Energy and Momentum Conserving Algorithms in Continuum Mechanics

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INTRODUCTION

Main Concern

Time integration of the general system

$$\dot{\boldsymbol{z}} = \boldsymbol{J}(\boldsymbol{z})\nabla H(\boldsymbol{z}) - \boldsymbol{D}(\boldsymbol{z})\nabla H(\boldsymbol{z})$$

$$\boldsymbol{z} \in \boldsymbol{R}^m, \qquad H : \boldsymbol{R}^m \to \boldsymbol{R},$$

$$\boldsymbol{J} = -\boldsymbol{J}^T \in \boldsymbol{R}^{m\times m}, \qquad \boldsymbol{D} = \boldsymbol{D}^T \geq 0 \in \boldsymbol{R}^{m\times m}$$

- includes general Hamiltonian systems
- analogous infinite-dimensional case

Key Features

Energy decay/conservation

$$\dot{H} = \nabla H \cdot \dot{\boldsymbol{z}} = \nabla H \cdot [\boldsymbol{J}\nabla H - \boldsymbol{D}\nabla H]$$

$$\boxed{\dot{H} = -\nabla H \cdot \boldsymbol{D}\nabla H \leq 0 \qquad \text{and} \qquad \dot{H} = 0 \quad \text{when} \quad \boldsymbol{D} \equiv \boldsymbol{O}}$$

Momentum conservation (linear/angular momentum)

Suppose

- $H = \widehat{H} \circ \boldsymbol{\zeta}$
- $\boldsymbol{\zeta} : \boldsymbol{R}^m \to \boldsymbol{R}^k$ invariants under a symmetry group, e.g.

$$\boldsymbol{\zeta}(\boldsymbol{z}) = (|\boldsymbol{q}|^2, \boldsymbol{q} \cdot \boldsymbol{p}, |\boldsymbol{p}|^2), \quad \boldsymbol{z} = (\boldsymbol{q}, \boldsymbol{p}) \in \boldsymbol{R}^6$$

"rotational invariants"

- $\exists\ F(z)$ such that $\boldsymbol{J}\nabla F \in \ker[\nabla \boldsymbol{\zeta}]$

Then

$$\boxed{\dot{F} = 0 \quad \text{when} \quad \boldsymbol{D} \equiv \boldsymbol{O}}$$

OBJECTIVE & MOTIVATION

Objective

To develop time integration schemes with :

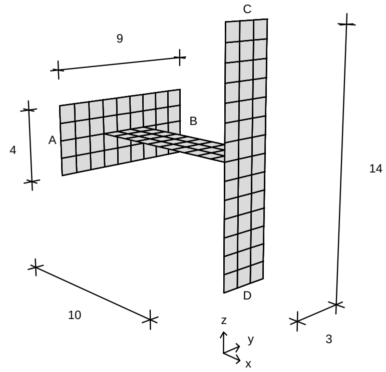
- mild or no restrictions on time step (stable implicit schemes)
- energy/momentum conservation when no damping present
- physical energy decay when damping present

