Asynchronous simulation of high-explosive detonations

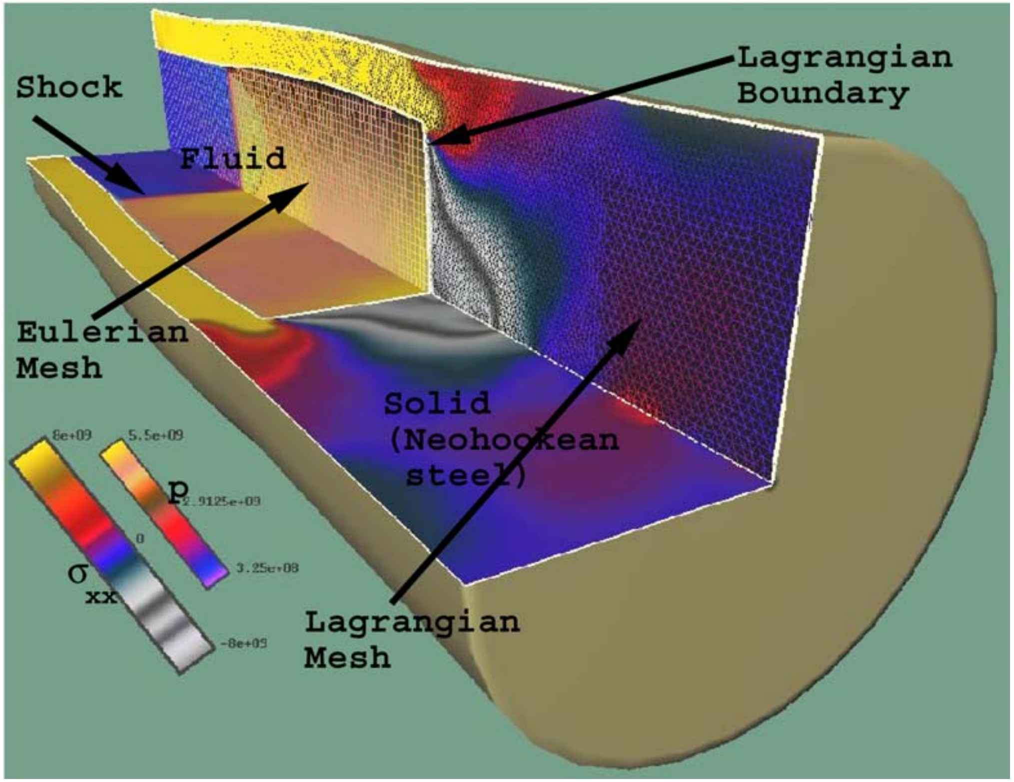
Adrián J. Lew
Graduate Aeronautical Laboratories, Caltech

April 2003

Jointly with: J. Marsden, M. Ortiz, M. West

Outline

- Asynchronous Variational Integrators (AVI)
- Artificial Viscosity for largely deforming shocked solids
- Detonation front simulation with AVIs

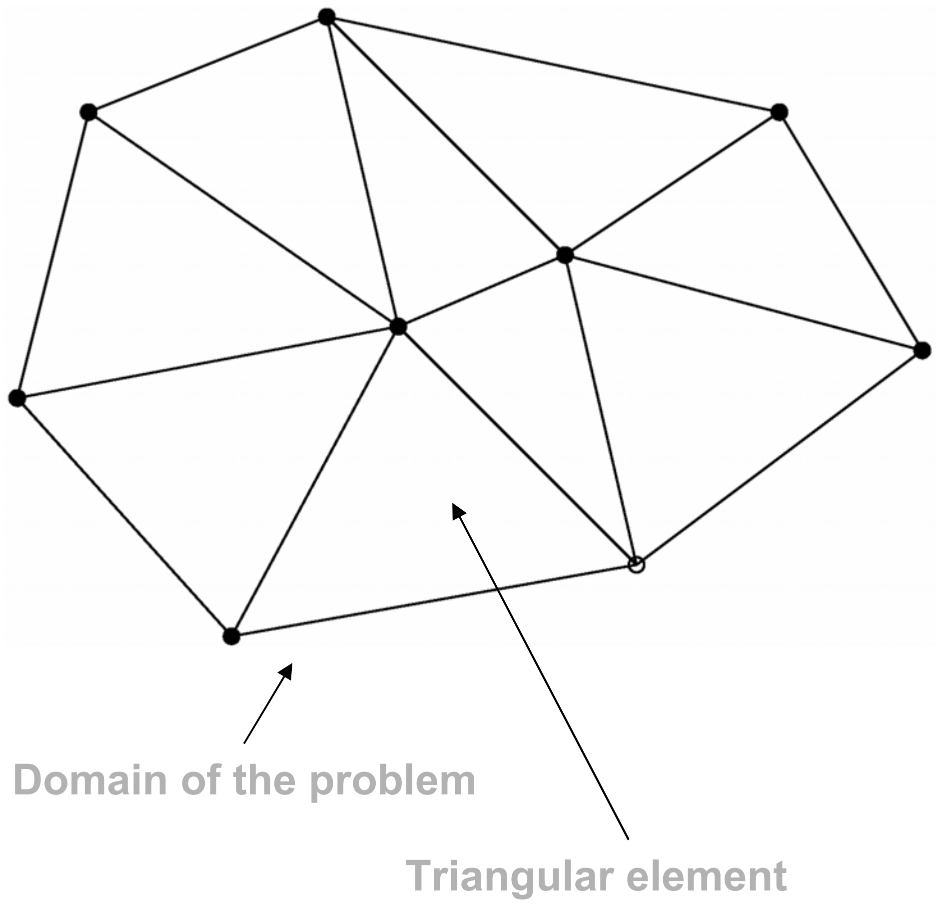


Asynchronous Variational Integrators

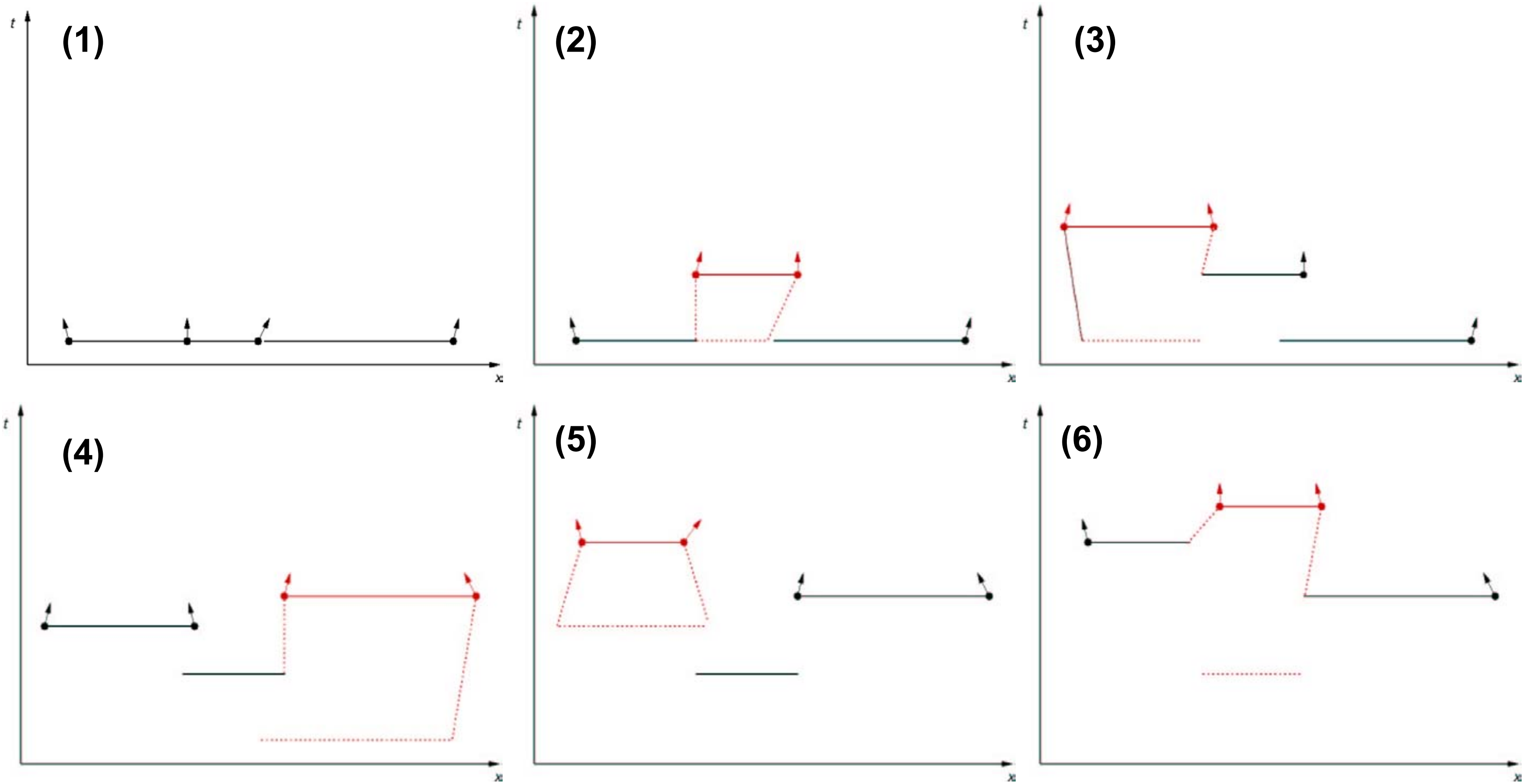
- Advance in time complex systems with multiple time scales
- Algorithms are derived from a variational principle
- Remarkable conservation properties
  - There is a discrete Noether's theorem
    - Symplectic-energy-momentum preserving
- Examples:
  - Finite Elements:
    - Allow elements to progress asynchronously
    - In the spirit of subcycling and element-by-element algorithms
  - Molecular Dynamics:
    - Multi-time step methods
    - Allow group-wise interactions to advance asynchronously

Finite elements at a glance

- Steps
  - Decompose the domain of the problem into elements (triangles, tetrahedra, etc)
  - Associate to each node a basis function $N_a(x)$
  - Construct the functional space V_h containing all linear combinations of $N_a(x)$
  - Seek solutions satisfying a constrained variational principle in V_h
- Example
  - In an elasticity problem, the unknowns are the displacements, which belong to the space V_h

