An Overview of Variational Integrators

A. Lew, M. West

Stanford University

J. Marsden, M. Ortiz

Caltech

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Variational Integrators

- What?
  - Theory to generate space and time integrators
- Why?
  - Conservation properties
    - Linear and angular momenta, energy, symplecticity, *J*-and *L*-integrals… (Discrete Noether's theorem). Get the definition of the discrete conserved quantity as well.
  - Pervasive applications
    - Elasticity, Fluids, Electromagnetism, General Relativity, Collisions, dissipative systems ….
  - Get the "physics" right
    - Get key statistical quantities right even in the face of chaotic dynamics (e.g., temperature)
- How much?
  - No extra cost than traditional approach
    - High-order, similar accuracy vs. cost, implicit/explicit …

Biased References

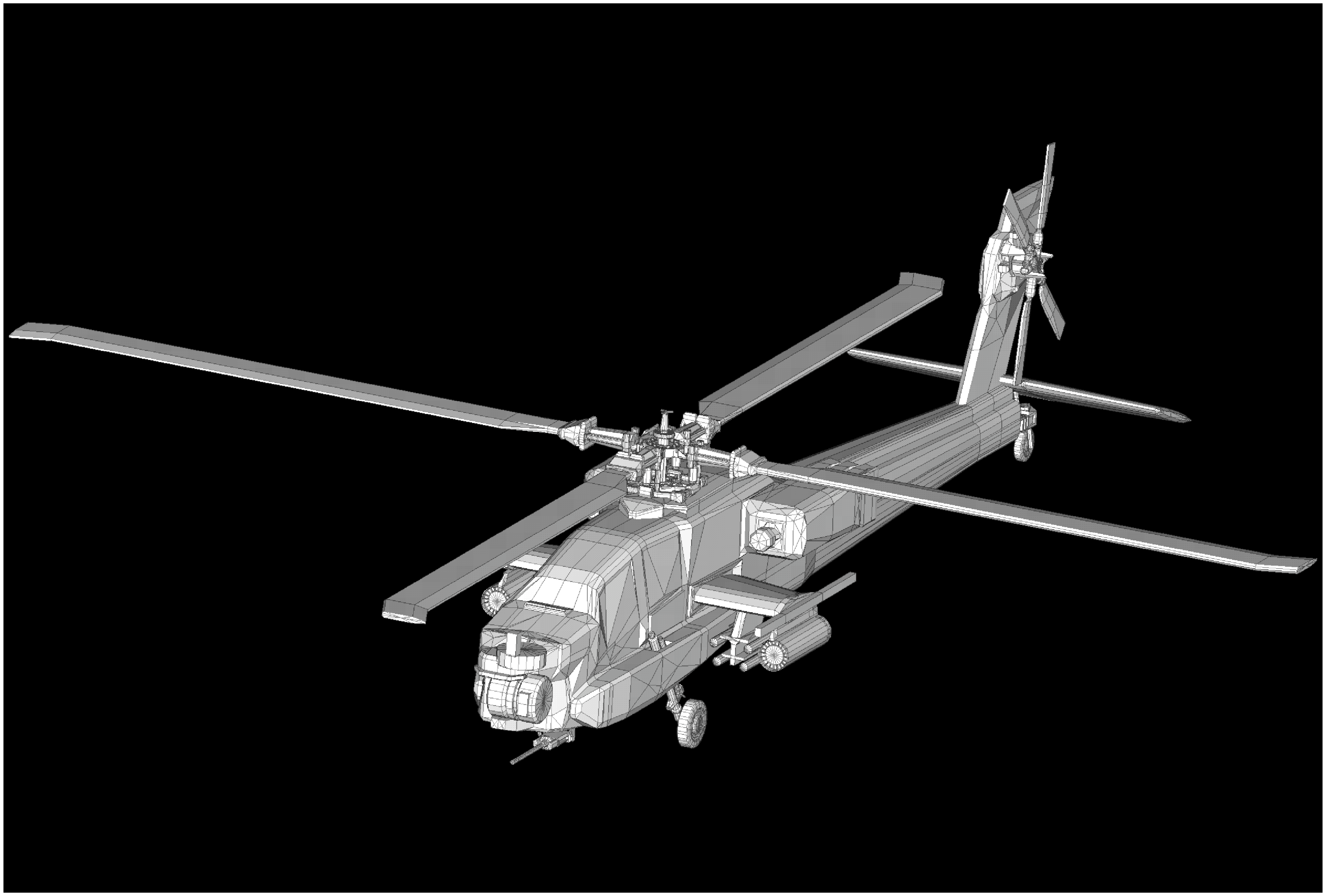
- On Variational Integrators:
  - Veselov [1988]
  - Moser and Veselov [1991]
  - Marsden and Wedlandt [1997]
  - Kane, Marsden, Ortiz [1999]
  - Marsden and West [2001]
  - Lew, Marsden, Ortiz, West [2003]
  - Fetecau, Marsden, Ortiz, West [2003]
  - Lew, Marsden, Ortiz, West [2004]
- Closely related:
  - Gonzalez and Simo [1996]
  - Gonzalez [1996]
  - Simo, Tarmow and Wang [1992]

Outline

First, some illustrative examples

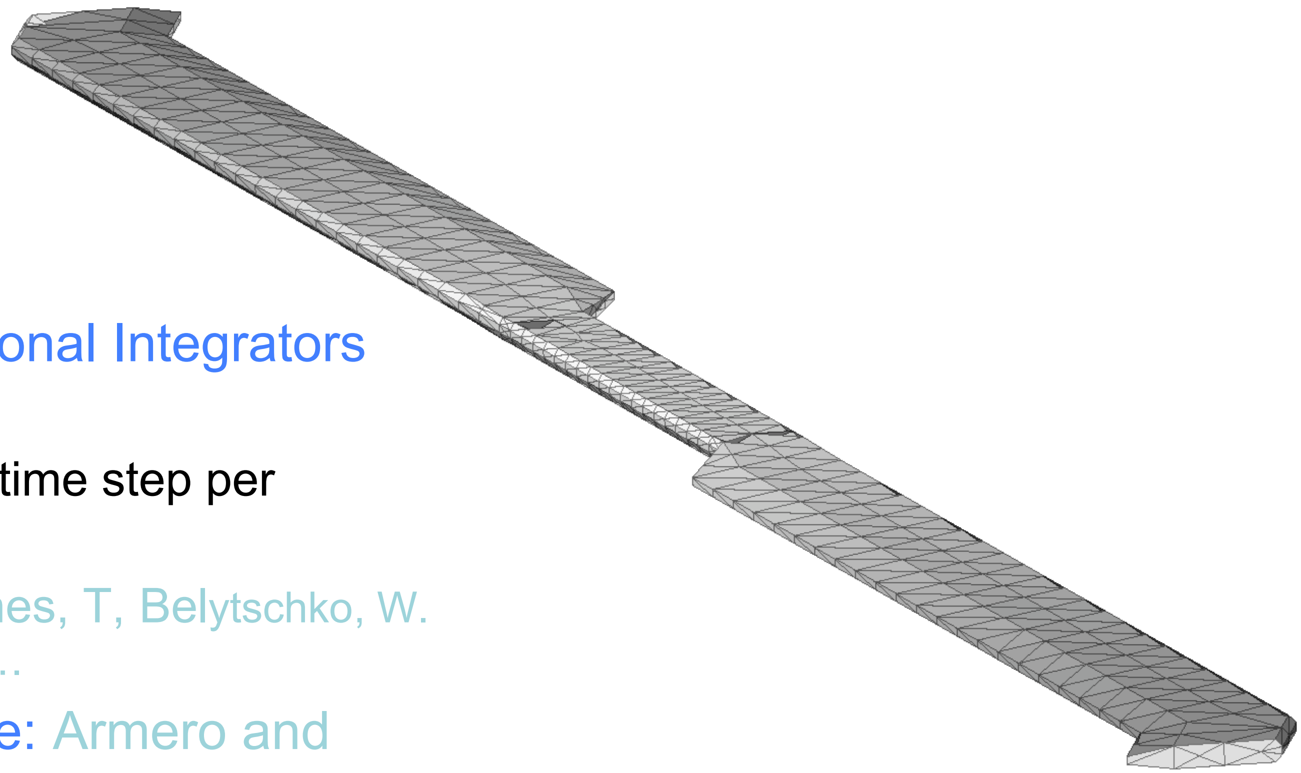
Then, the theory…..

