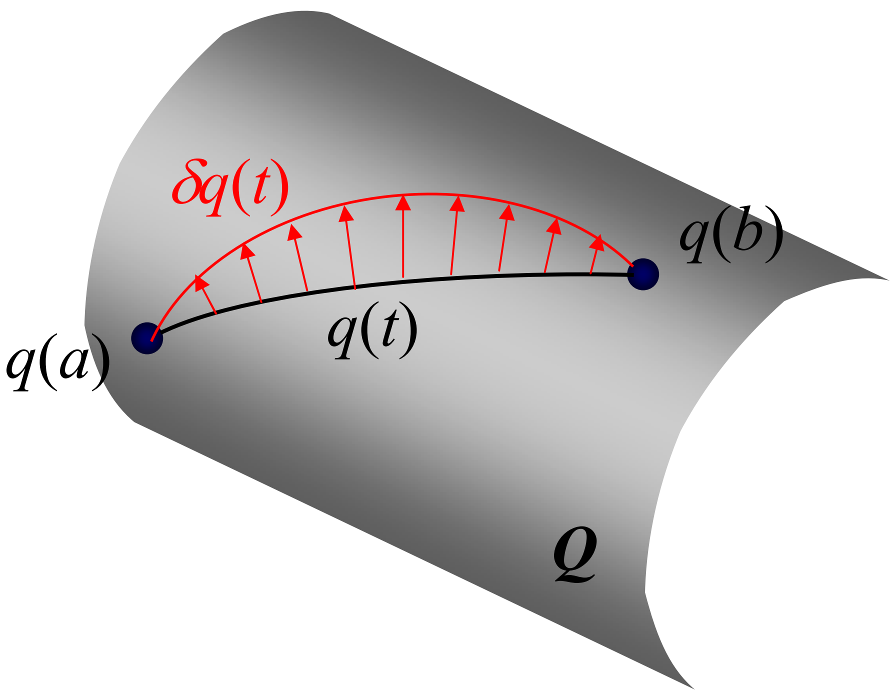
$$\frac{\partial L_d(q_k, q_{k+1})}{\partial q_k} + \frac{\partial L_d(q_{k-1}, q_k)}{\partial q_{k+1}} = 0$$

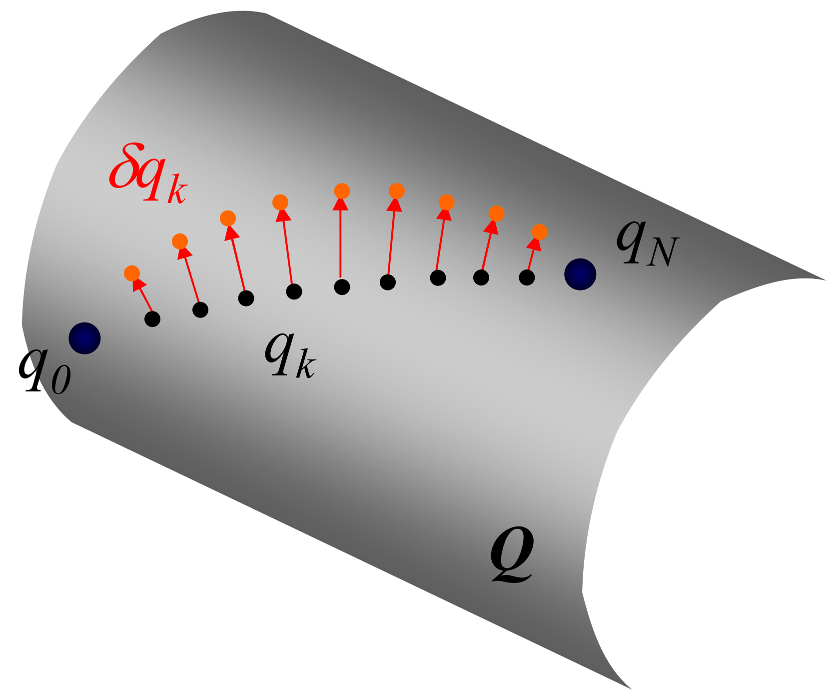
- For the Lagrangian given on slide 10 the discrete Euler-Lagrange equation becomes a **discretization of Newton's equation**

$$M\left(\frac{q_{k+1} - 2q_k + q_{k-1}}{(\Delta t)^2} \right) = -\nabla V(q_k)$$

Discrete Lagrange Mechanics

- In pictures . . .