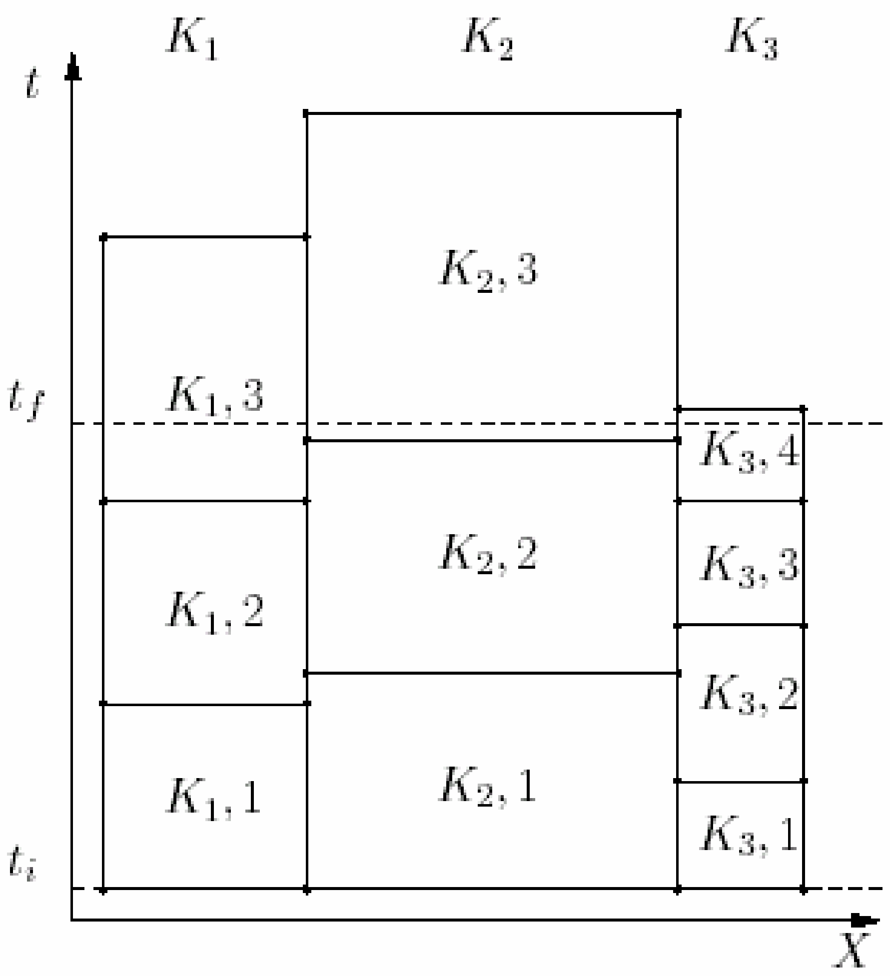


AVI in a nutshell



One-dimensional example of AVI

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

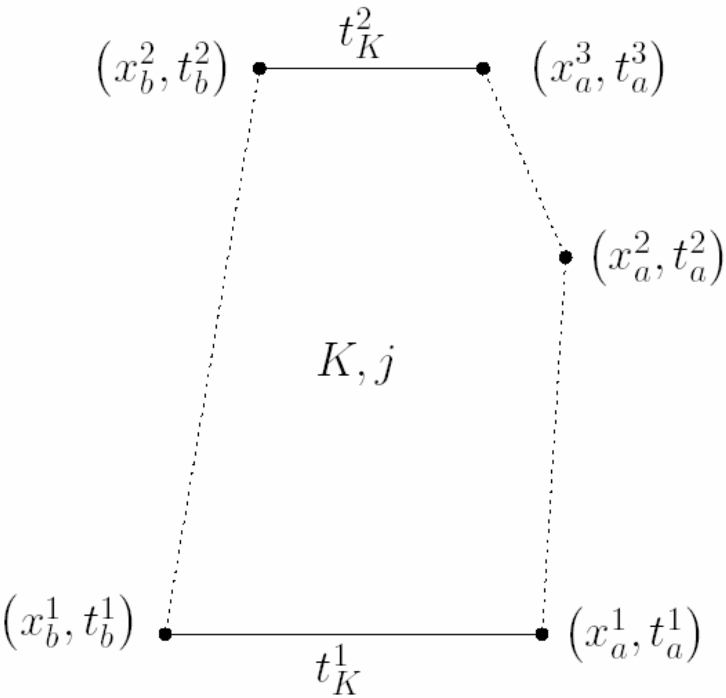
$$D_{a,i} S_d = 0 \qquad \forall \boldsymbol{x}_a^i \in \mathcal{X}_{admissible}$$

This is the algorithm !

Example

- Choose Discrete Lagrangians

$$L_d^{K,j} = \frac{1}{2m_{a,K}} \left| \boldsymbol{p}_{a,K}^{3/2} \right|^2 \left(t_a^2 - t_a^1 \right) + \frac{1}{2m_{a,K}} \left| \boldsymbol{p}_{a,K}^{5/2} \right|^2 \left(t_a^3 - t_a^2 \right) + \frac{1}{2m_{b,K}} \left| \boldsymbol{p}_{b,K}^{3/2} \right|^2 \left(t_b^2 - t_b^1 \right) - \Phi_K \left[\boldsymbol{\varphi}_h \left(t_K^2 \right) \right] \left(t_K^2 - t_K^1 \right)$$

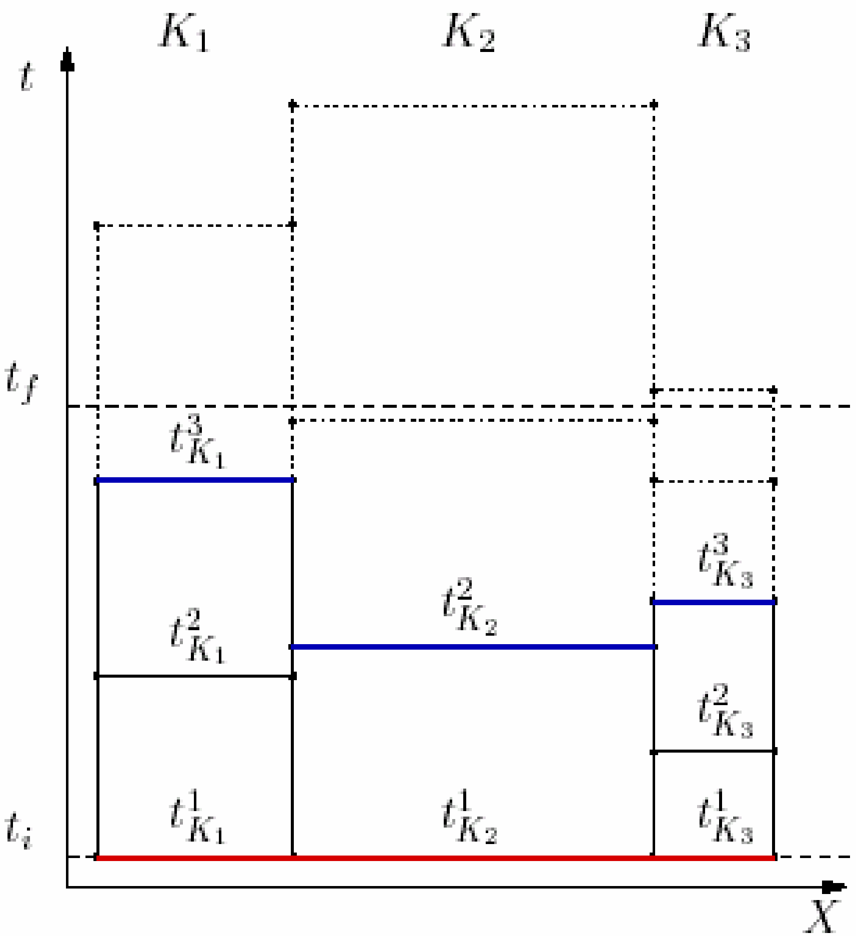


where

$$\boldsymbol{p}_{a,K}^{i+1/2} = m_{a,K} \frac{\boldsymbol{x}_a^{i+1} - \boldsymbol{x}_a^i}{t_a^{i+1} - t_a^i}$$

$$\Phi_K \left[\boldsymbol{\varphi}_h \right] = \int_K W(\nabla_0 \boldsymbol{\varphi}_h)\, dV + \textbf{f.t.}$$