Conservation Properties Example



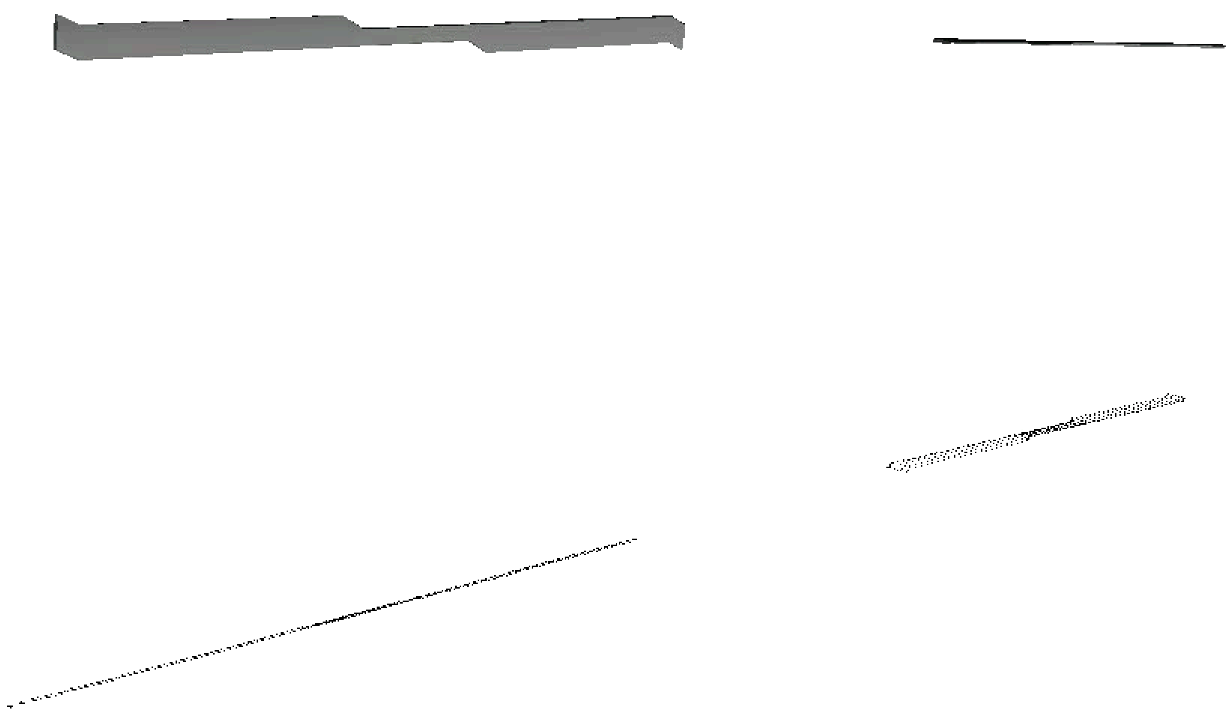
Apache AH-64

Helicopter Blades

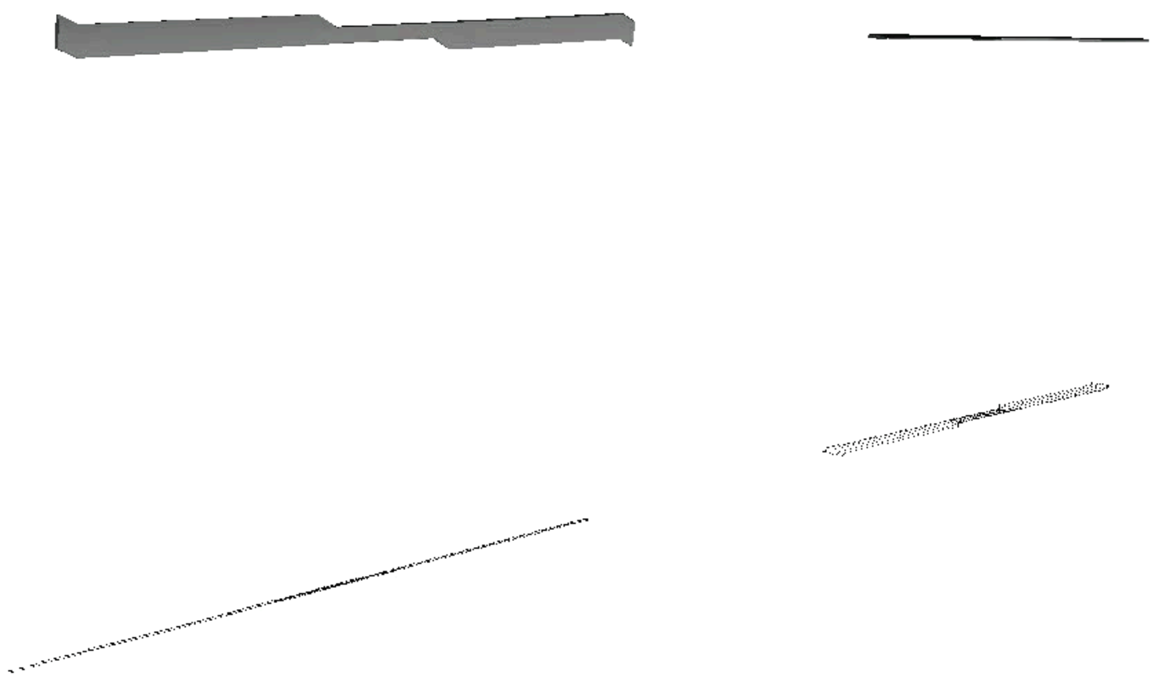


- Asynchronous Variational Integrators (AVI)
  - A possibly-different time step per element
  - Subcycling: T. Hughes, T, Belytschko, W. K. Liu, P. Smolinsky,….
- Classical test example: Armero and Romero[2001], Bottasso and Bauchau [2001]
- In Lew, Marsden, Ortiz and West [2004]