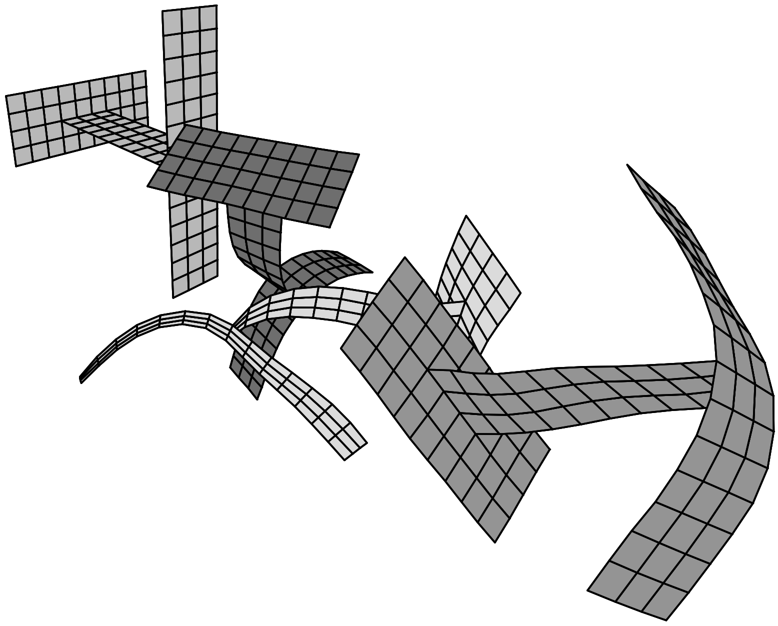
Motivation

- classic schemes generally fail on all three points

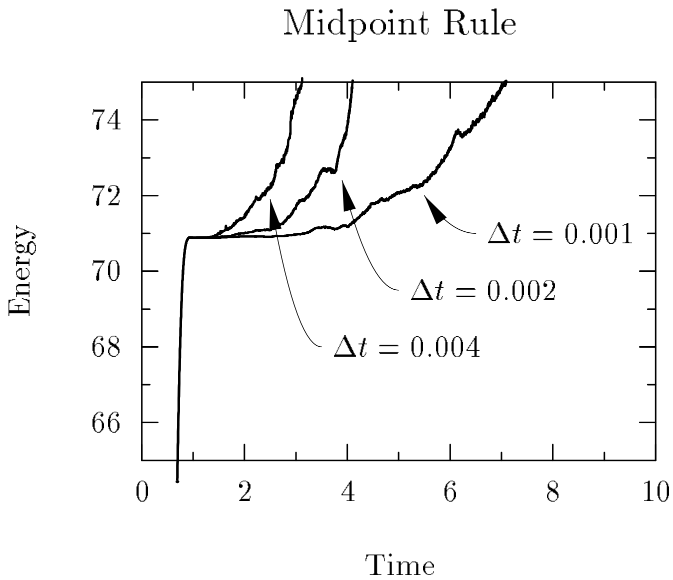
Example: "$\dot{H} = 0$"

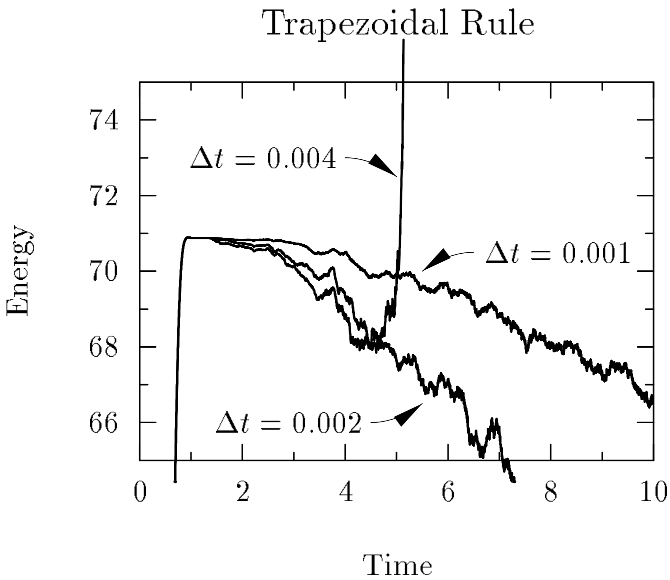
Nonlinear Shells (Simo & Tarnow 1992)





Energy vs Time: Mid-Point Rule & Trapezoidal Rule





OUTLINE

I. Introduction and motivation

II. Why does the Mid-Point Rule fail?

- Kepler model problem
- Elastodynamics model problem
  - Illustration of difficulties
  - Remedies

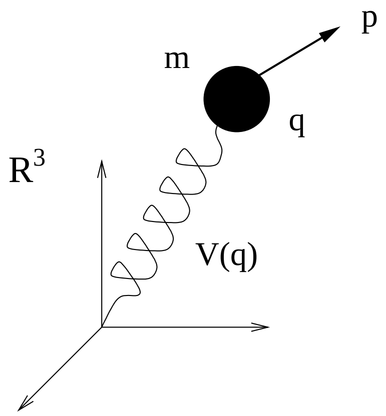
III. Abstract framework for conserving schemes