Conservation Properties



- Disc. Linear Momentum

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

$$\Downarrow$$

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

$$\Downarrow$$

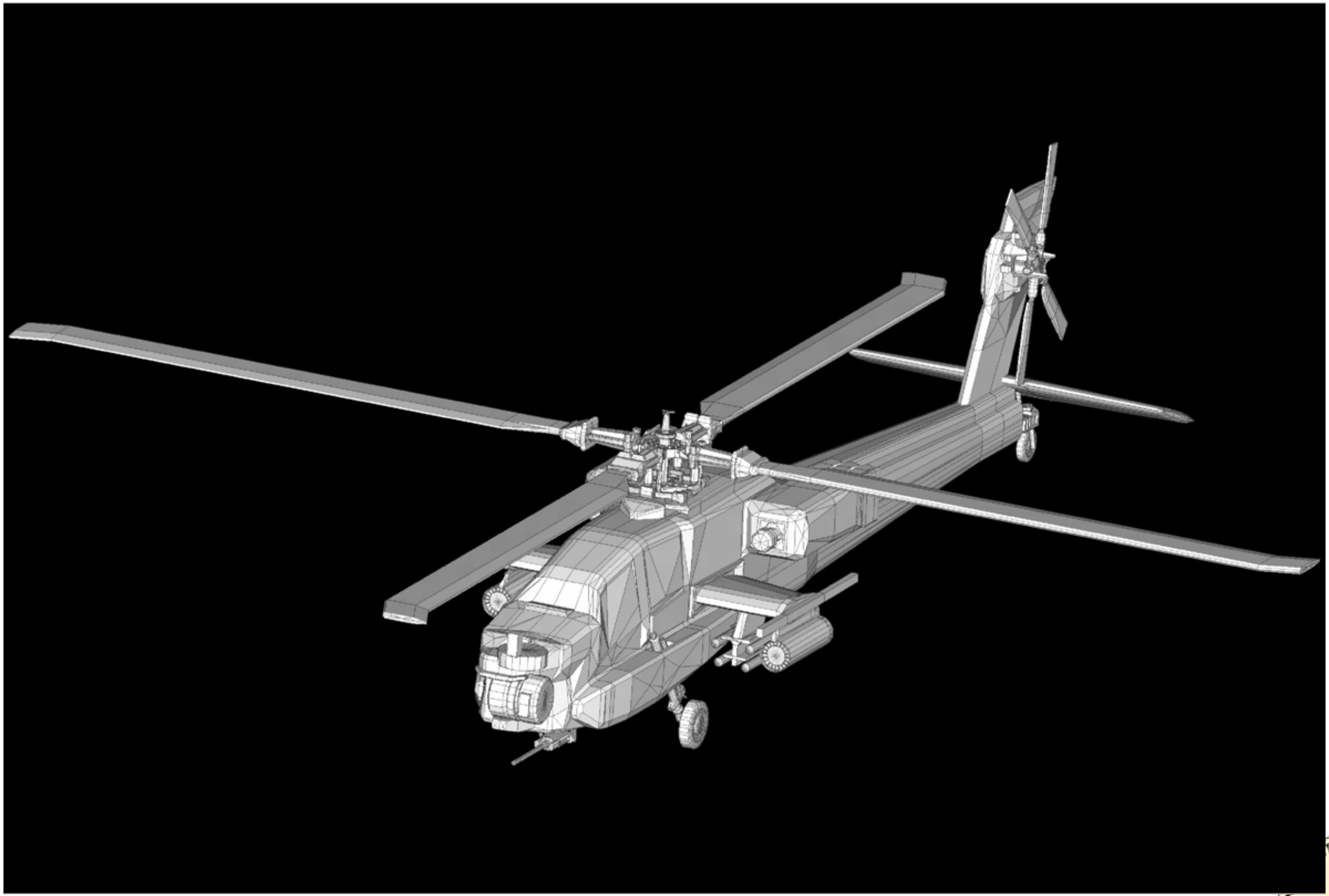
DEL equations, N.B.C

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

- Disc. Angular Momentum

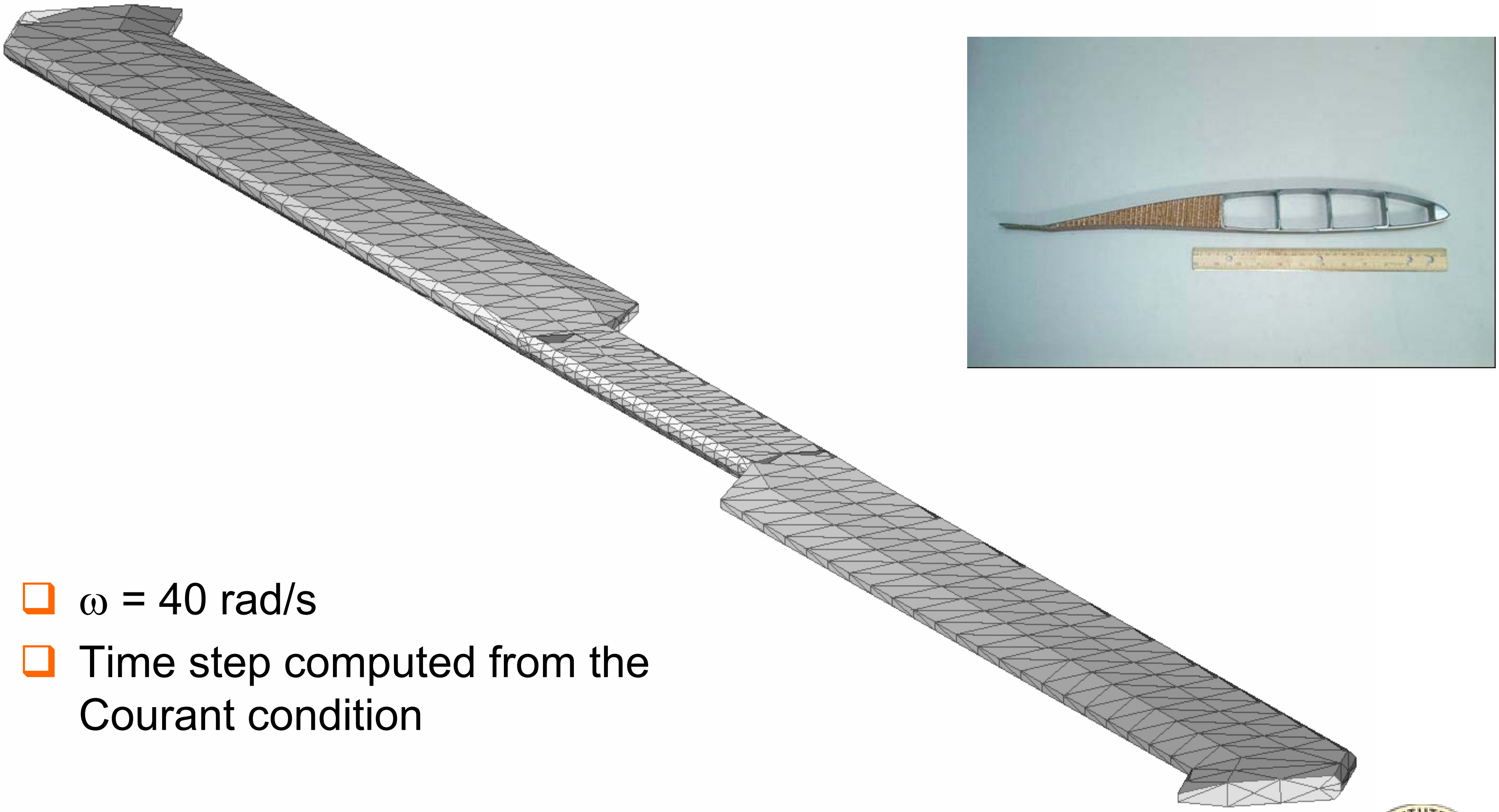
This is the discrete Noether's theorem !