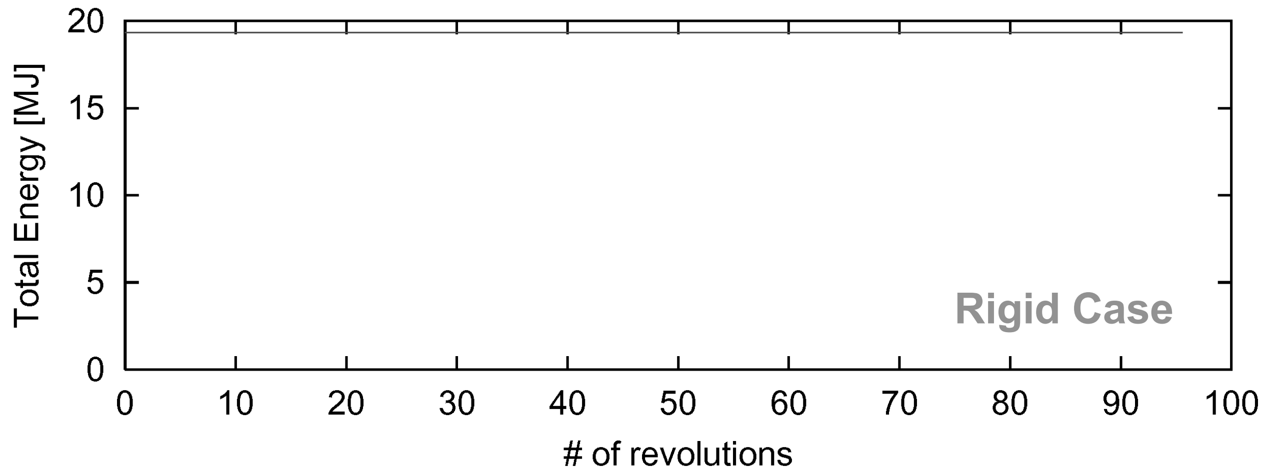
Rigid Case



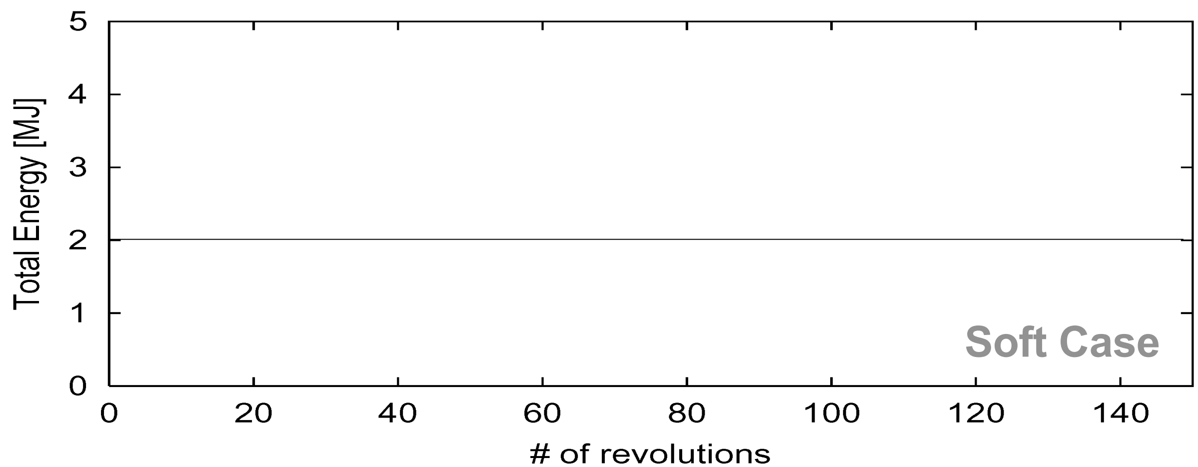
Soft Case



Energy conservation



Energy behavior characteristic
of Variational Integrators

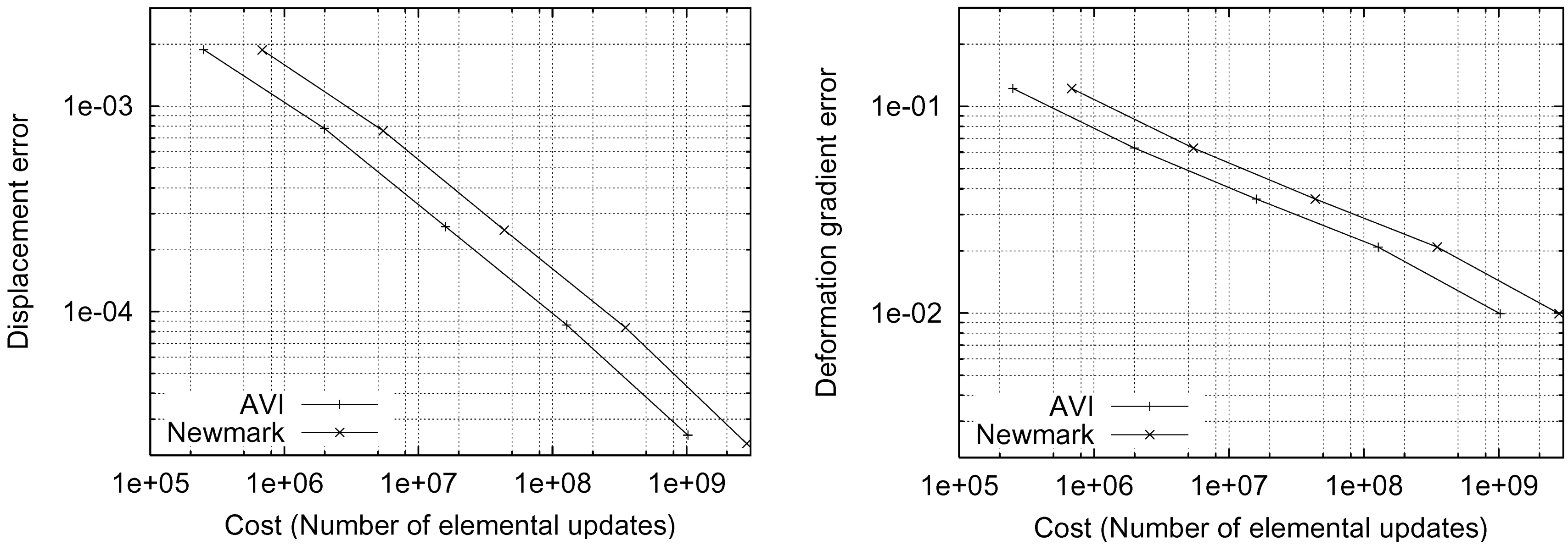


235 millions
updates of the
fastest element !

(Backward error analysis: Hairer and Lubich [2000], Neishtadt [1984])

Accuracy

- Convergence of AVIs proved in Lew, Marsden, Ortiz and West [2004].