Hamilton's Principle

Variational Integrators

- Using the discrete Euler-Lagrange equations we now have a map to take us from q_0 to q_1, i.e., integrate the trajectory
- Integrators which use the discrete Euler-Lagrange equations are known as **variational integrators**
- Before we move to an example, we note that IVP problems are usually not specified with two initial position, but instead an initial position and velocity

Variational Integrators

- Thus, we define a discretize conjugate momentum as

$$p_k = -\frac{\partial L_d(q_k, q_{k+1})}{\partial q_k} \qquad (*)$$

$$p_{k+1} = \frac{\partial L_d(q_k, q_{k+1})}{\partial q_{k+1}} \qquad (**)$$

- This allows us to go from (q_0, p_0) to (q_k, p_k)
  - Use (*) to find q_k (usually an implicit routine)
  - Then use the explicit equation (**) to find p_k

Finding $L_d(q_k, q_{k+1})$

- All the equations described so far requires a discrete Lagrangian, but how do we find the discrete version given the continuous Lagrangian
- Quadrature rule of interpolating functions $L_d(q_k, q_{k+1}) \approx \int_{t_k}^{t_{k+1}} L(q, \dot{q})\, dt$
  - Many method exist, i.e., rectangular rule, midpoint rule, Newmark method which is common in structural dynamics,
  - But we will focus on the Trapezoidal Rule (Verlet or Störmer rule) which is commonly used in molecular dynamics and provide explicit relations for (*)

$$L_d(q_k, q_{k+1}) = \frac{1}{2}\left[L\left(q_k, \frac{q_{k+1} - q_k}{\Delta t} \right) + L\left(q_{k+1}, \frac{q_{k+1} - q_k}{\Delta t} \right) \right] \Delta t$$

$$= \frac{1}{2}\left[\left(\frac{q_{k+1} - q_k}{\Delta t} \right)^T M \left(\frac{q_{k+1} - q_k}{\Delta t} \right) + V(q_{k+1}) - V(q_k) \right] \Delta t$$

Example 1: PCR3BP

- Planar Circular Restricted 3-Body Problem (PCR3BP)

- The normalized equations of motions are

$$\ddot{x} - 2\dot{y} - x = -(1-\mu)\frac{x - x_1}{r_1^3} - \mu\frac{x - x_2}{r_2^3} = -\frac{\partial V}{\partial x}$$

$$\ddot{y} + 2\dot{x} + y = -(1-\mu)\frac{y}{r_1^3} - \mu\frac{y}{r_2^3} = -\frac{\partial V}{\partial y}$$

where $\mu = m_2/(m_1 + m_2)$

- The Lagrangian is given as

$$L = \frac{1}{2}\left[(\dot{x} - y)^2 + (\dot{y} + x)^2\right] + \frac{1-\mu}{r_1} + \frac{\mu}{r_2}$$

Example 1: PCR3BP

- Discretizing the Lagrangian we get

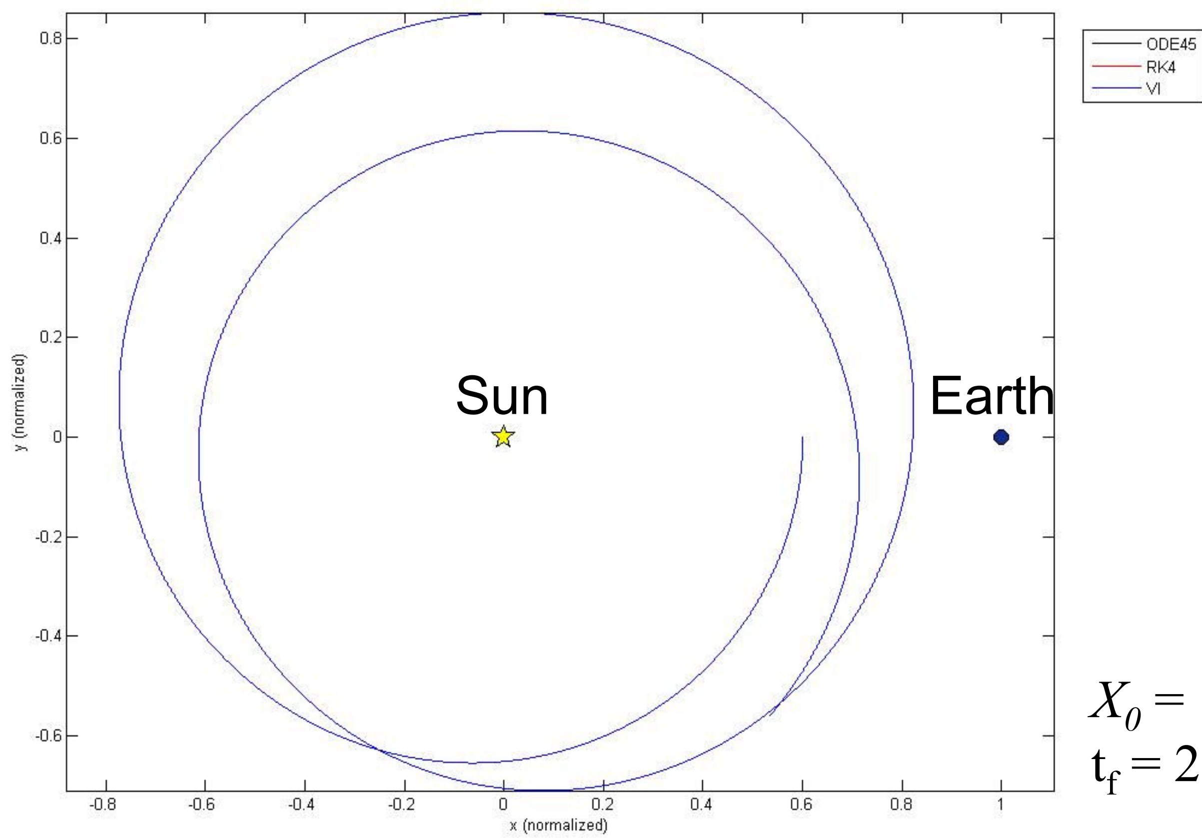
$$L_d = \frac{1}{2}\left[\frac{1}{2}\left[\left(\frac{x_{k+1}-x_k}{\Delta t} - y_k\right)^2 + \left(\frac{y_{k+1}-y_k}{\Delta t} + x_k\right)^2\right] + \frac{1-\mu}{r_{k,1}} + \frac{\mu}{r_{k,2}}\right.$$
$$\left. + \frac{1}{2}\left[\left(\frac{x_{k+1}-x_k}{\Delta t} - y_{k+1}\right)^2 + \left(\frac{y_{k+1}-y_k}{\Delta t} + x_{k+1}\right)^2\right] + \frac{1-\mu}{r_{k+1,1}} + \frac{\mu}{r_{k+1,2}}\right]\Delta t$$