Structural Dynamics Example



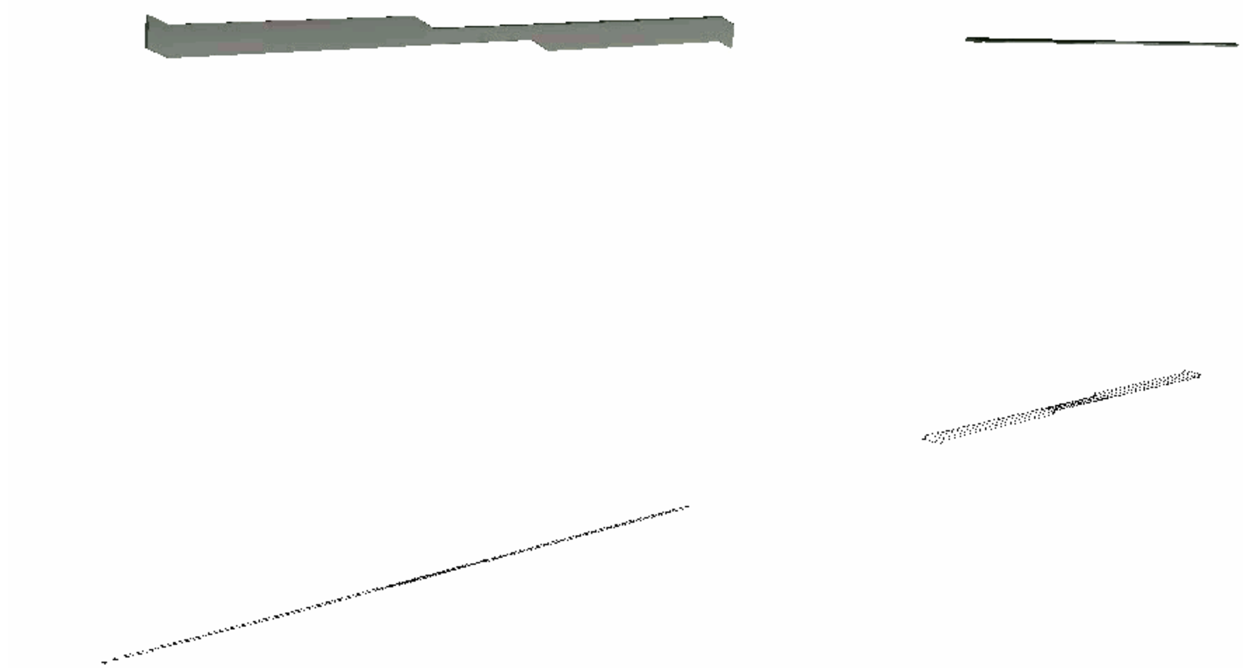
Apache AH-64

Helicopter Blades

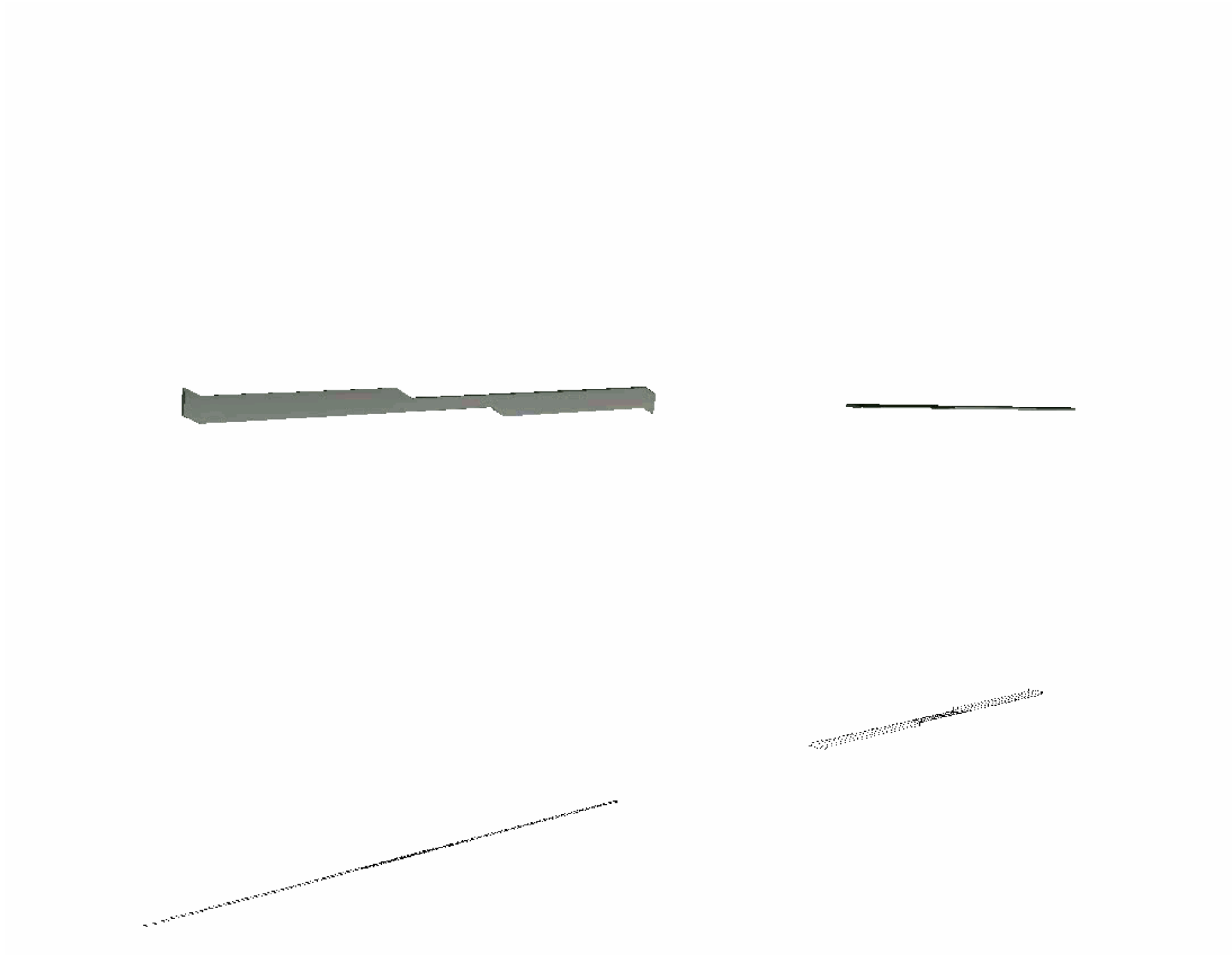


- ω = 40 rad/s
- Time step computed from the Courant condition

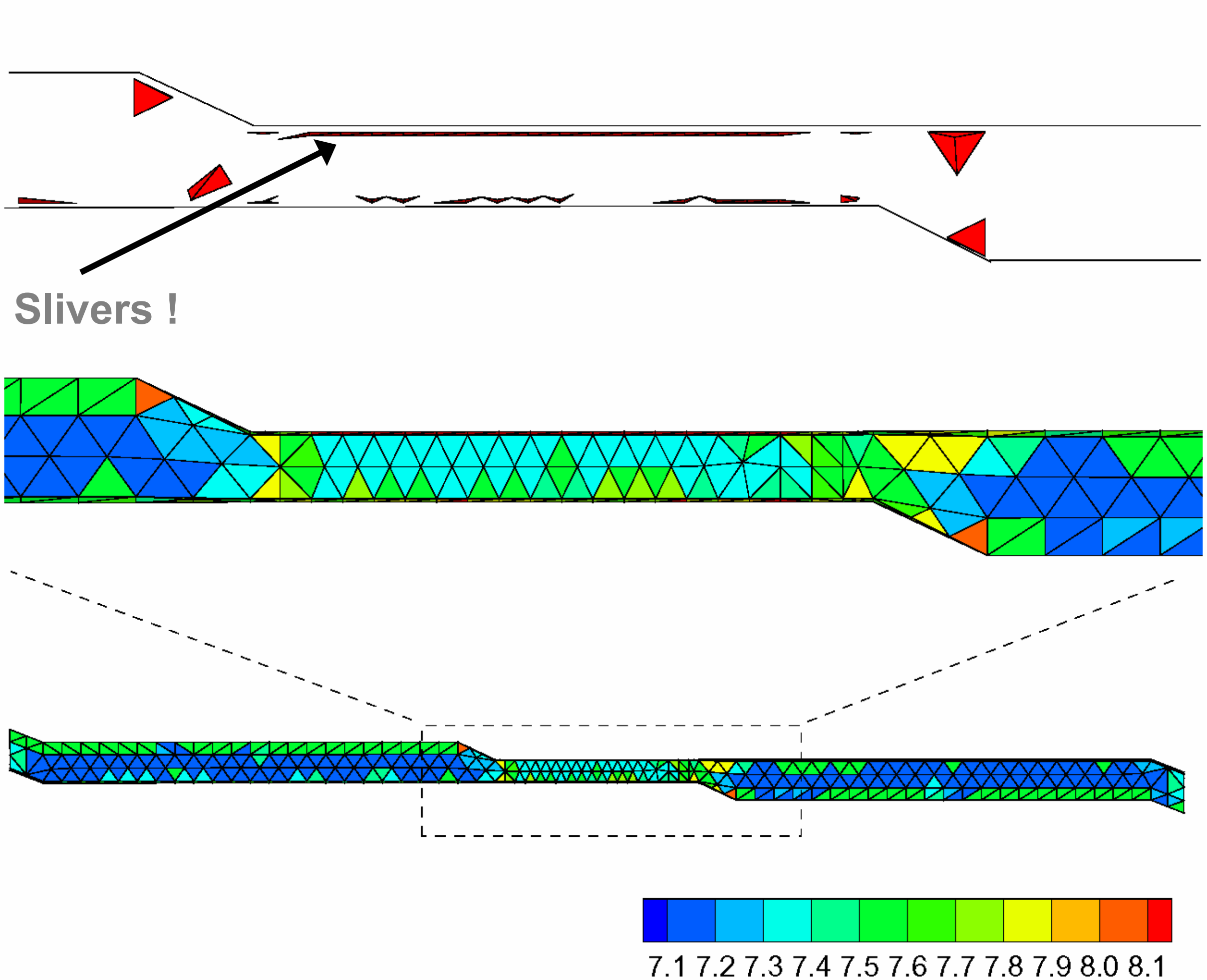
Rigid Case



Soft Case



Number of Updates



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

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

Symplectic Flow

- Every variational time integrator is symplectic
- Continuous case – Free Action Variations

Action → $$S(q(t)) = \int_0^t L(q,\dot{q})\,dt$$

Free Action variations → $$dS(q(t))\cdot\delta q(t) = \int_0^t \left(\frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i}\right)\delta q^i dt + \underbrace{\frac{\partial L}{\partial \dot{q}^i}\delta q^i}_{\Theta_L\cdot\delta q}\Big|_0^t$$

Zero over trajectories (the term $\frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i}$ inside the integral)

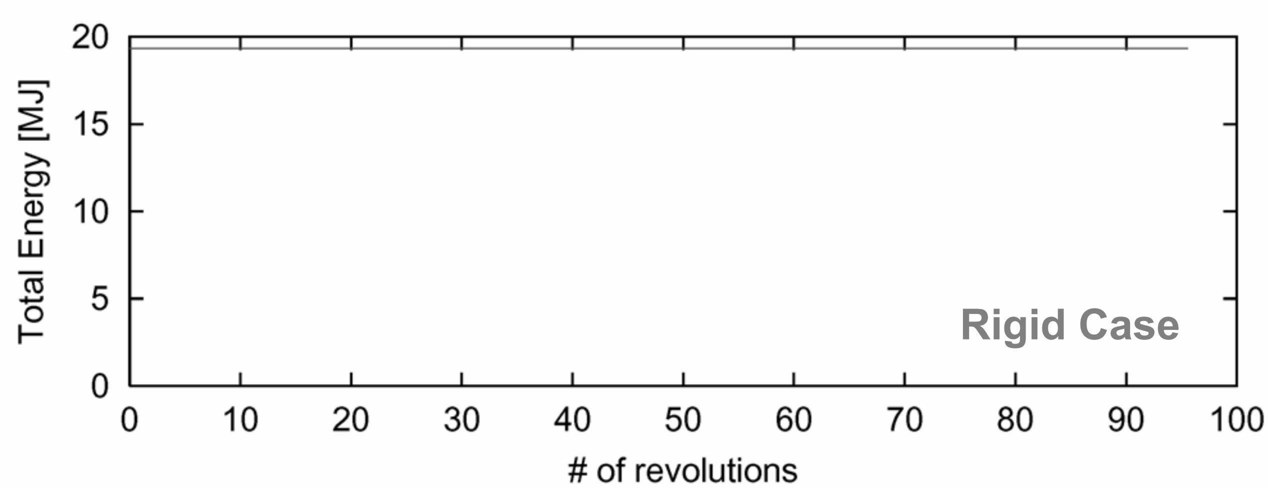
$$d^2 S = 0 \Longrightarrow \underbrace{d\Theta_L\cdot\delta q(t)}_{F_t^* d\Theta_L\cdot\delta q(0)} = d\Theta_L\cdot\delta q(0)$$

Symplectic form ($d\Theta_L$)

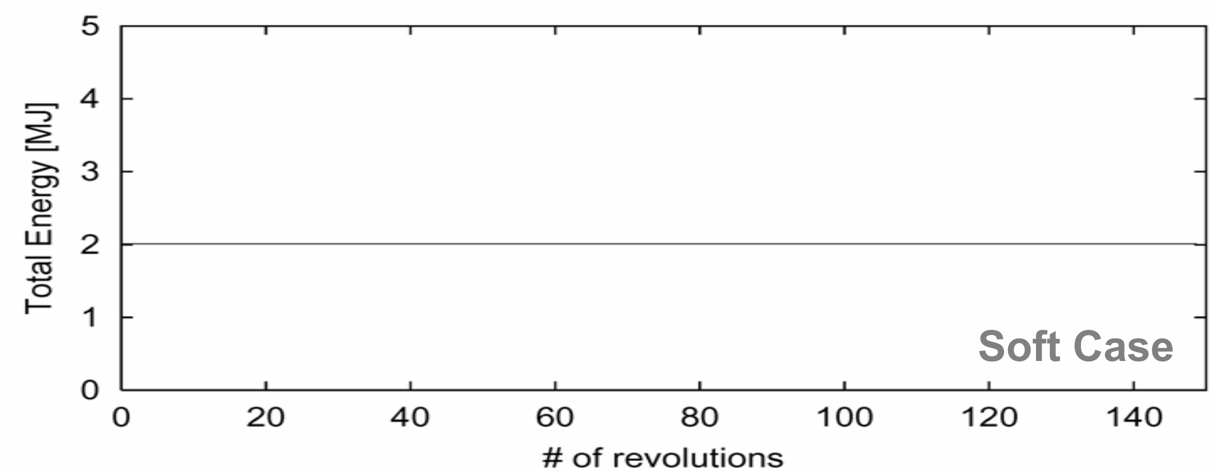
Canonical one-form (Θ_L)

- Discrete case - Free discrete action variations
- Consequences
  - Liouville's theorem, good long-time energy behavior