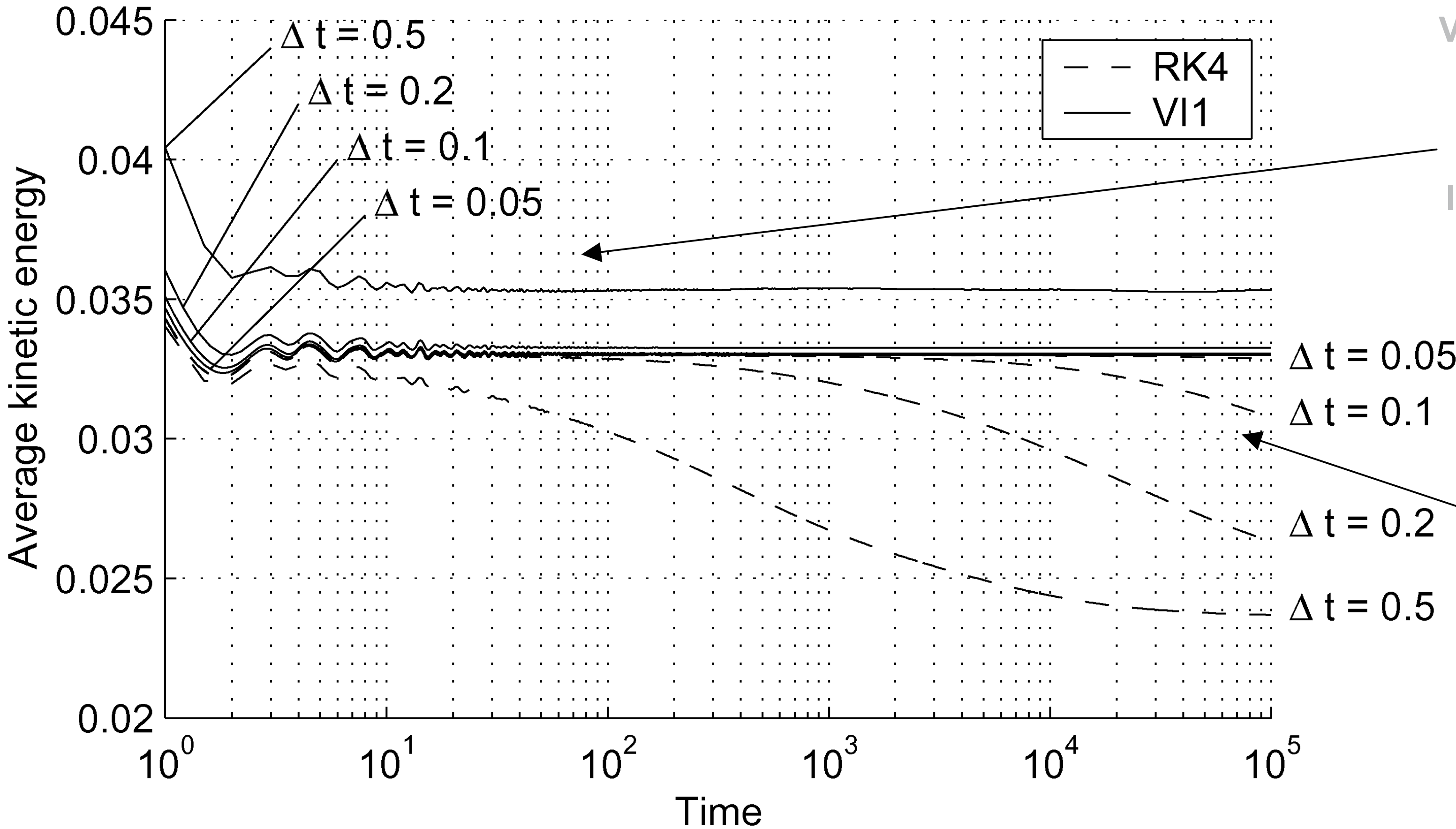


Convergence behavior of AVI

Computing what matters

- Get statistical quantities right, such as temperature, even in the face of chaotic dynamics and errors in the computation of individual trajectories
- ODE Example
  - Compute the temperature, time averaged kinetic energy, of a system of interacting particles in the plane.
  - System of 16 point masses, 4 x 4, in the plane joined by springs. The system starts from the regular configuration with random initial velocities.

Computing what matters



VI1 converges to the average kinetic energy even for fairly large time steps

RK4 suffers substantial numerical dissipationi

Average kinetic energy as a function of time and time step size for a 4th order non-symplectic Runge-Kutta and a 1st order variational integrator.

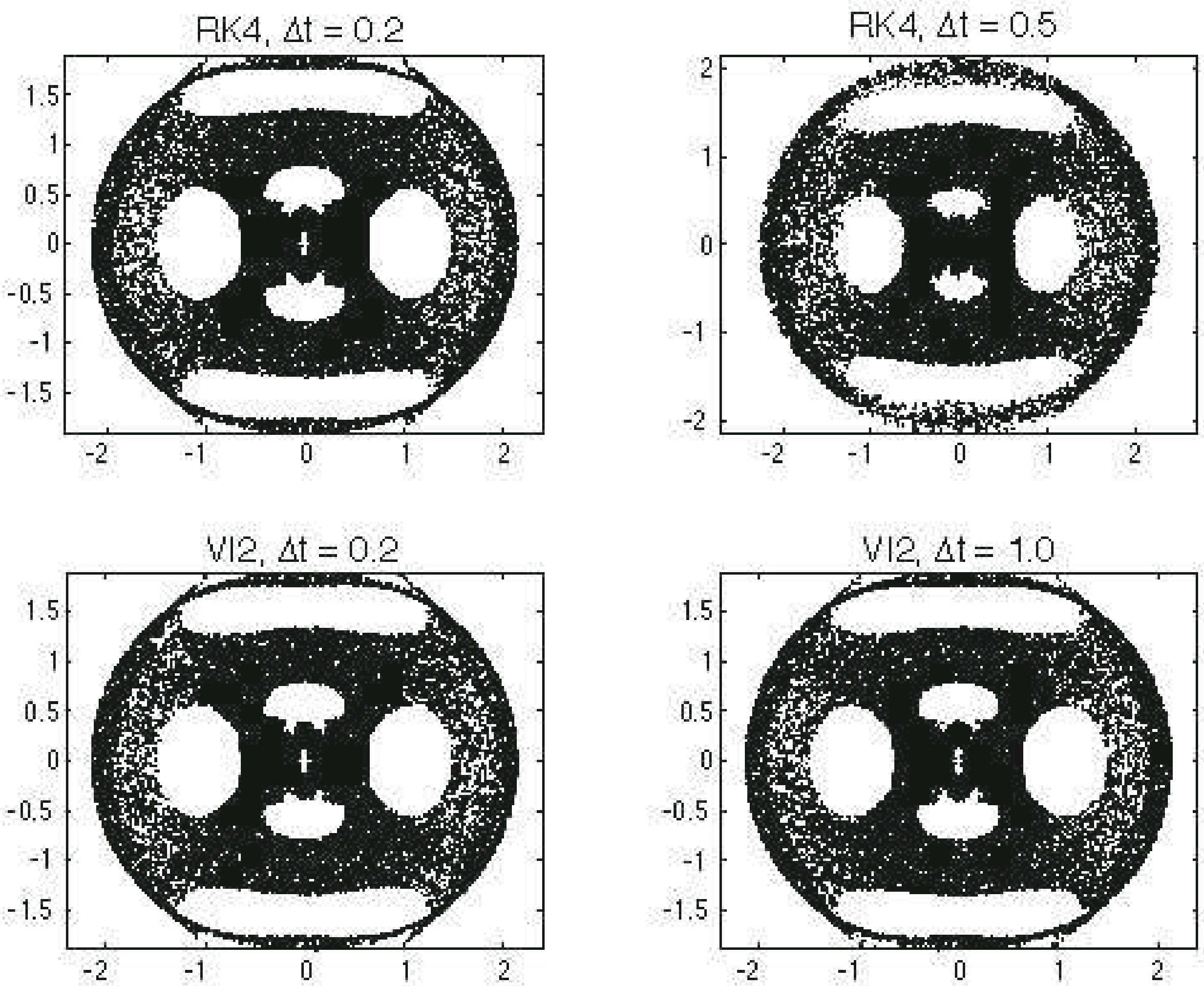
Computing what matters

Error due to the finite time averaging

VI4 is always better, and VI1 is better than RK4 for large time steps !

Temperature error as a function of computational cost comparison between a 1st(VI1) and 4th(VI4) order variational integrator and a 4th order non-symplectic Runge-Kutta (RK4). The three plots correspond to different averaging time lengths