- Discrete gradients
- General scheme

IV. Closing remarks

KEPLER MODEL PROBLEM

$$\boxed{\begin{aligned} \dot{\boldsymbol{q}} &= \quad m^{-1}\boldsymbol{p} \\ \dot{\boldsymbol{p}} &= -\frac{V'(|\boldsymbol{q}|)}{|\boldsymbol{q}|}\boldsymbol{q} \end{aligned}}$$



$$\boldsymbol{z} = (\boldsymbol{q}, \boldsymbol{p}), \quad H(\boldsymbol{z}) = \tfrac{1}{2}m^{-1}|\boldsymbol{p}|^2 + V(|\boldsymbol{q}|), \quad \boldsymbol{J} = \begin{pmatrix} O & I \\ -I & O \end{pmatrix}$$

FEATURES

- $H(\boldsymbol{z})$ invariant under rotation group
- $H(\boldsymbol{z})$, $\boldsymbol{j}(\boldsymbol{z}) = \boldsymbol{q} \times \boldsymbol{p}$ are integrals
- $\boldsymbol{q}, \boldsymbol{p} \in \boldsymbol{R}^3$ evolve in plane normal to $\boldsymbol{\mu} = \boldsymbol{j}(\boldsymbol{z}_0)$
- the radial variables $\lambda = |\boldsymbol{q}|$ and $\pi = \boldsymbol{p} \cdot \boldsymbol{q}/|\boldsymbol{q}|$ satisfy

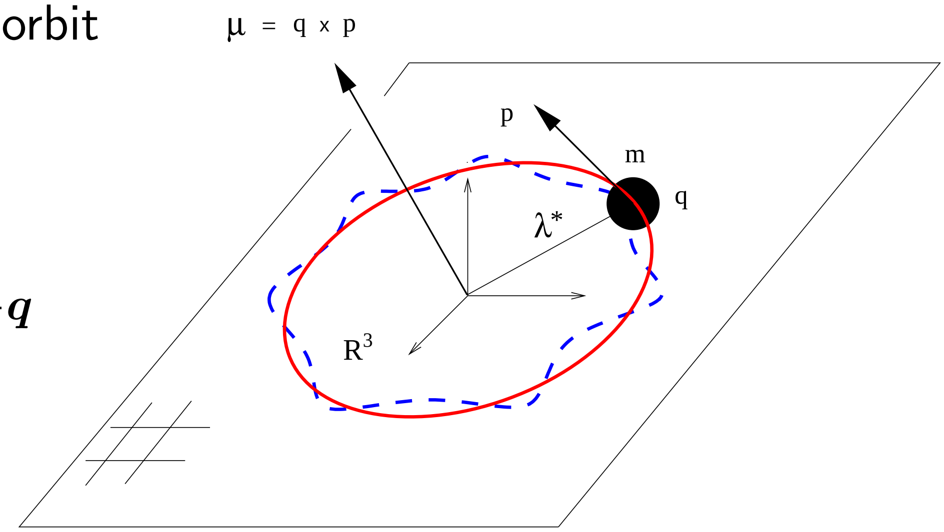
$$\boxed{\begin{aligned} \dot{\lambda} &= \quad m^{-1}\pi \\ \dot{\pi} &= -V'_\mu(\lambda) \end{aligned}} \qquad \text{“reduced equations”}$$

where

$$V_\mu(\lambda) = V(\lambda) + \tfrac{1}{2}|\boldsymbol{\mu}|^2/m\lambda^2 \quad \text{“Smale's amended potential”}$$

Relative Equilibria

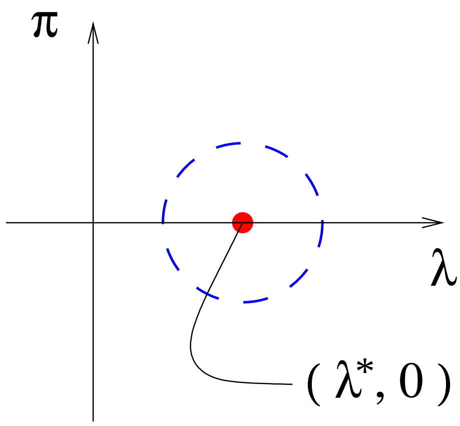
steady, circular orbit



$$\dot{\boldsymbol{q}} = m^{-1}\boldsymbol{p}$$
$$\dot{\boldsymbol{p}} = -\frac{V'(|\boldsymbol{q}|)}{|\boldsymbol{q}|}\boldsymbol{q}$$