Energy conservation



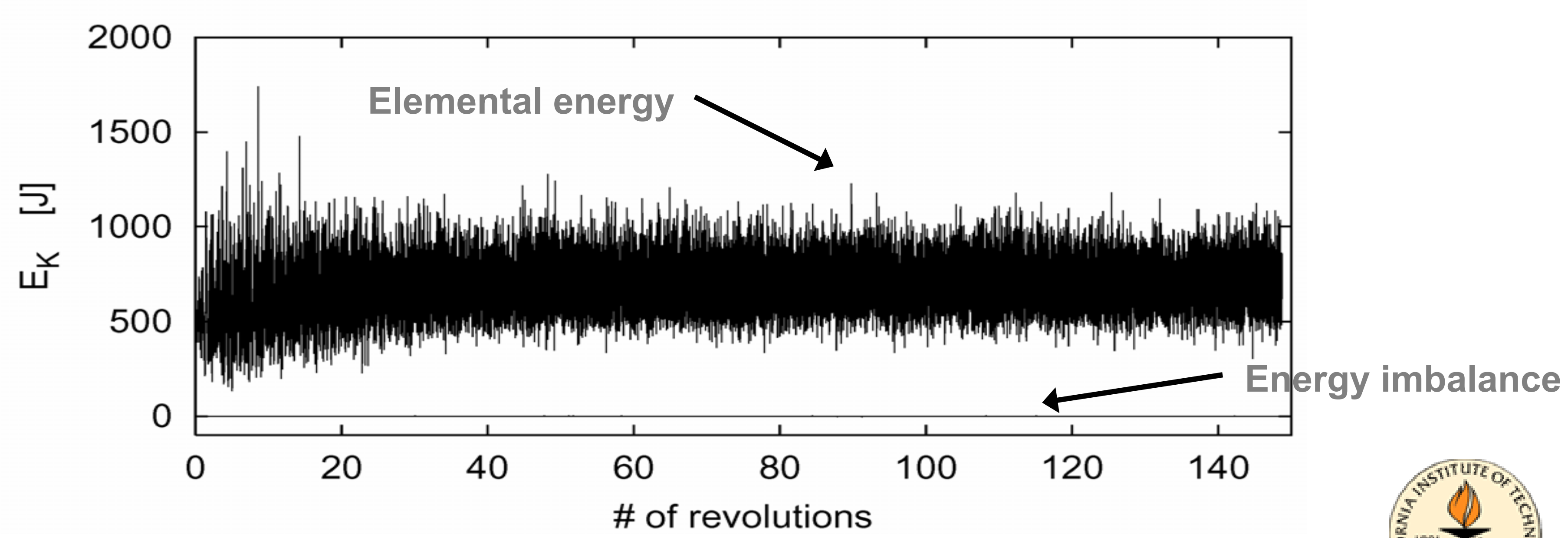
Characteristic energy behavior
of Variational Integrators



235 millions
updates of the
fastest element !

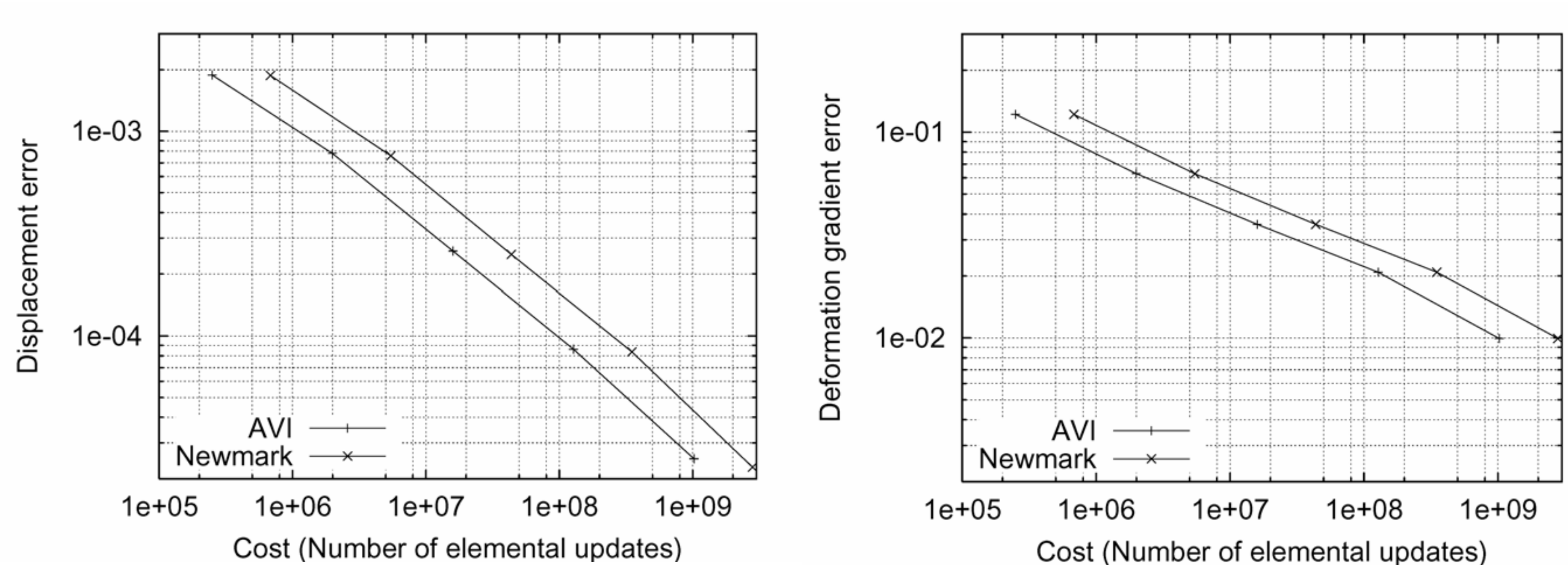
Local Energy Behavior

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



Convergence

- Convergence of AVIs proved in Lew, Marsden, Ortiz and West (2003), to appear in IJNME (West).



Convergence behavior of AVI

Configurational Forces

- Configurational forces are derivatives of the energy with respect to changes in the configuration of the mechanical system
  - Crack propagation, phase transformations
- Invariance of the elastic energy under rigid translations and rotations of the particles in the reference configuration leads to the path independent J-integral and L-integral respectively
- Discrete case
  - Configurational forces are conjugate to the positions of the nodes in the mesh
  - Resulting algorithms lead to variational mesh adaption (Thoutireddy and Ortiz, 2003)
  - Discrete Noether's theorem define discrete path independent J and L integrals

Discrete Conserved J-Integral

- Ω_g is the shaded domain.

Set of nodal coordinates

$$I_g[\varphi_h, \mathbb{X} + \boldsymbol{v}] = I_g[\varphi_h, \mathbb{X}]$$

This is S_d

$$\Downarrow$$

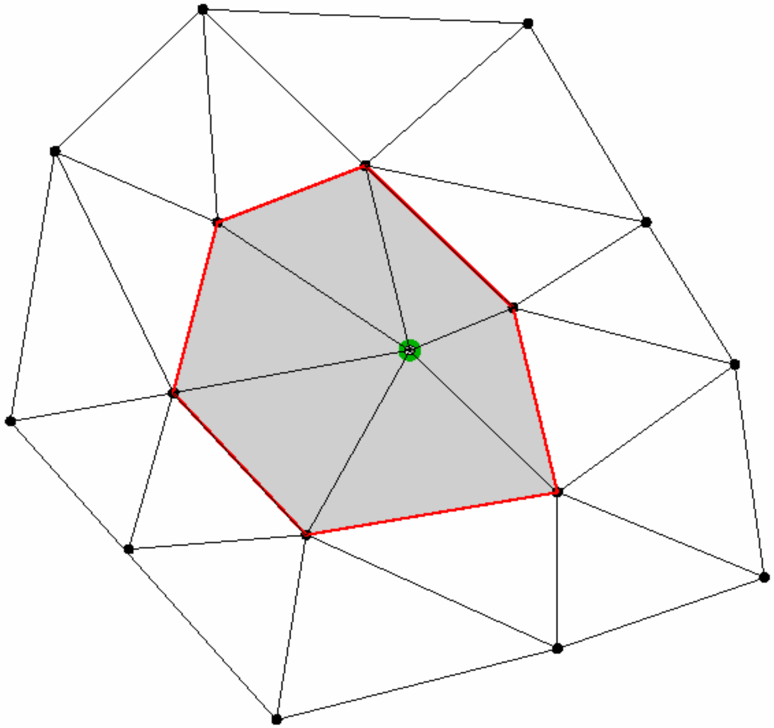
$$\sum_a D_{X_a} I_g = 0$$

VALE (Thoutireddy and Ortiz, 2003)