Chaotic dynamics



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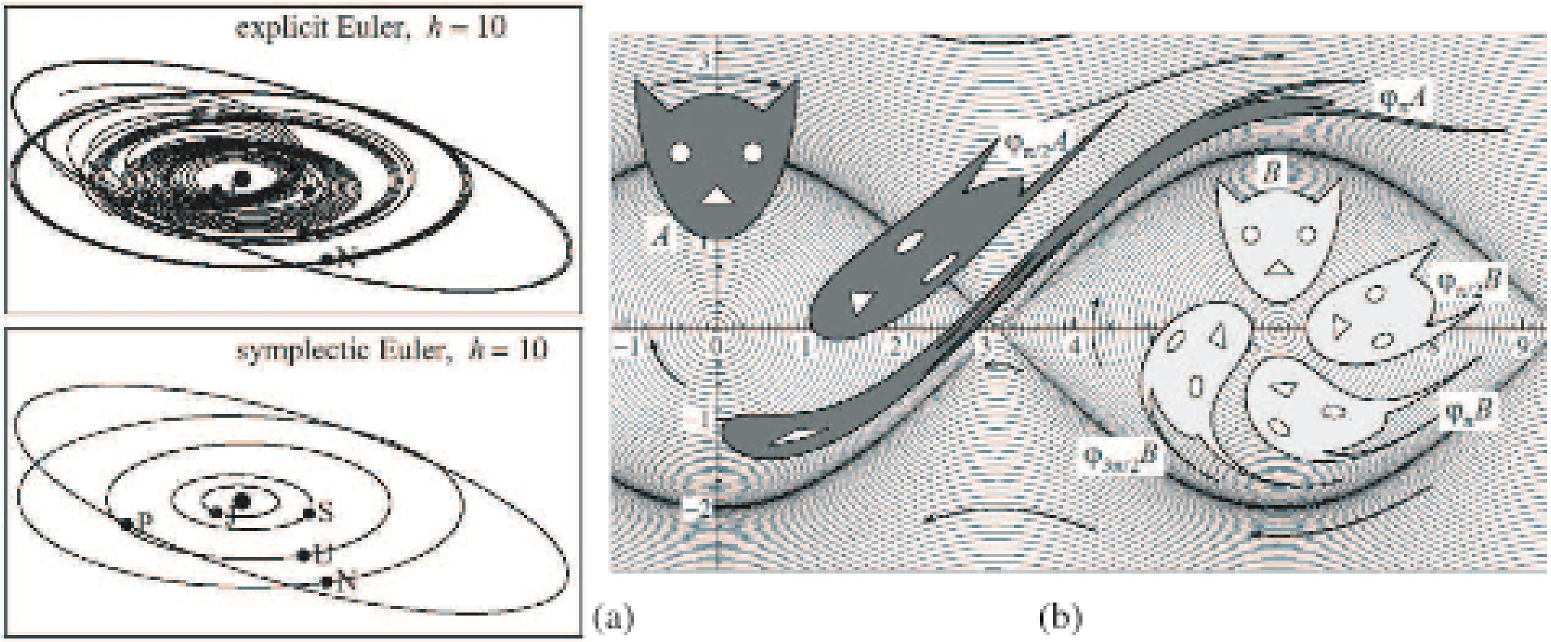
Symplecticity



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VI For Elastodynamics

Lagrangian mechanics

- Lagrangian density

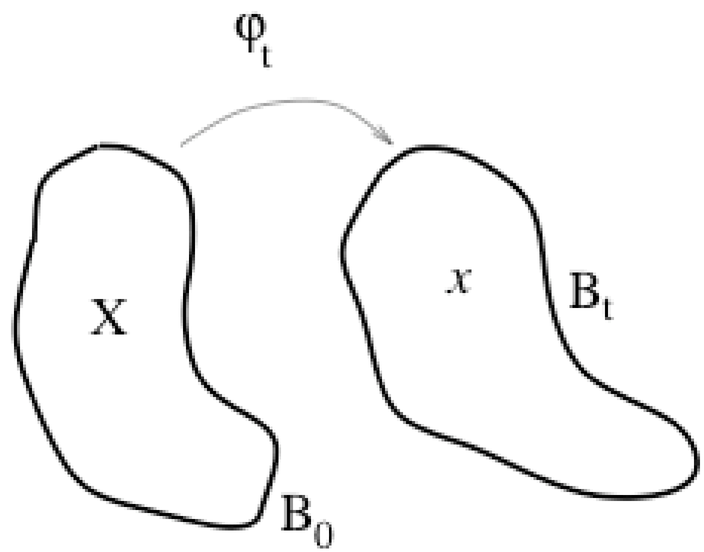
$$\mathcal{L}(\varphi, \dot{\varphi}) = \frac{1}{2}\rho_0|\dot{\varphi}|^2 - W(\nabla_X \varphi)$$

- Action

$$S[\varphi] = \int_{B_0 \times (t_i, t_f)} \mathcal{L}\, dt\, dX$$

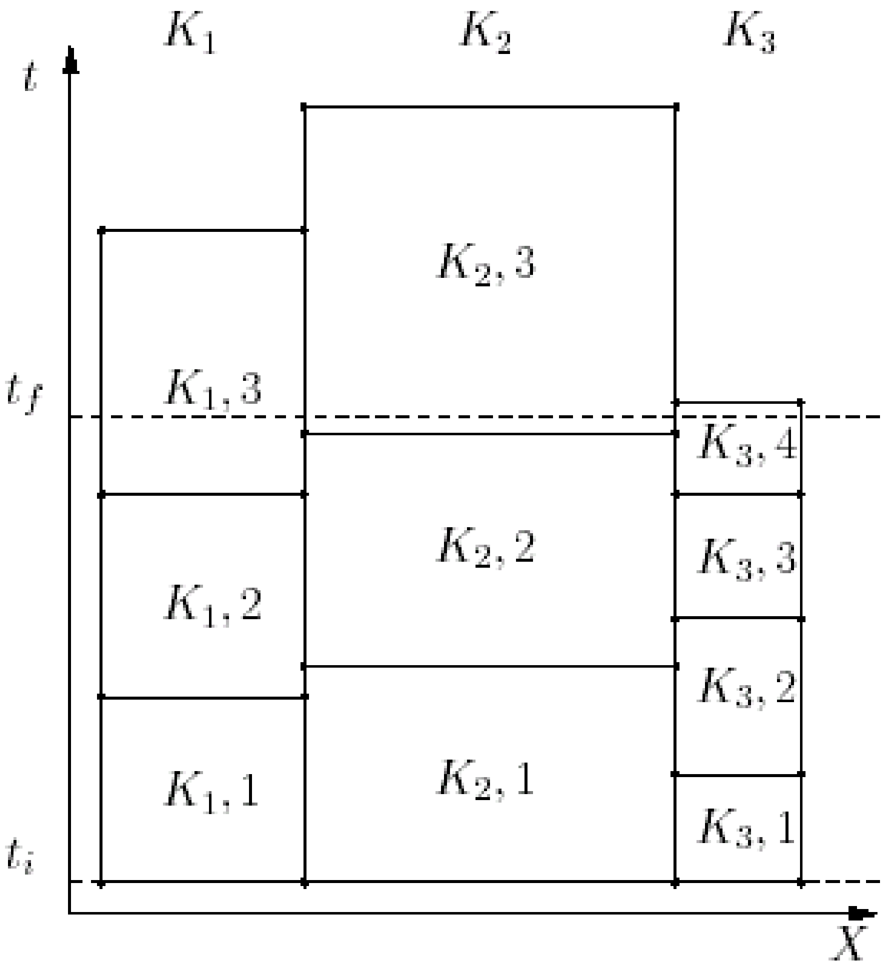
- Hamilton's variational principle

$$\delta S = 0$$



- Same formulation for Electromagnetism, Fluids, General Relativity, etc.

Variational Formulation



- Discrete Lagrangians

$$L_d^{K,j} \approx \int_{K,j} \mathcal{L} \, dt dX$$

- Discrete Action Sum

$$S_d = \sum_{K,j} L_d^{K,j}$$

Variational Formulation

- Discrete Variational Principle:

"The discrete motion renders the Discrete Action Sum stationary with respect to admissible spatial variations of the nodal trajectories"