$\Downarrow$

fixed point



$$\dot{\lambda} = m^{-1}\pi$$
$$\dot{\pi} = -V'_\mu(\lambda)$$

$$V'_\mu(\lambda^*) = 0$$

Stability

stable relative equilibria = stable fixed point

= local min of $V_\mu(\lambda)$

Analysis of the Mid-Point Rule

MID-POINT RULE

$$\left.\begin{aligned} \frac{\boldsymbol{q}_{n+1}-\boldsymbol{q}_n}{\Delta t} &= \quad m^{-1}\boldsymbol{p}_{n+\frac{1}{2}} \\ \frac{\boldsymbol{p}_{n+1}-\boldsymbol{p}_n}{\Delta t} &= -\frac{V'(|\boldsymbol{q}_{n+\frac{1}{2}}|)}{|\boldsymbol{q}_{n+\frac{1}{2}}|}\boldsymbol{q}_{n+\frac{1}{2}} \end{aligned}\right\} \tag{1}$$

where $\boldsymbol{q}_{n+\frac{1}{2}} = \frac{1}{2}(\boldsymbol{q}_{n+1}+\boldsymbol{q}_n)$.

- preserves $\boldsymbol{j}(\boldsymbol{z}_n) = \boldsymbol{q}_n \times \boldsymbol{p}_n$
- does not preserve $H(\boldsymbol{z}_n) = \frac{1}{2}m^{-1}|\boldsymbol{p}_n|^2 + V(|\boldsymbol{q}_n|)$.

REDUCED EQUATIONS

Introduce reduced variables as before

$$\lambda_n = |\boldsymbol{q}_n|, \qquad \pi_n = \boldsymbol{p}_n \cdot \boldsymbol{q}_n / |\boldsymbol{q}_n|.$$

Then (1) implies the implicit reduced equation

$$\boldsymbol{G}_{\mathrm{MP}}(\lambda_{n+1},\pi_{n+1};\lambda_n,\pi_n) = \boldsymbol{0}. \tag{2}$$

- look for fixed points $(\widehat{\lambda}^*, 0)$ $\quad\Leftrightarrow\quad$ relative equilibria
- study stability

Results

Existence of Relative Equilibria:

Fixed points $\widehat{\lambda}^*$ are stationary points of a perturbed potential:

$$\widehat{V}_\mu(\lambda, \Delta t) \approx V_\mu(\lambda)$$

Stability of Relative Equilibria:

Fixed points $\widehat{\lambda}^*$ are only conditionally stable in general:

- linearly stable when $\Delta t < \Delta t_{critical}$
- unstable when $\Delta t > \Delta t_{critical}$

Two questions:

- What's causing the instability?
- Is there a cure?

Source of Instability

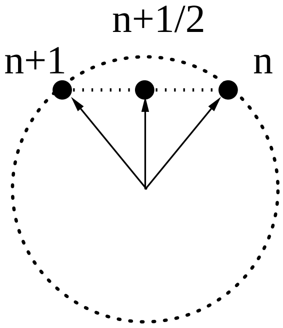
coupling between internal forces and rotations

Exact Problem:

$$\frac{V'(|\boldsymbol{q}|)}{|\boldsymbol{q}|} \text{ rotationally invariant when } \boldsymbol{q} = \boldsymbol{\Lambda}(t)\boldsymbol{q}_0$$

Mid-point discretization:

$$\frac{V'(|\boldsymbol{q}_{n+\frac{1}{2}}|)}{|\boldsymbol{q}_{n+\frac{1}{2}}|} \text{ not rotationally invariant when } \boldsymbol{q}_{n+1} = \boldsymbol{\Lambda}\boldsymbol{q}_n$$



A Remedy

$$\text{replace} \quad V'(|\boldsymbol{q}_{n+\frac{1}{2}}|)\,\frac{1}{|\boldsymbol{q}_{n+\frac{1}{2}}|}$$

$$\text{by} \qquad \frac{V(|\boldsymbol{q}_{n+1}|) - V(|\boldsymbol{q}_n|)}{|\boldsymbol{q}_{n+1}| - |\boldsymbol{q}_n|}\,\frac{1}{\frac{1}{2}(|\boldsymbol{q}_{n+1}| + |\boldsymbol{q}_n|)}$$