where $r_{k,1} = \sqrt{(x_k+\mu)^2 + y_k^2}$ $\quad r_{k,2} = \sqrt{(x_k - 1 + \mu)^2 + y_k^2}$

- Using Eqs. (*) and (**) rearranging the equations a little we get an explicit set of expression for the position and momentum at time step *k*+1 provided a set of initial conditions at step *k* (see paper).

Example 1: PCR3BP

- Sun-Earth system example, μ = 3.04036e-006

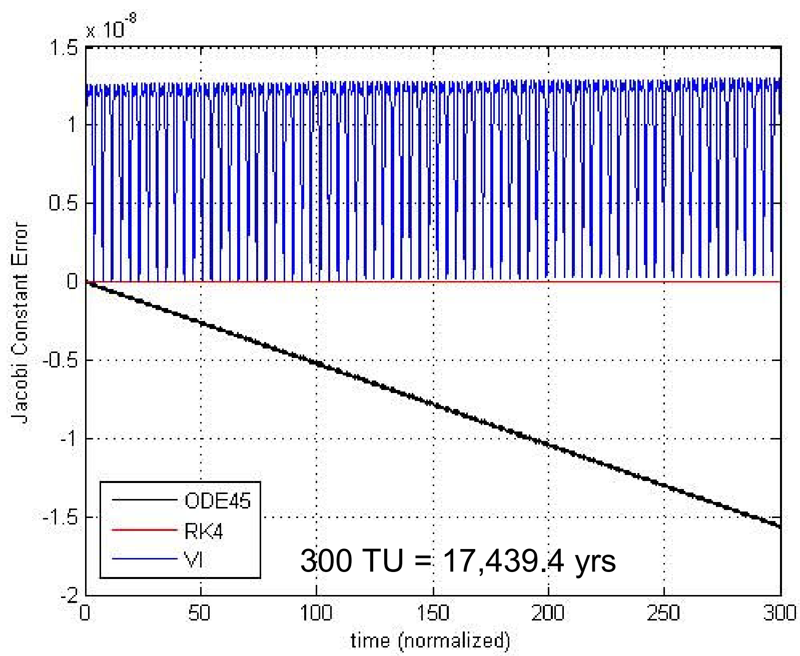


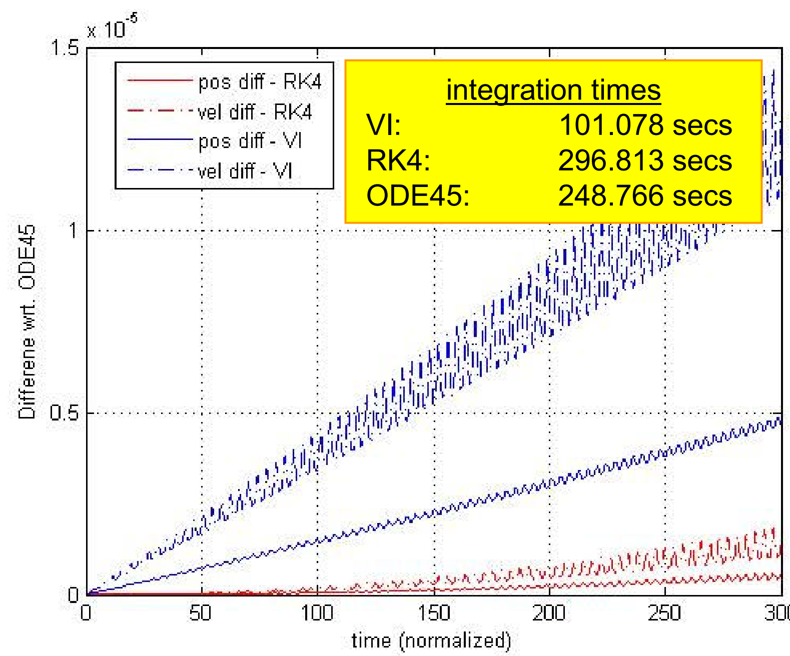
$X_0 = [0.6, 0, 0, -2]$
$t_f = 291$ years

Example 1: PCR3BP

- Note that for this system there is only one conserved quantity, the Jacobi constant

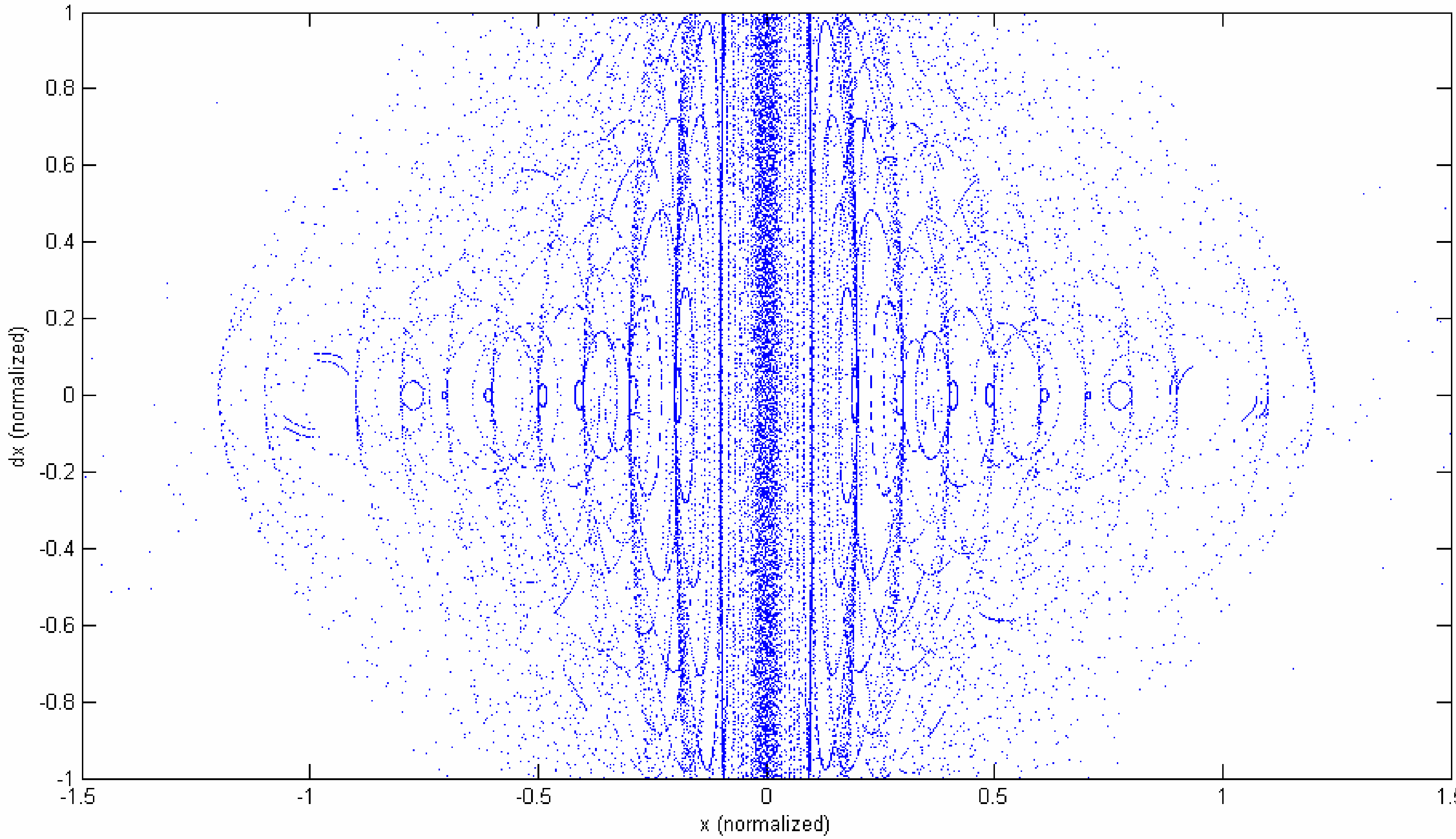
$$J_C = \left(x^2 + y^2\right) + 2\left(\frac{1-\mu}{r_1} + \frac{\mu}{r_2}\right) - \left(\dot{x}^2 + \dot{y}^2\right)$$