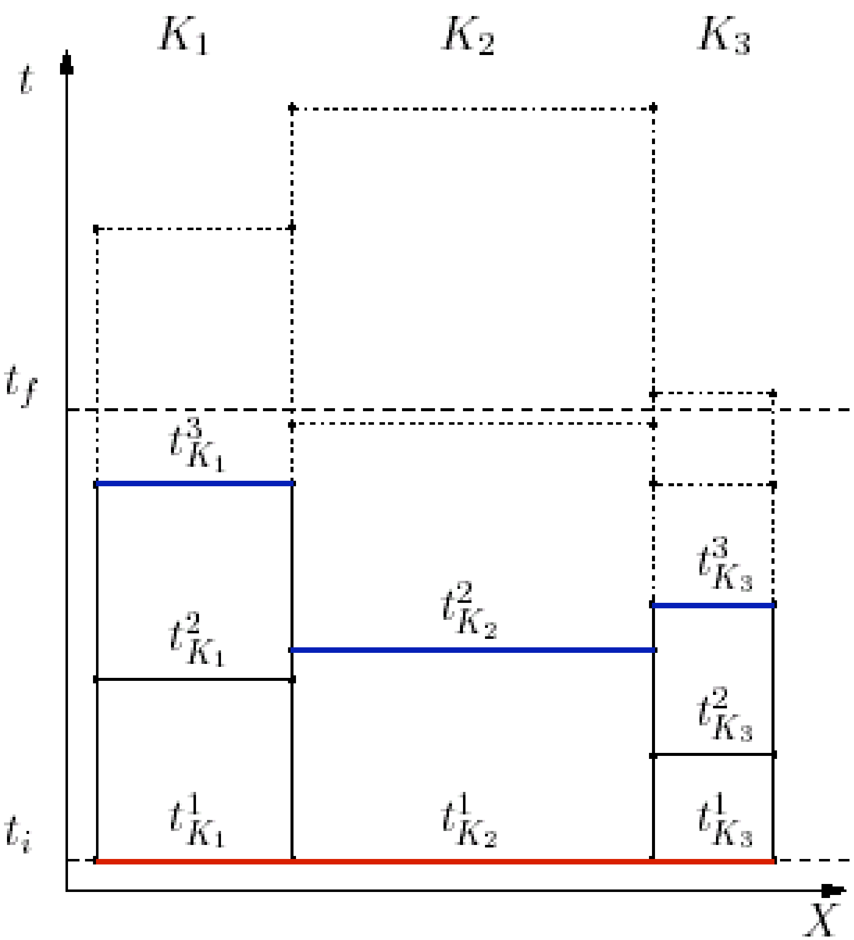
More precisely,

Discrete Euler-Lagrange equations

$$D_{a,i} S_d = 0 \qquad \forall \boldsymbol{x}_a^i \in \mathcal{X}_{admissible}$$

This is the algorithm !

Conservation Properties



- Disc. Linear Momentum

$$S_d(\mathcal{X} + \boldsymbol{v}) = S_d(\mathcal{X})$$

$$\Downarrow$$

$$\sum_{x_{i,a} \in \mathcal{X}} D_{i,a} S_d(\mathcal{X}) = 0$$

$$\Downarrow$$

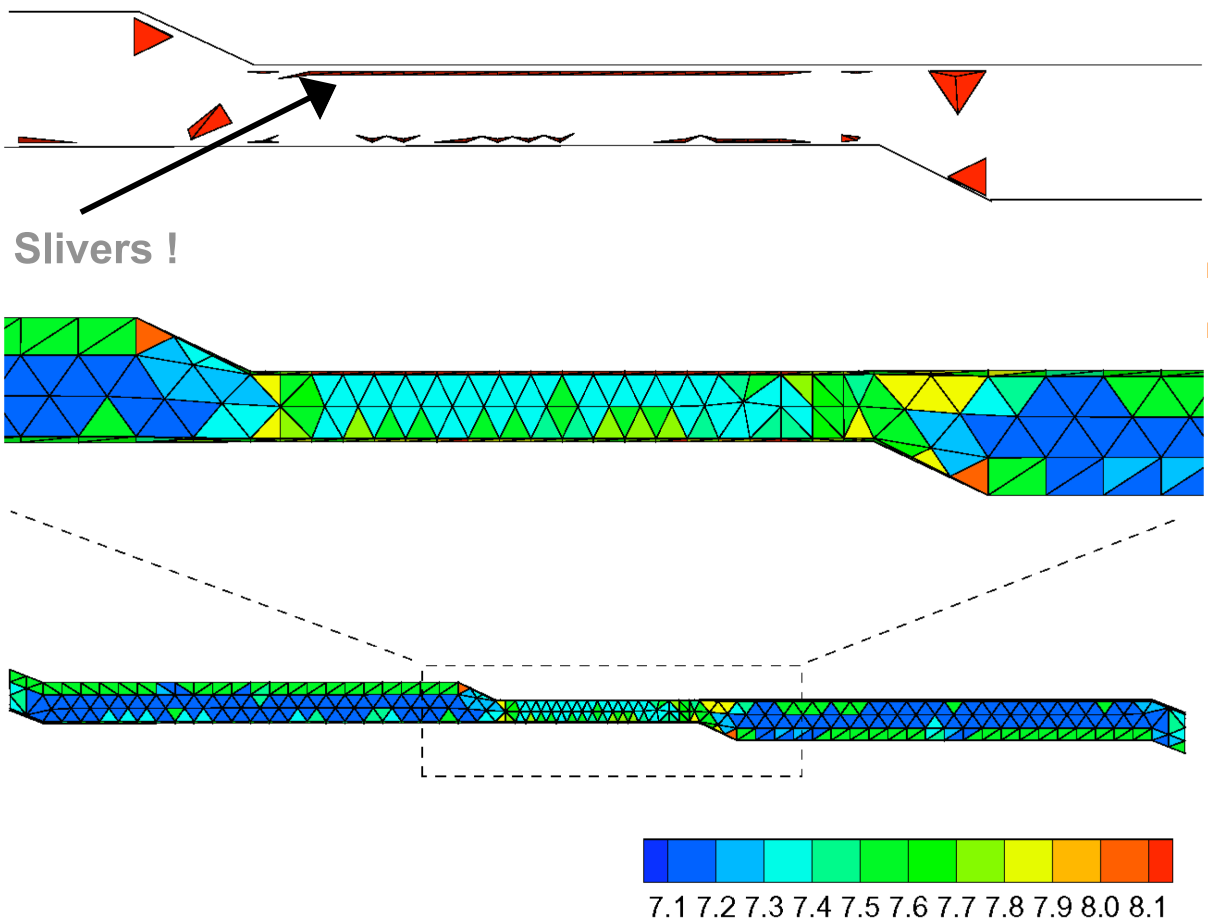
DEL equations, N.B.C

$$-\sum_{x_{i,a} \in \mathcal{X}_r} D_{i,a} S_d = \sum_{x_{i,a} \in \mathcal{X}_b} D_{i,a} S_d$$

- Disc. Angular Momentum

This is the discrete Noether's theorem !