A Conserving Scheme

Conserving Scheme

$$\left.\begin{aligned} \frac{\boldsymbol{q}_{n+1}-\boldsymbol{q}_n}{\Delta t} &= \quad m^{-1}\boldsymbol{p}_{n+\frac{1}{2}} \\ \frac{\boldsymbol{p}_{n+1}-\boldsymbol{p}_n}{\Delta t} &= -\frac{V(|\boldsymbol{q}_{n+1}|)-V(|\boldsymbol{q}_n|)}{|\boldsymbol{q}_{n+1}|-|\boldsymbol{q}_n|}\;\frac{\boldsymbol{q}_{n+\frac{1}{2}}}{\frac{1}{2}(|\boldsymbol{q}_{n+1}|+|\boldsymbol{q}_n|)} \end{aligned}\right\} \tag{3}$$

- preserves $\boldsymbol{j}(\boldsymbol{z}_n) = \boldsymbol{q}_n \times \boldsymbol{p}_n$
- preserves $H(\boldsymbol{z}_n) = \frac{1}{2}m^{-1}|\boldsymbol{p}_n|^2 + V(|\boldsymbol{q}_n|)$.

Reduced Equations

Introduce reduced variables as before

$$\lambda_n = |\boldsymbol{q}_n|, \qquad \pi_n = \boldsymbol{p}_n \cdot \boldsymbol{q}_n / |\boldsymbol{q}_n|.$$

Then (3) implies the implicit reduced equation

$$\boldsymbol{G}_{\mathrm{EM}}(\lambda_{n+1}, \pi_{n+1}; \lambda_n, \pi_n) = \boldsymbol{0} \tag{4}$$

- look for fixed points $(\widehat{\lambda}^*, 0)$ $\quad\Leftrightarrow\quad$ relative equilibria
- study stability

Results

Existence of Relative Equilibria:

Fixed points $\widehat{\lambda}^*$ are exact, i.e. stationary points of $V_\mu(\lambda)$.

Stability of Relative Equilibria:

i. The reduced equations preserve the integral

$$H_\mu(\lambda, \pi) = \tfrac{1}{2} m^{-1} \pi^2 + V_\mu(\lambda) \quad \text{“reduced Hamiltonian”}$$

ii. V_μ local min at $\widehat{\lambda}^*$ $\Rightarrow$ H_μ local min at $(\widehat{\lambda}^*, 0)$

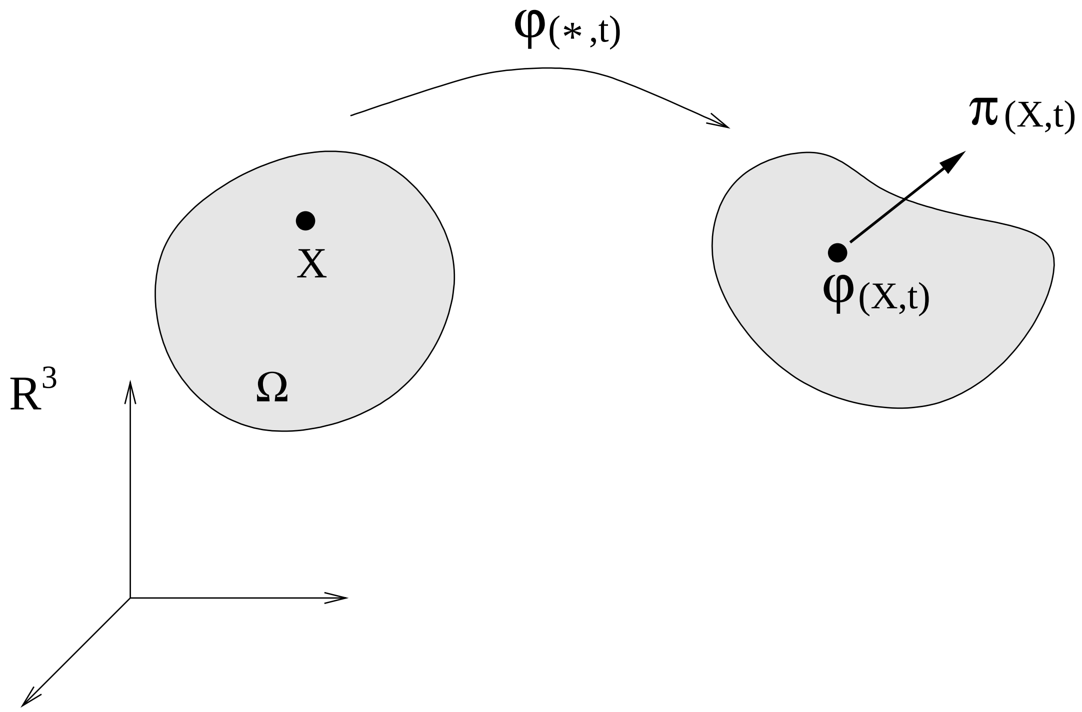
$\Rightarrow$ H_μ is a Lyapunov function