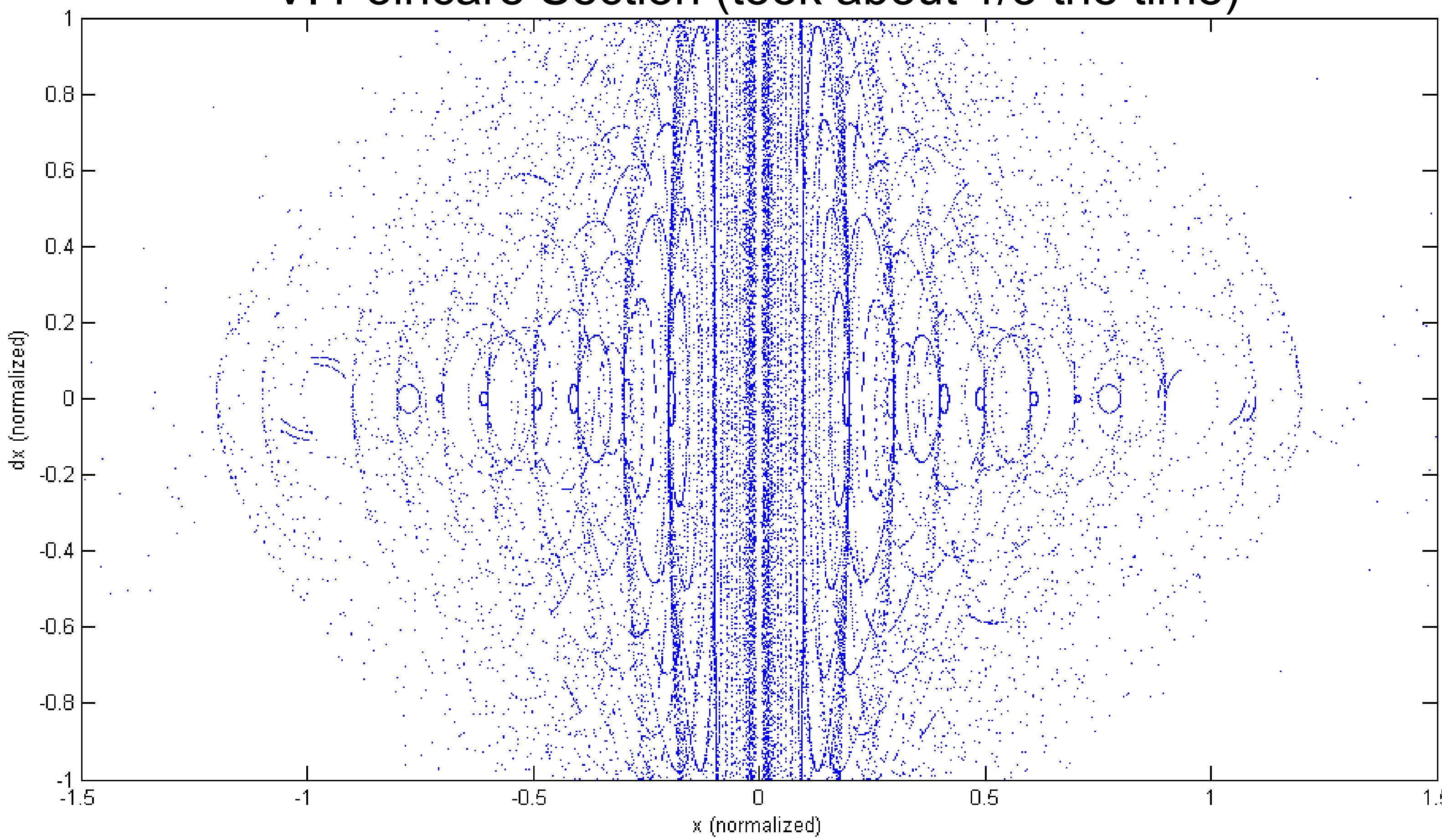
Example 1: PCR3BP

ODE45 Poincaré Section



Example 1: PCR3BP

VI Poincaré Section (took about 1/3 the time)



Example 2: 4-Body Problem

- 4-body simplified solar system model including the Sun, Jupiter, Saturn, and Uranus with their initial conditions specified in the J2000 frame with respect to the solar system barycenter on 01-JAN-2000