$$\text{But } D_{X_a} I_g = 0 \text{ if } X_a \in \mathring{\Omega}_g$$

$$\Downarrow$$

$$\sum_{a \in \partial\Omega} D_{X_a} I_g = 0$$



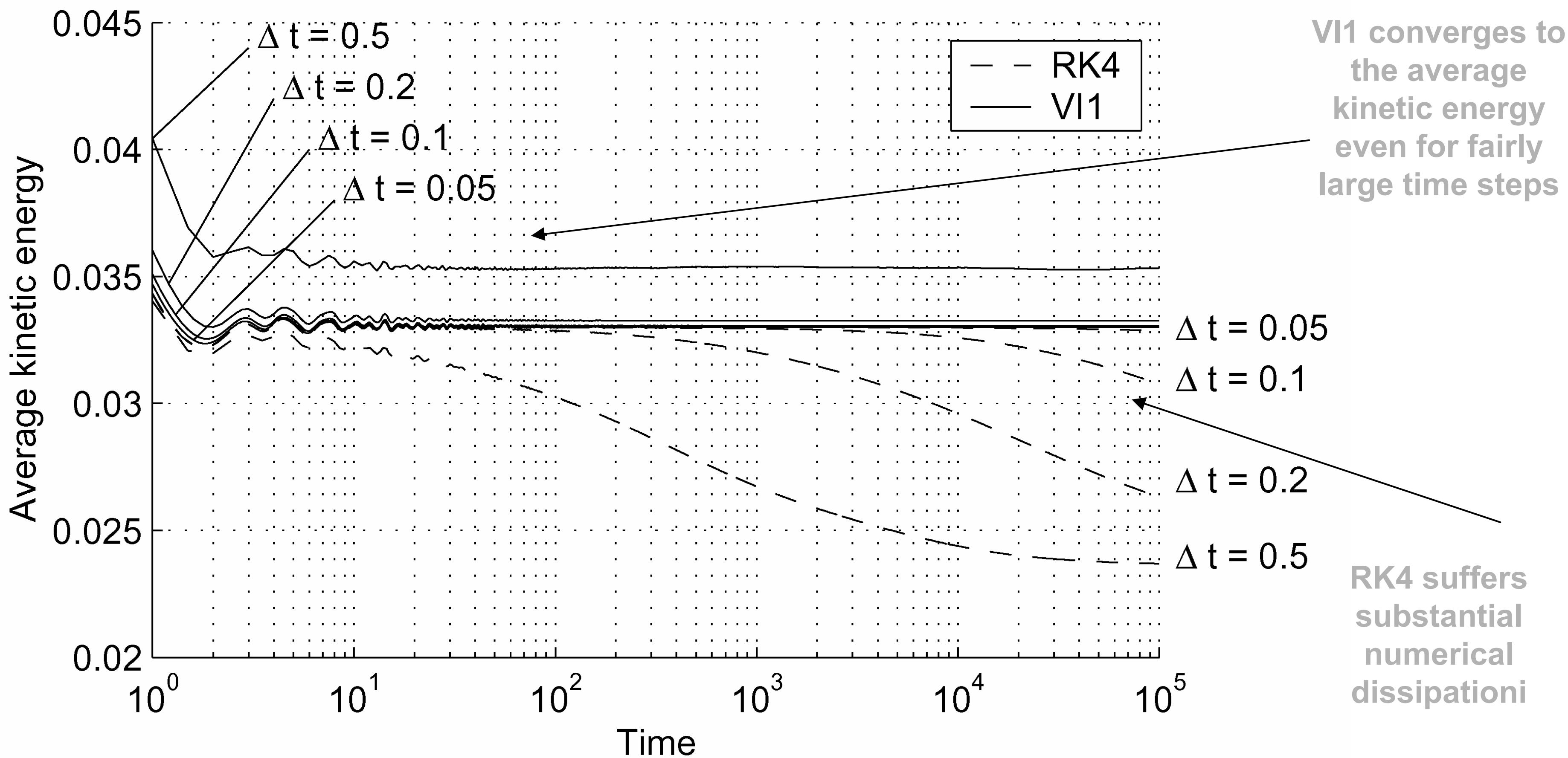
- Discrete L-integral

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 (In LMOW '03, computations by M. West)
  - 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.
- ODE Discrete Lagrangian

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

Computing what matters

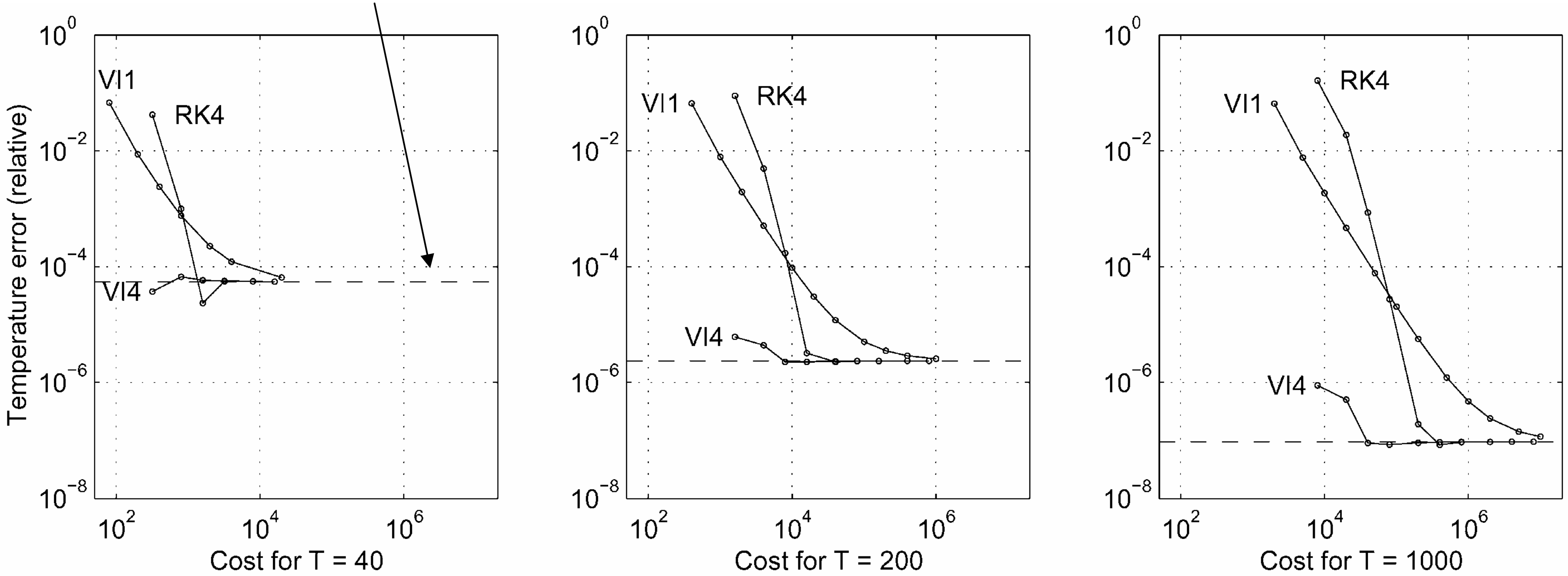


Average kinetic energy as a function of time and time step size for a 4th order non-symplectic Runge-Kutta and a 1st order variational integrator. (West, to appear in Lew, Ortiz, Marsden and West, 2003)

Computing what matters

Error due to the finite time averaging

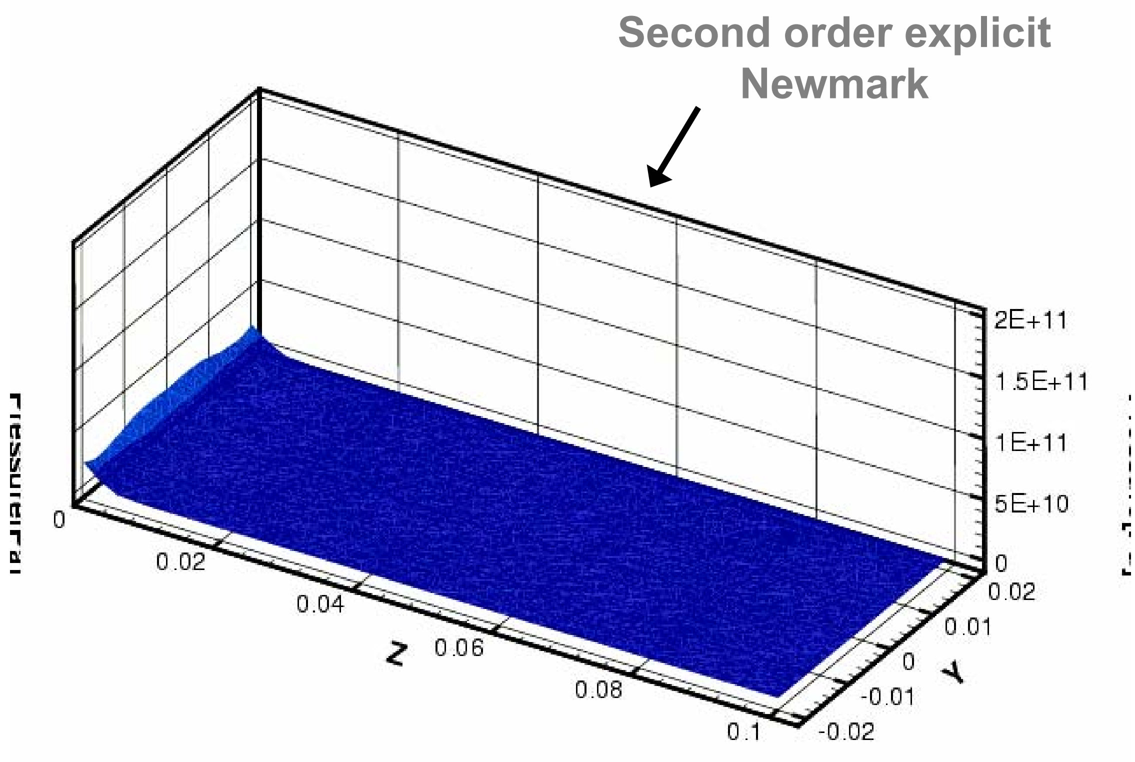
VI4 is always better, and VI1 is better than RK4 for large time steps !



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 (West, to appear in Lew, Ortiz, Marsden and West, 2003)

Shock Propagation in Solids

- When propagating a shock numerically a "stabilization" method is needed
- Artificial Viscosity is easily combined with existing finite element codes and used with non-structured meshes



- For largely deforming solids the Art Visc should:
  - Work well with high-order elements
  - Work well with Lagrangian formulations
  - Be Material Frame Indifferent

Artificial Viscosity Formulation

- Physical motivation
  - A viscous shock has a length-scale
  - Amount of dissipation is independent of the shape of the shock
- Locally add viscosity to make the shock width comparable to the mesh size
- Need to supply the dissipation that the discretization is not capturing (Von Neumann & Ritchmyer, 1950)
- Traditionally, the extra dissipation has been included as an “added” pressure term ➡ volumetric stress !!

Lew, Radovitzky and Ortiz, J. Comp. Aided Mat. Design, 8 (2-3):213-231, 2002.

Artificial Viscosity Formulation

- The total viscosity coefficient is

$$\eta_{\mathrm{h}} = \eta + \Delta\eta$$

Computed to asymptotically approximate the total dissipation in 1-D strong and weak shocks

- The artificial viscosity value is

$$\Delta\eta = \begin{cases} f(\Delta u, h) & \Delta u < 0 \\ 0 & \Delta u \geq 0 \end{cases}$$

Compression

Expansion

- For multidimensional computations:

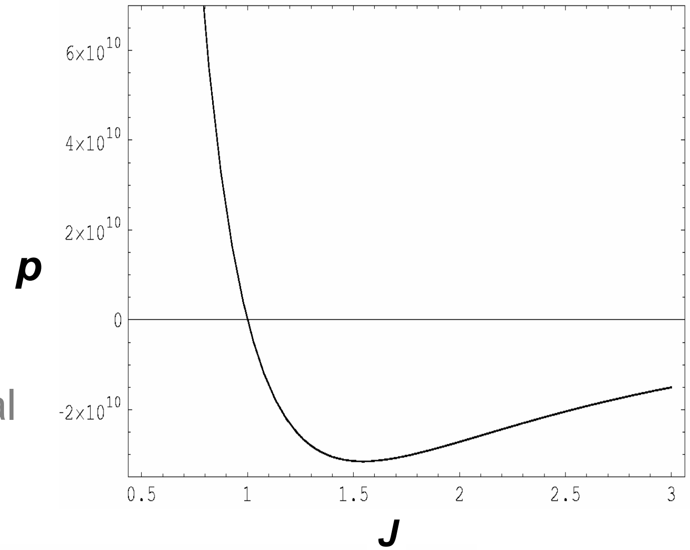
$$h = g(J, |K|, d) \qquad \Delta u = h \frac{\partial \log J}{\partial t}$$