Number of Updates

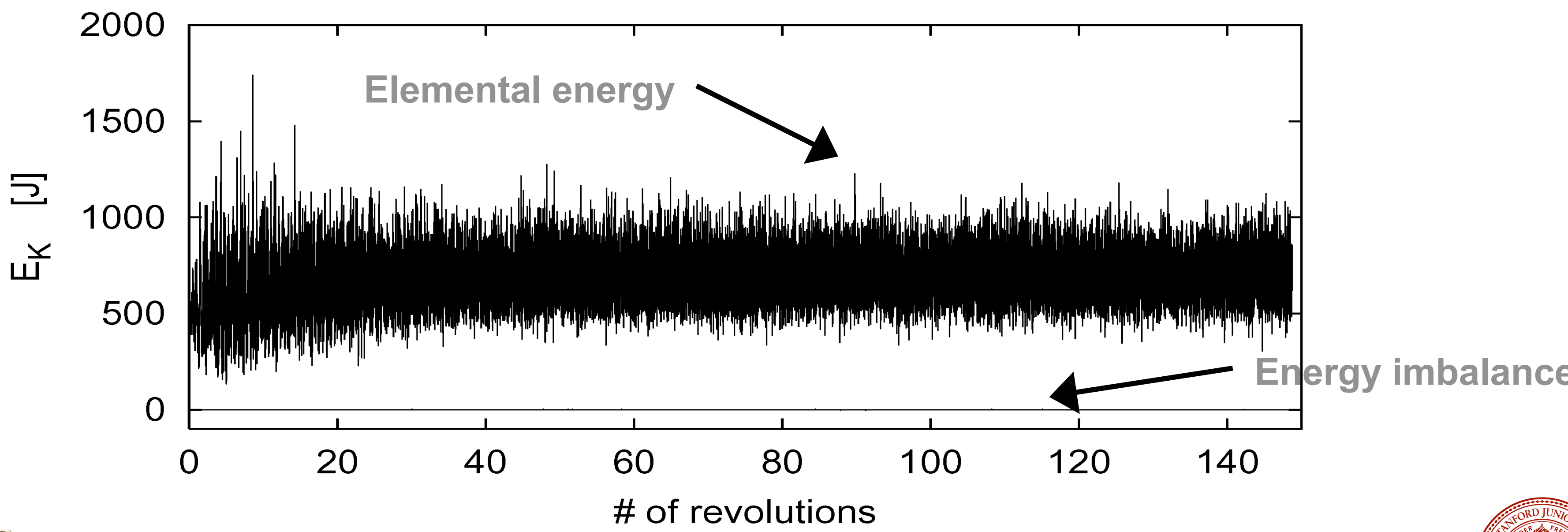


- 10-node tets, *slivers !*
- Speed-up ≈ 6

Contour plot of log(number of updates) for each element after 150 revolutions

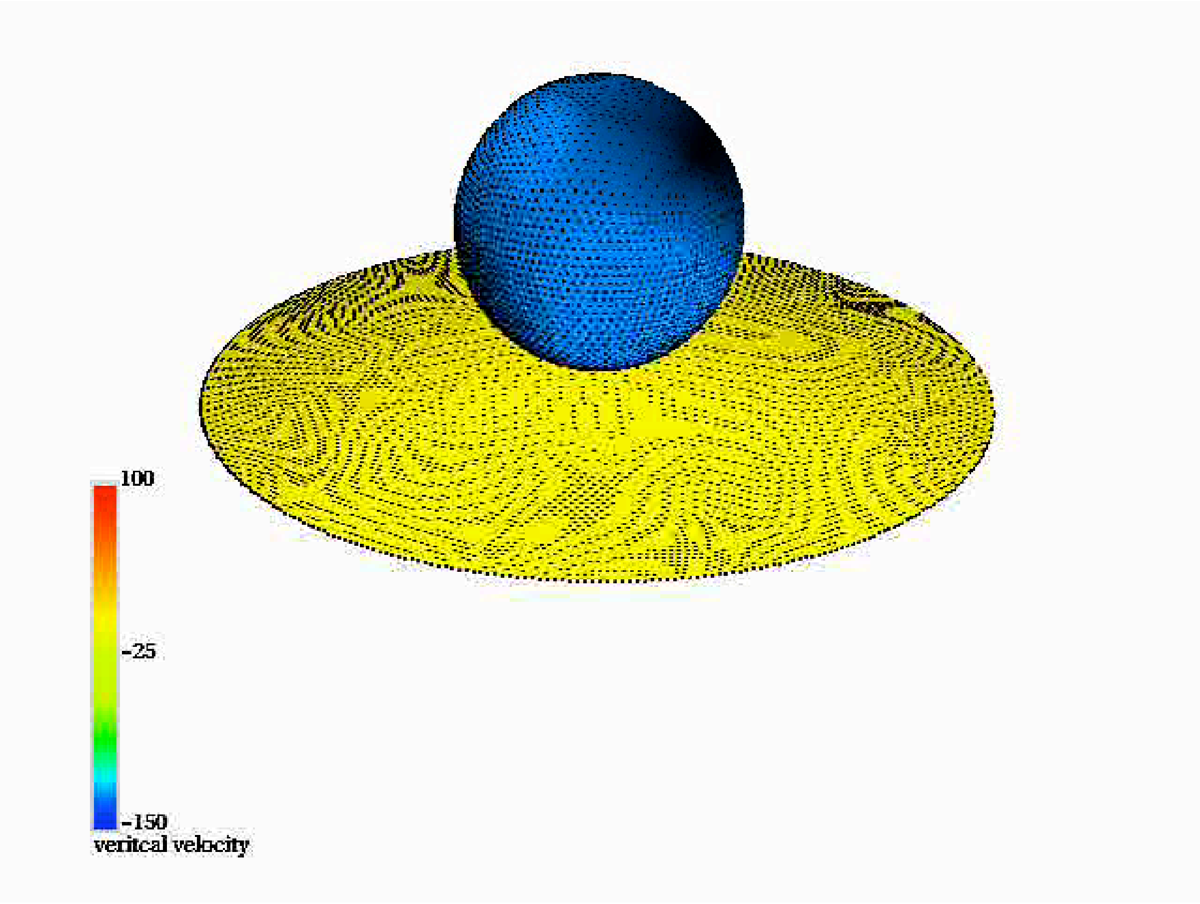
Local Energy Behavior

- A local energy balance equation is obtained as the Euler-Lagrange equation conjugate to the elemental time step.
- Local energy conservation and time-adaptivity