- The Lagrangian for this system is (for *N*=4)

$$L = \frac{1}{2}\sum_{i=1}^{N} m_i\left(\dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2\right) + G\sum_{i=1}^{N-1}\sum_{j>i}^{N}\frac{m_i m_j}{r_{ij}}$$

- Solving for the position and momentum at the next time step we have

$$q_{k+1} = q_k + (\Delta t)M^{-1}p_k - \frac{1}{2}(\Delta t)^2 M^{-1}(\nabla V(q_k))$$

$$p_{k+1} = p_k - \frac{1}{2}(\Delta t)(\nabla V(q_{k+1}) + \nabla V(q_k))$$

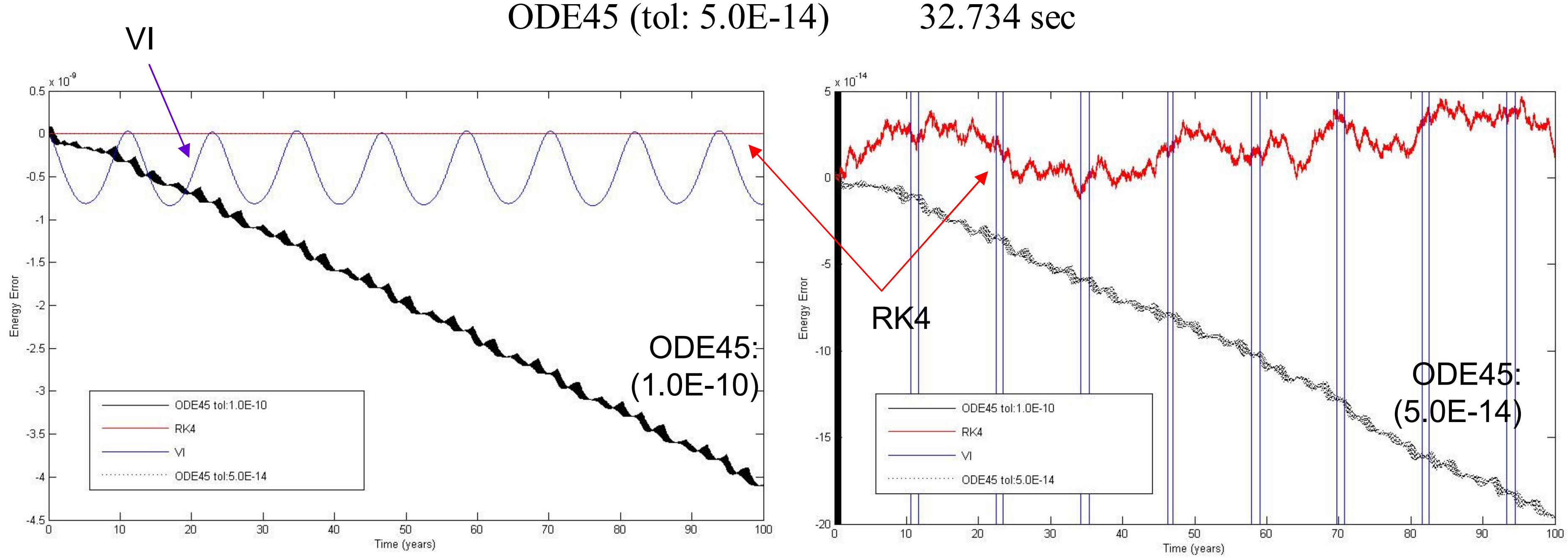
where the 12-by-1 vector $\nabla V(q_k) = \begin{bmatrix}\partial V/\partial q_{1,k} & \partial V/\partial q_{2,k} & \partial V/\partial q_{3,k} & \partial V/\partial q_{4,k}\end{bmatrix}^T$

Example 2: 4-Body Problem

- Short propagation of 100 years

scheme	runtime
VI	61.282 secs
RK4	222.594 sec
ODE45 (tol: 1.0E-10)	30.422 sec
ODE45 (tol: 5.0E-14)	32.734 sec

(VI and RK4: 1 day step sizes)