- Values computed at each Gauss point
- Observations
  - The artificial viscosity is computed at the “constitutive” level
  - Material Frame Indifferent
  - Order-independent formulation

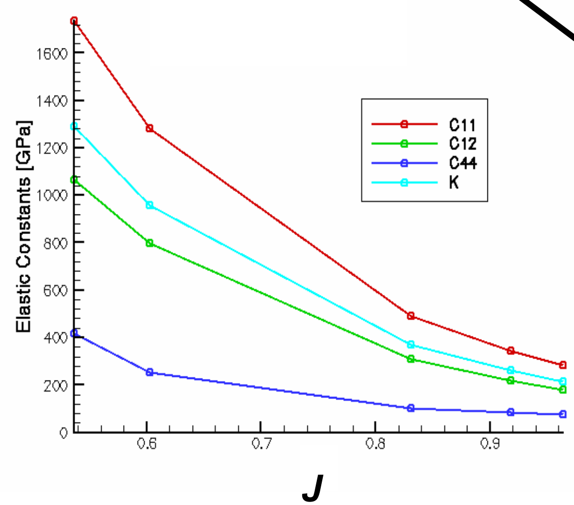
Tantalum model

- Ab-initio equation of state and elastic constants (Cohen, 2000)
- J2-isotropic plasticity
- Steinberg-Guinan model for the pressure dependence of the yield surface

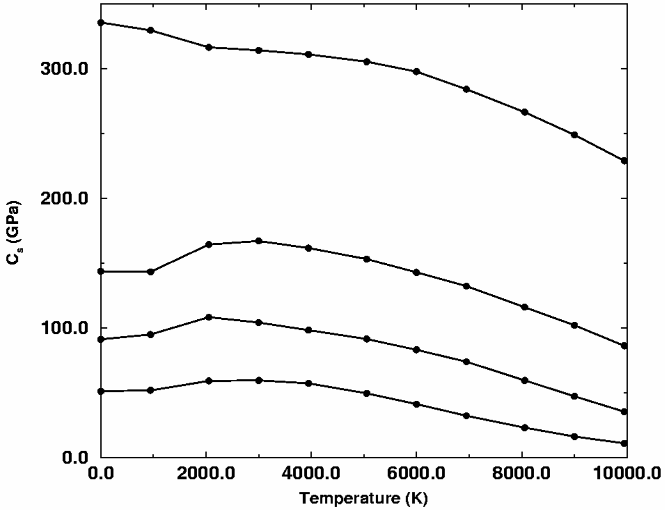
EoS isothermal



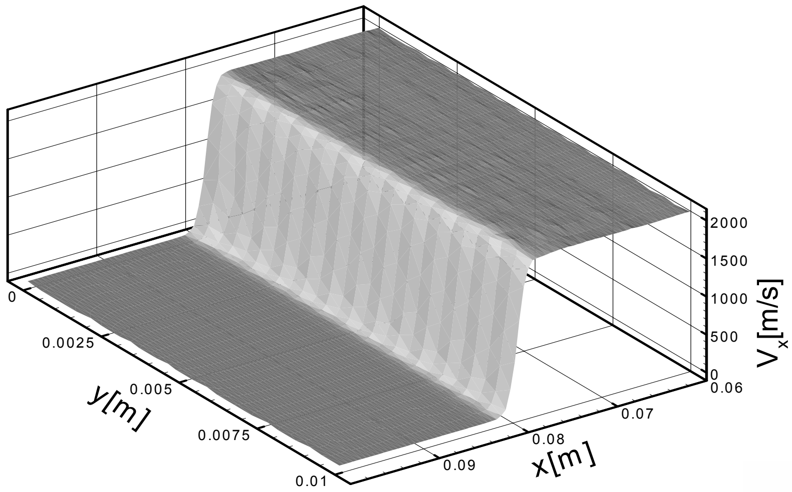
Isothermal elastic constants



Isochoric elastic constants

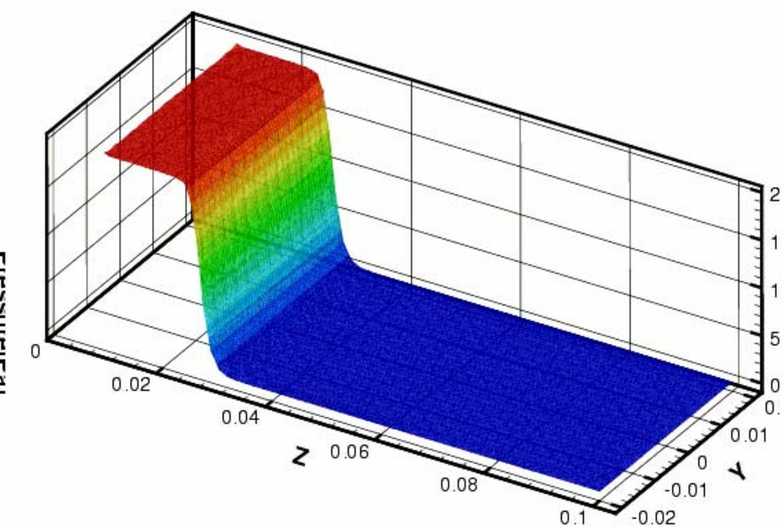


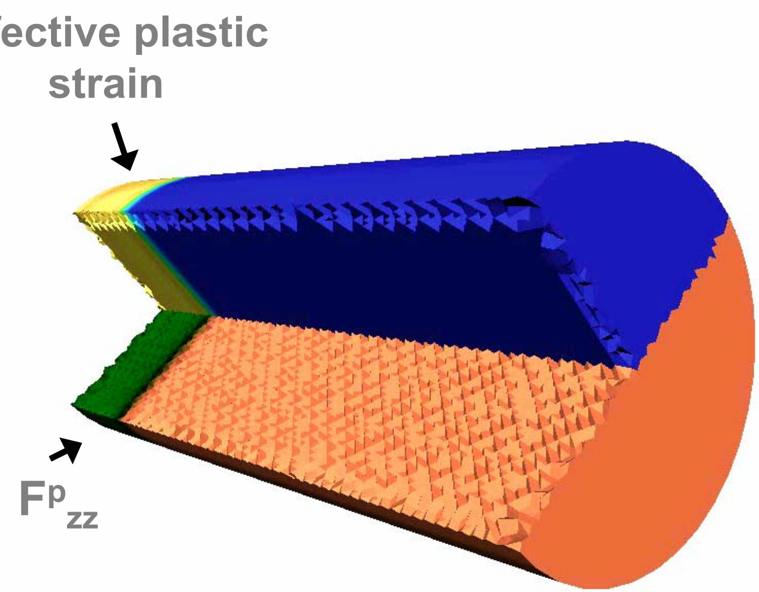
Shocked Ta - Validation and Verification



	Theoretical	Numerical
p_2[GPa]	194.86	194.8±0.1
v_2 [10^{-5} m^3/kg]	3.953	3.953±0.001
T_2[K]	5263	5260±30
D[m/s]	5852	5855±30

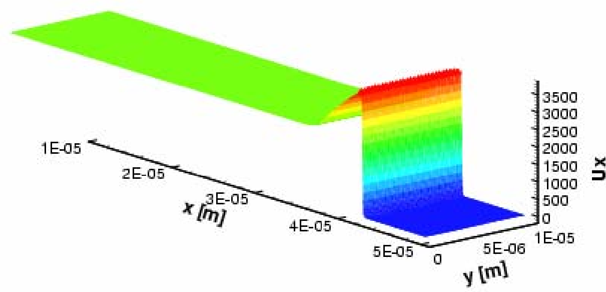
Jump Conditions



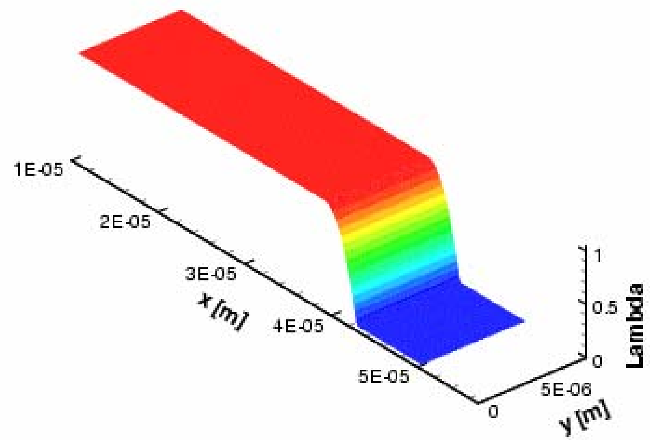


Engineering Model of HMX

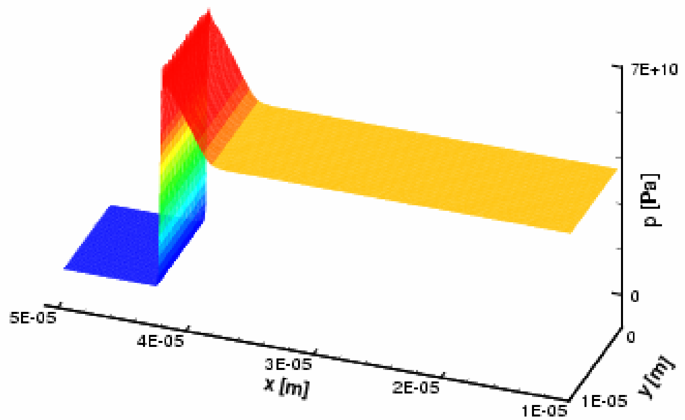
- Mie-Grüneisen equation of state designed to reproduce well the detonation front velocity (Morano and Shepherd, 1999)
- One-step chemistry