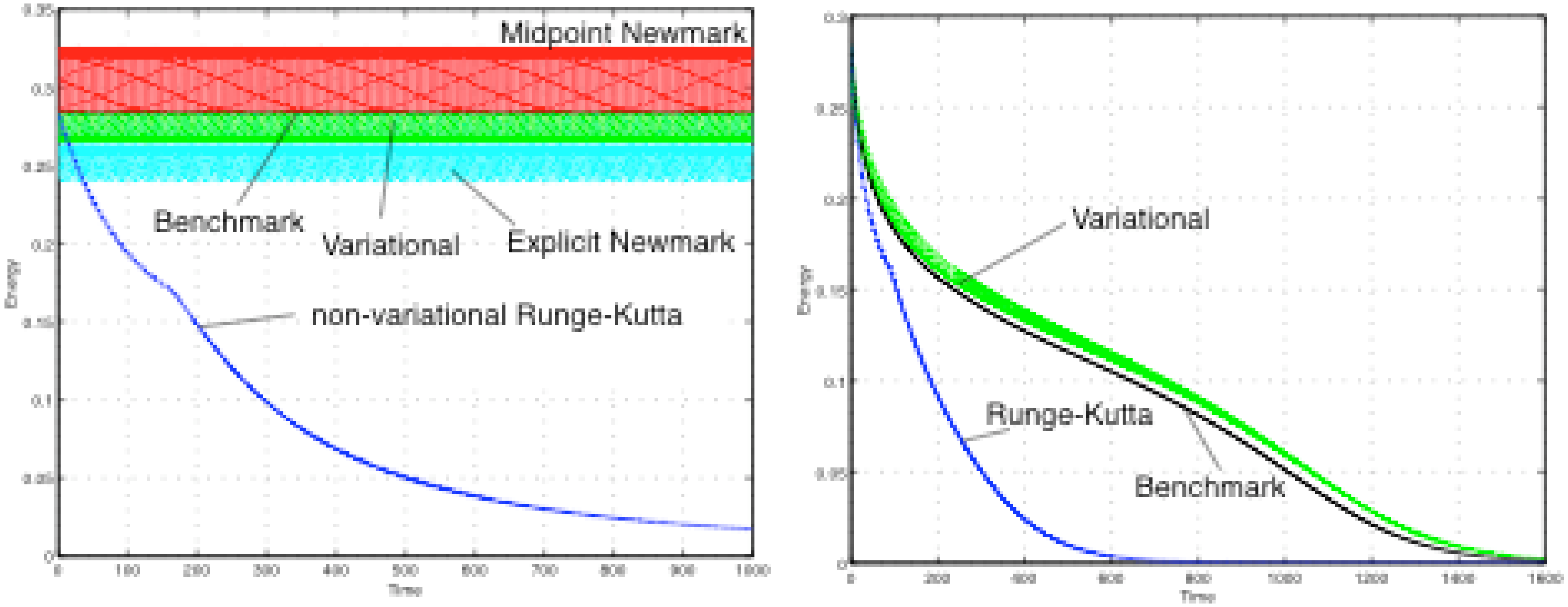
Examples: Collision

- Some remarks about the formulation



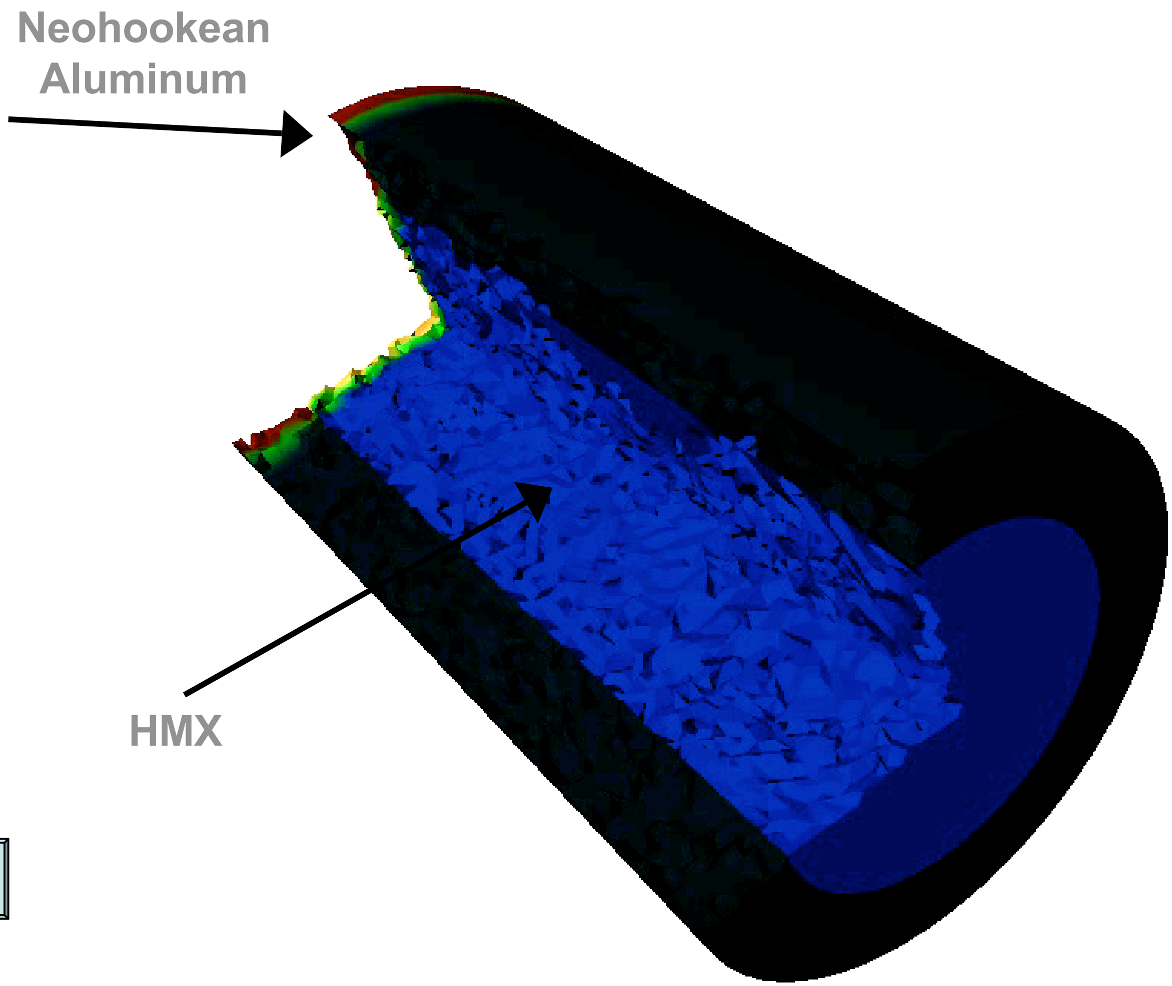
Example: Dissipative systems

- Lagrange-d'Alembert pple.
- Weak dissipative systems



(a) Conservative mechanics (b) Dissipative mechanics

Contained Detonation



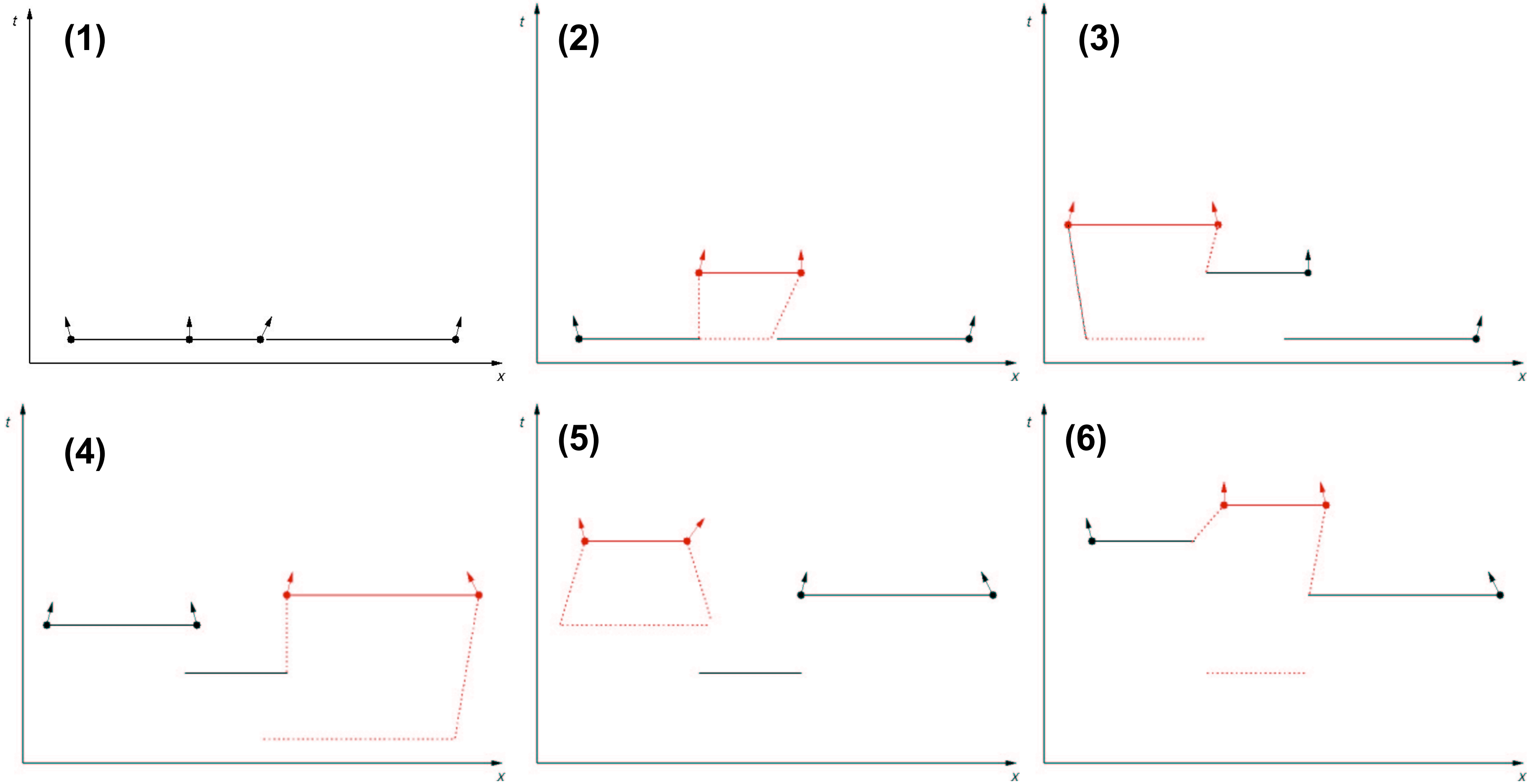
- Impact velocity

  2170 m/s
- Multiphysics
- AVI

Impact problem on a Canister with HMX

The End

AVI in a nutshell



One-dimensional example of AVI