$\Rightarrow$ nonlinear stability.

Three remarks on conserving scheme:

- 2nd order accurate, like Mid-Point rule
- “conserving” modification cures coupling/stability problem
- similar problem/cure in more complex systems

ELASTODYNAMICS MODEL PROBLEM

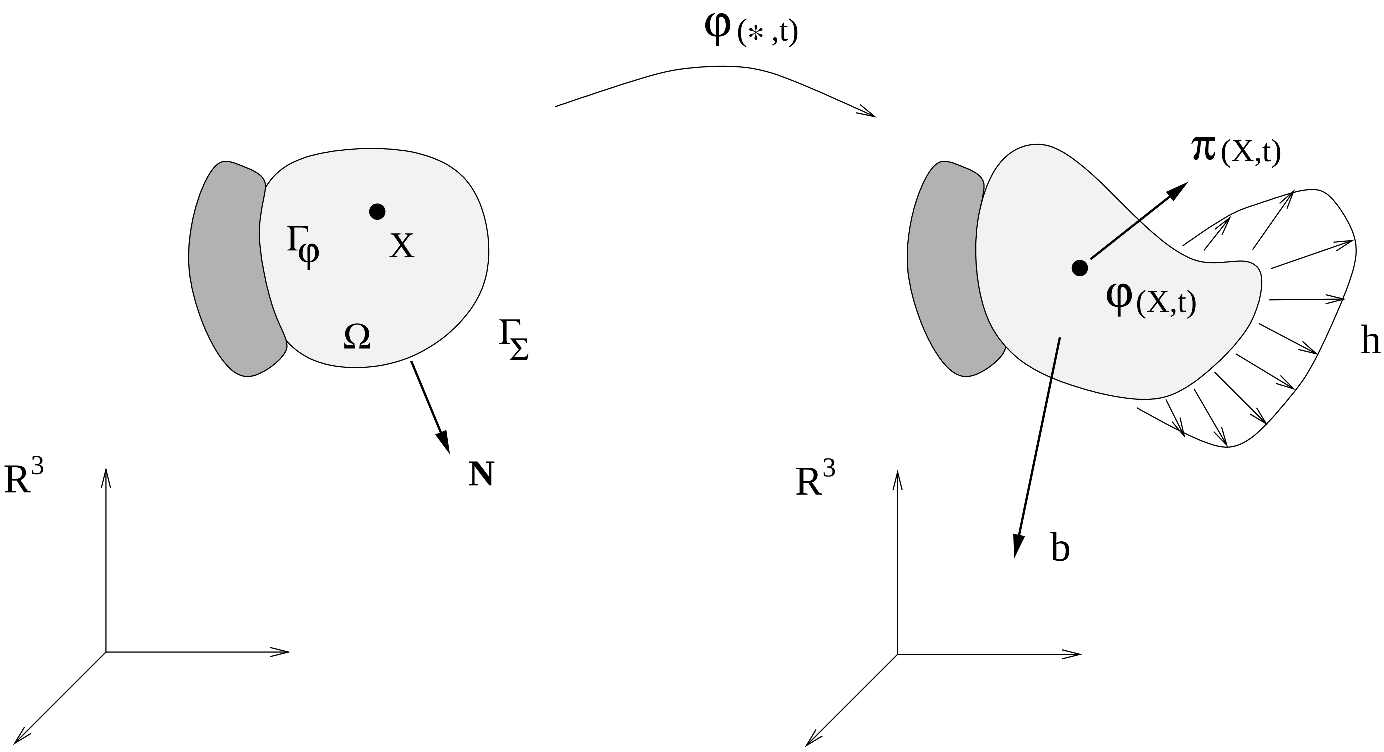


NOTATION

Deformation	$\boldsymbol{\varphi} : \bar{\Omega} \times [0,T] \to \boldsymbol{R}^3$
(Linear) Momentum Density	$\boldsymbol{\pi} : \bar{\Omega} \times [0,T] \to \boldsymbol{R}^3$
Deformation Gradient	$\boldsymbol{F}(\boldsymbol{\varphi}) = \nabla\boldsymbol{\varphi}$
Cauchy Strain	$\boldsymbol{C}(\boldsymbol{\varphi}) = \boldsymbol{F}(\boldsymbol{\varphi})^T \boldsymbol{F}(\boldsymbol{\varphi})$
Strain Energy Function	$W(\boldsymbol{C})$
Second Piola-Kirchhoff Stress	$\boldsymbol{\Sigma}(\boldsymbol{\varphi})$

$$\boldsymbol{\Sigma}(\boldsymbol{\varphi}) = 2\, DW(\boldsymbol{C}(\boldsymbol{\varphi}))$$

Typical IBVP



Find $\boldsymbol{\varphi}, \boldsymbol{\pi} : \bar{\Omega} \times [0,T] \to \boldsymbol{R}^3$ such that

$\dot{\boldsymbol{\varphi}} = \rho^{-1}\boldsymbol{\pi}$	in	$\Omega \times (0,T]$
$\dot{\boldsymbol{\pi}} = \nabla \cdot [\boldsymbol{F}(\boldsymbol{\varphi})\boldsymbol{\Sigma}(\boldsymbol{\varphi})] + \boldsymbol{b}$	in	$\Omega \times (0,T]$
$\boldsymbol{\varphi} = \boldsymbol{g}$	in	$\Gamma_\varphi \times (0,T]$