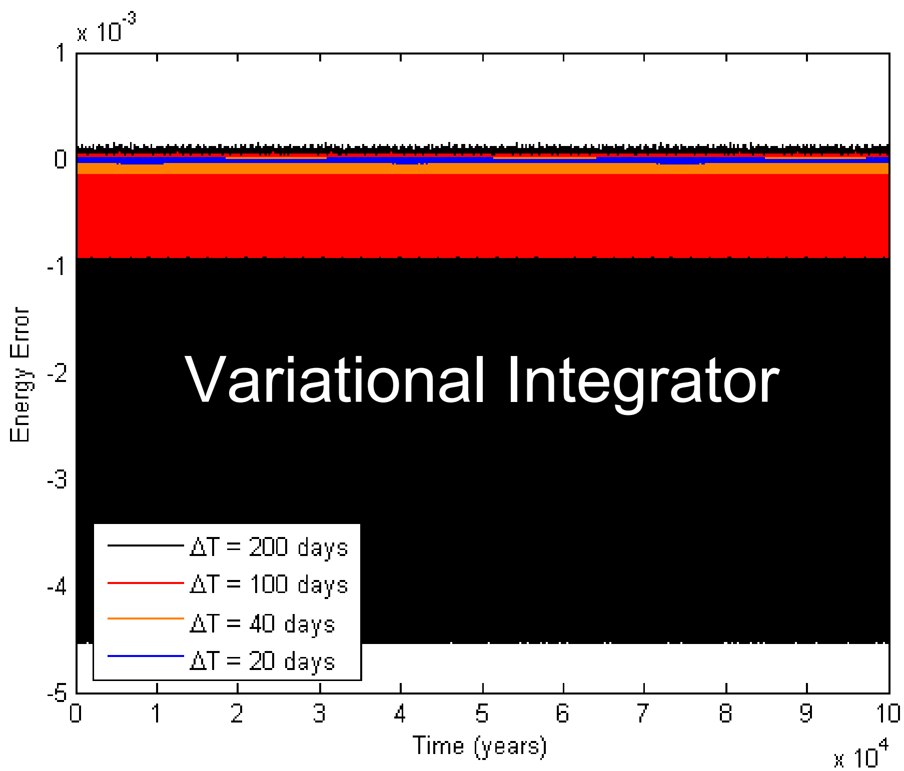
Example 2: 4-Body Problem

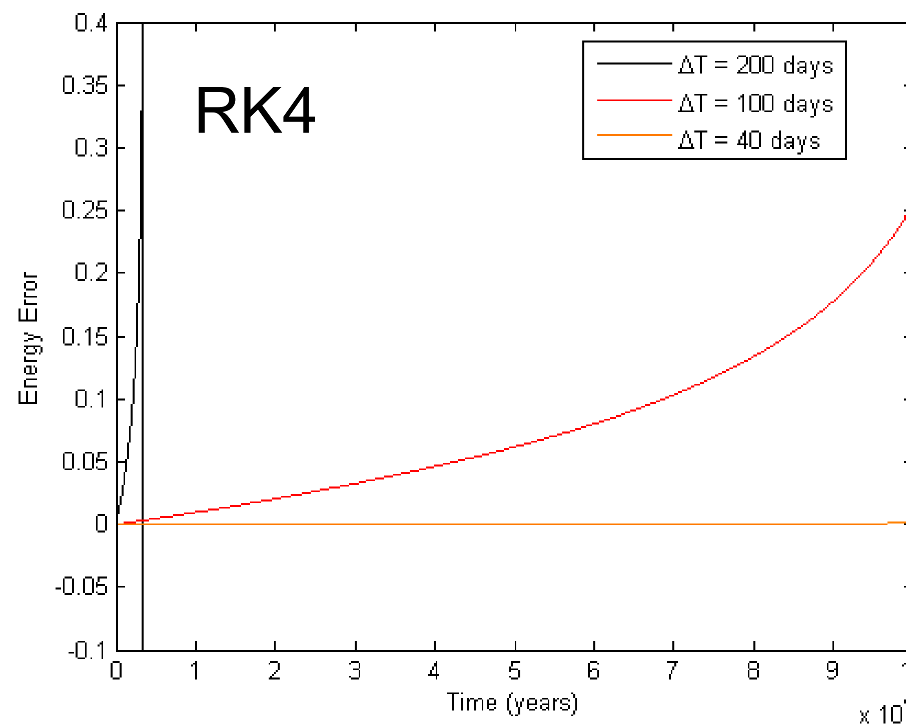
- It appears that the high tolerance ODE45 and the RK4 scheme has better energy conservation that of the variational integrator for propagations under 100 year (but this is only due to the short integration time)

- What happens when we start propagating for 1000s of years or millions?
  - Note that there is a drift in the ODE45 scheme
  - But is there such drift in the RK4 scheme?