Particle velocity



Products mass fraction

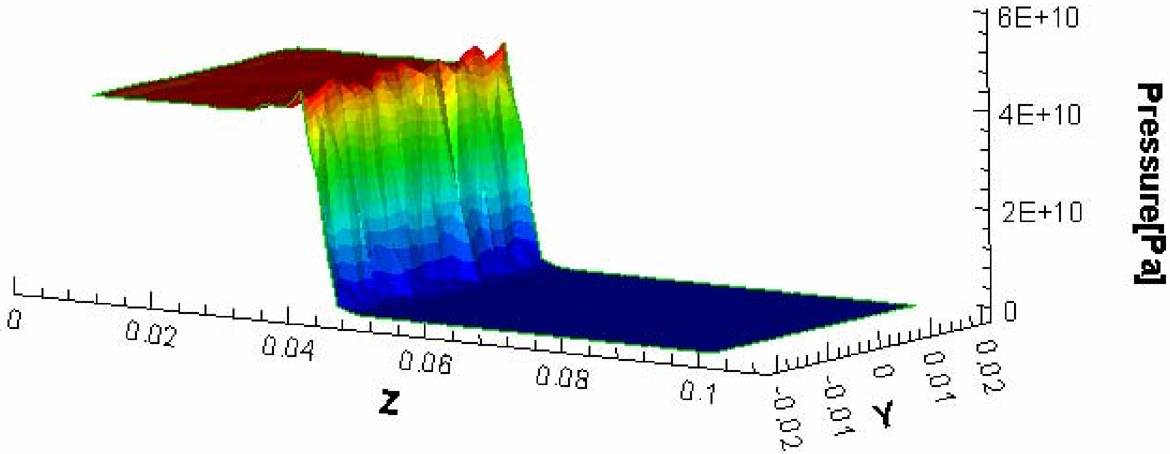


Pressure

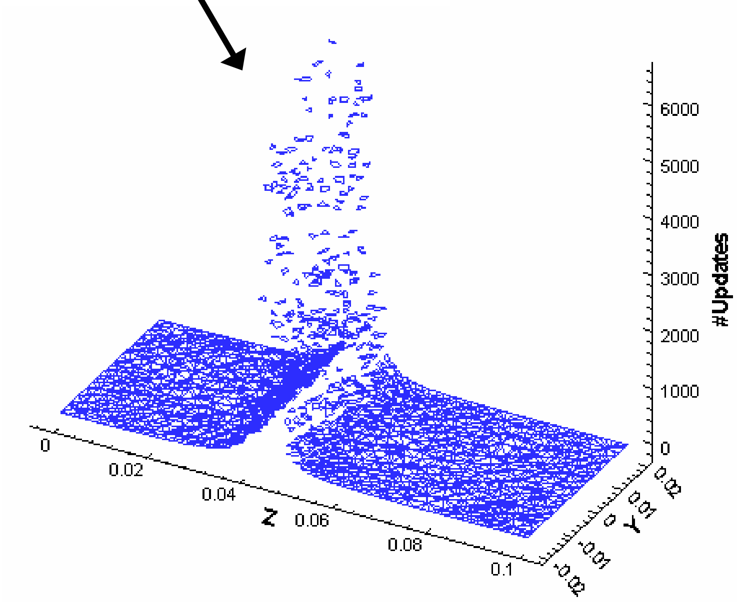
Detonation front with AVI

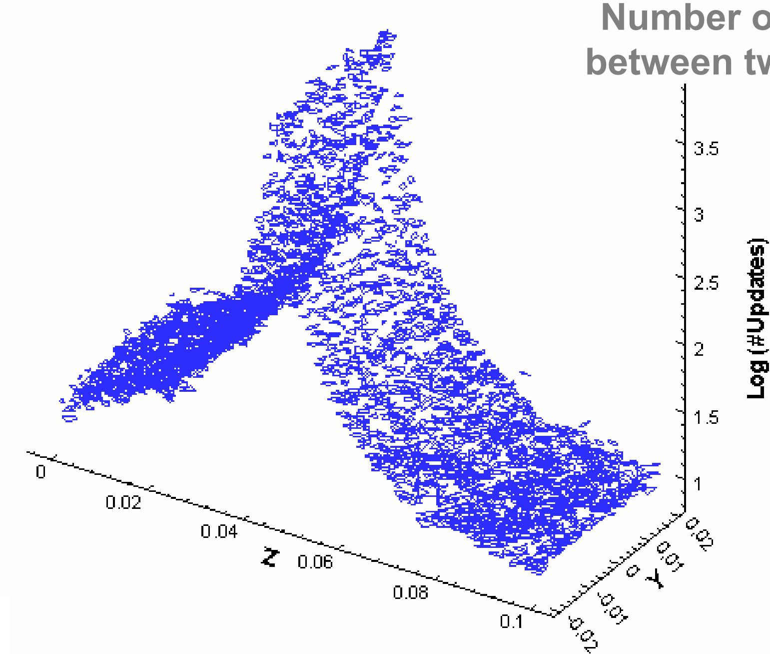
The computational effort is localized where the action is !!

Max/Min Ratio = 10^3

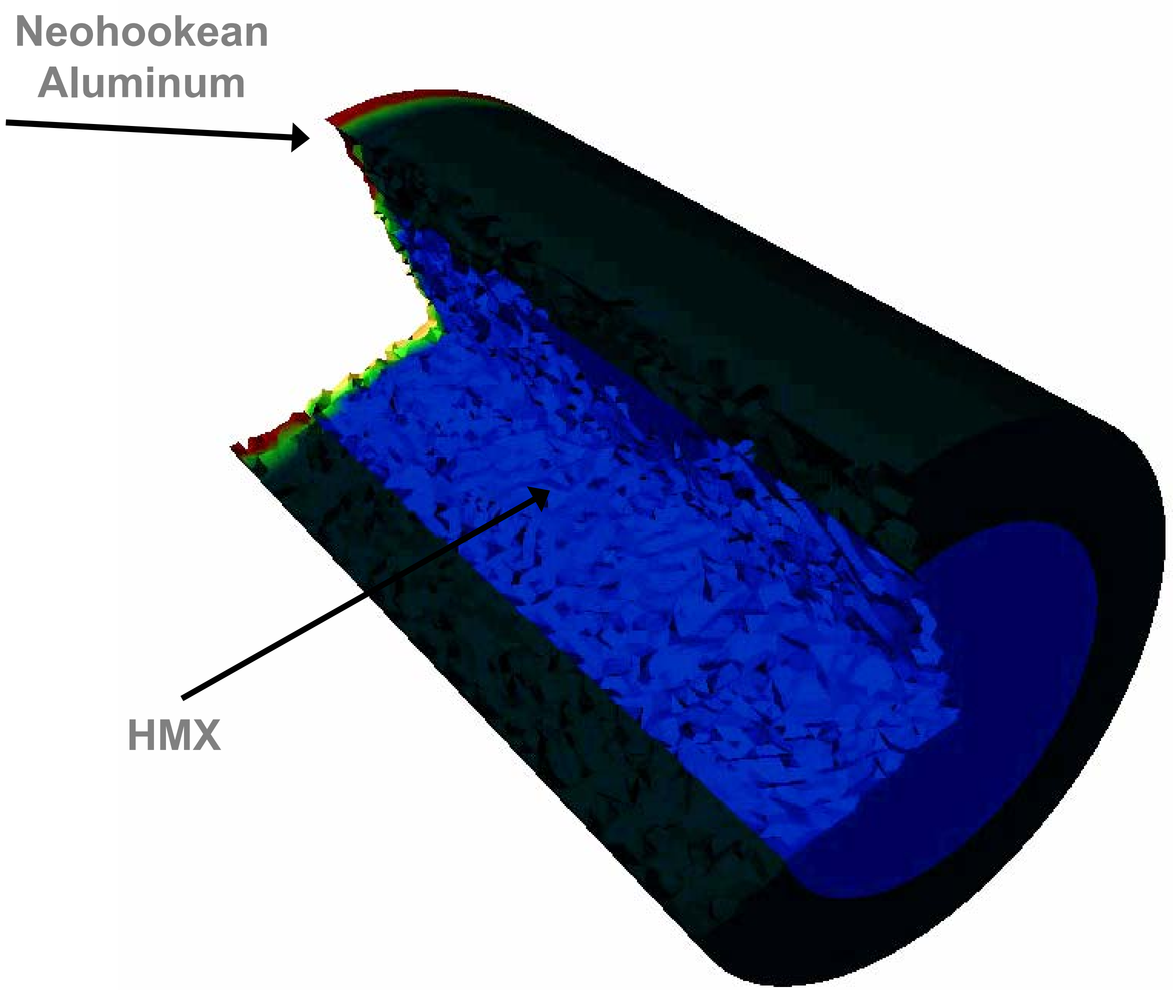


Number of updates between two outputs





Integration into the VTF

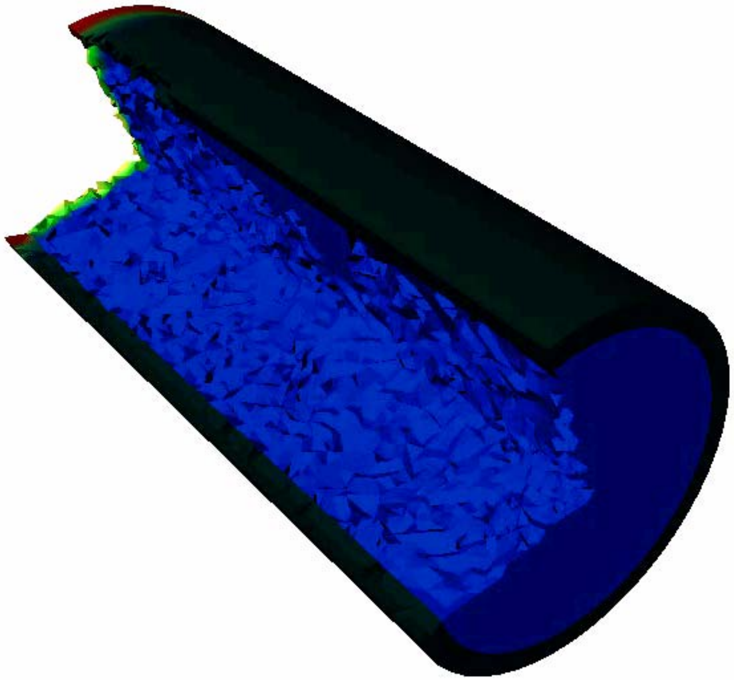


- Impact velocity

  2170 m/s
- Artificial Viscosity
- AVI

Impact problem on a Canister with HMX

Thinner-walled tube



Impact problem on a Canister with HMX

Selected References

- Marsden and West, *Acta Numerica*, 10, 2001
- Marsden, Patrick and Shkoller, *Comm. Math. Phys.*, 199, 351-395, 1998.
- Kane, Marsden and Ortiz, *J. Math. Phys.*, 40, 3353-3371, 1999.
- Lew, Marsden, Ortiz and West, *Archive for Rational Mechanics & Analysis*, (2), 85-146, 2003.
- Lew, Radovitzky and Ortiz, *Journal of Computer-Aided Material Design*, 8, 213-231, 2001.
- Arienti, Morano and Shepherd, GALCIT Report FM99-8, 1999
- Reich S., *SIAM J. Numer. Anal.*, 36(5), 1549-1570, 1999.