Long-term Energy Behavior

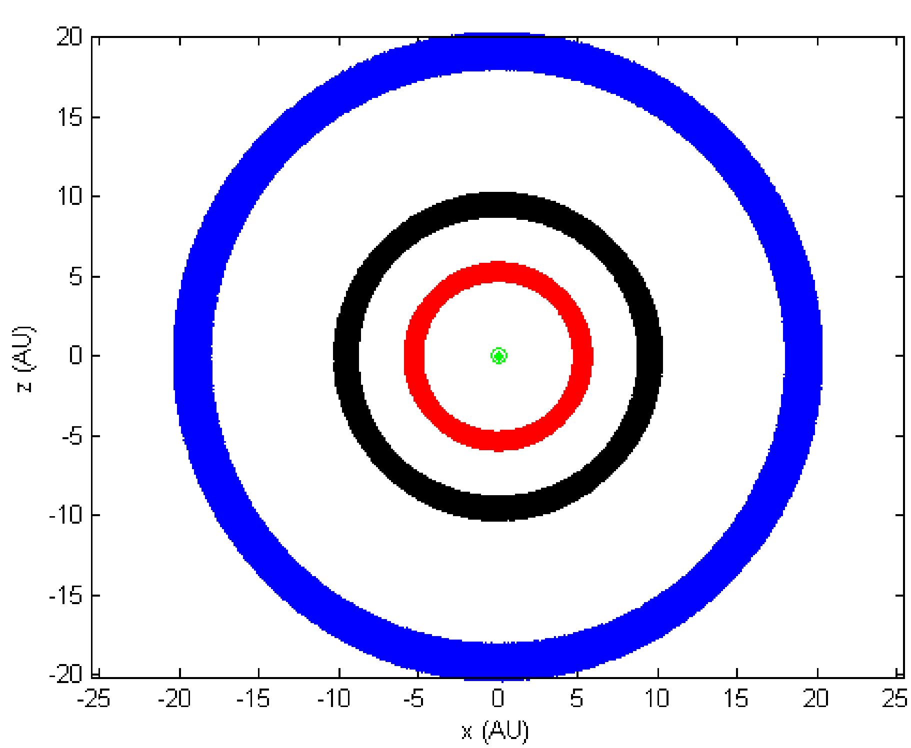
- Average energy for the VI remains fairly constant for a wide range of time steps
- Energy drift for the RK4 which can be minimize by taking smaller time steps

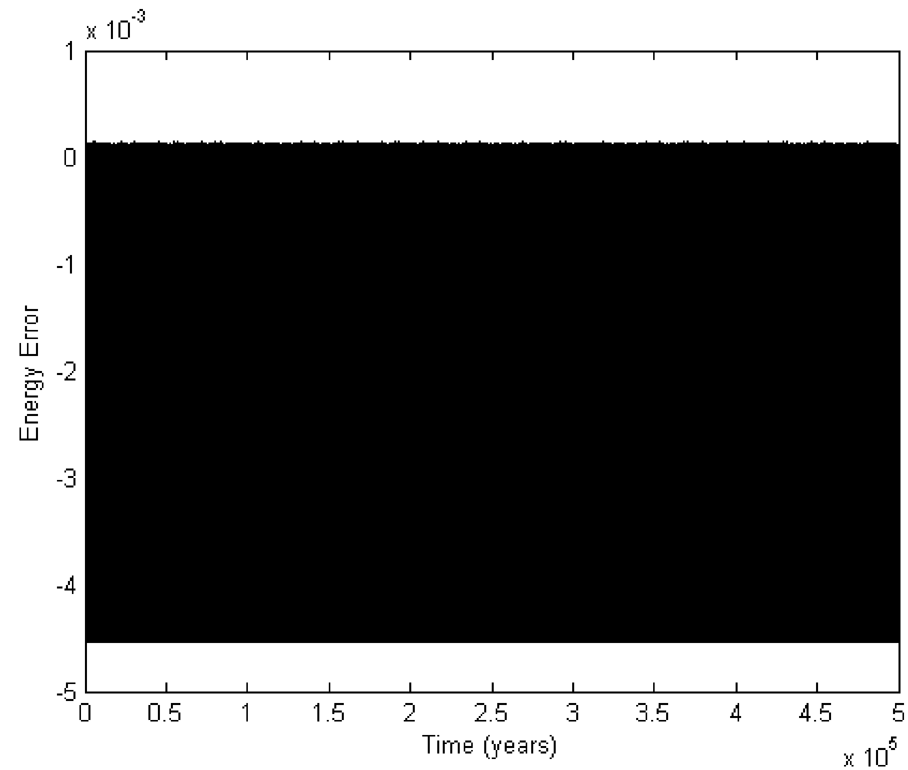




What if Local Accuracy is Important?

- VI: **500,000 year** propagation with a step size of **200 days**
- Remarkably stable for such a coarse step size, which RK4 could not accomplish





Conclusions and Comments

- Variational integrators are straight forward to design and implement for simple dynamical systems
- Variational integrators inherently conserved important quantities of dynamical system
- RK4 perform surprising very well (for small time steps) for many mission design and navigation applications when short integration times are sufficient.
- For longer term propagations and for larger step sizes, variational integrators are very beneficial
  - No energy drifts
  - Faster integration time
  - Reasonably accurate solutions

If I had time . . .

- Re-write code in Fortran or Python instead of Matlab
- Look at adding non-conservative forces
- Look at the application of using variation integrators for highly stiff dynamical problems, i.e., systems with many kinematics constraints