$\boldsymbol{F}(\boldsymbol{\varphi})\boldsymbol{\Sigma}(\boldsymbol{\varphi})\boldsymbol{N} = \boldsymbol{h}$	in	$\Gamma_\Sigma \times (0,T]$

plus initial conditions

Key Features

- Infinite-dimensional version of general system with

$$\boldsymbol{z} = (\boldsymbol{\varphi}, \boldsymbol{\pi}), \quad \boldsymbol{J} = \begin{pmatrix} O & I \\ -I & O \end{pmatrix}$$

$$H(\boldsymbol{z}) = \int_{\Omega} \left[\tfrac{1}{2}\rho^{-1}|\boldsymbol{\pi}|^2 + W(\boldsymbol{C}(\boldsymbol{\varphi})) - \boldsymbol{\varphi} \cdot \boldsymbol{b} \right] d\Omega$$
$$- \int_{\Gamma_{\Sigma}} \boldsymbol{\varphi} \cdot \boldsymbol{h} \, d\Gamma$$

- Typical integrals

Energy	$H(\boldsymbol{z})$
Linear Momentum	$\boldsymbol{l}(\boldsymbol{z}) = \int_{\Omega} \boldsymbol{\pi} \, d\Omega$
Angular Momentum	$\boldsymbol{j}(\boldsymbol{z}) = \int_{\Omega} \boldsymbol{\varphi} \times \boldsymbol{\pi} \, d\Omega$

Note: For the Neumann problem with no external loads

$$\text{i.e.} \qquad \Gamma_{\Sigma} = \partial\Omega, \quad \boldsymbol{h} = \boldsymbol{0} \quad \text{and} \quad \boldsymbol{b} = \boldsymbol{0}$$

all of the above quantities are integrals.

Mid-Point Rule Time Discretization

Given $\boldsymbol{\varphi}_n, \boldsymbol{\pi}_n$ find $\boldsymbol{\varphi}_{n+1}, \boldsymbol{\pi}_{n+1}$ such that

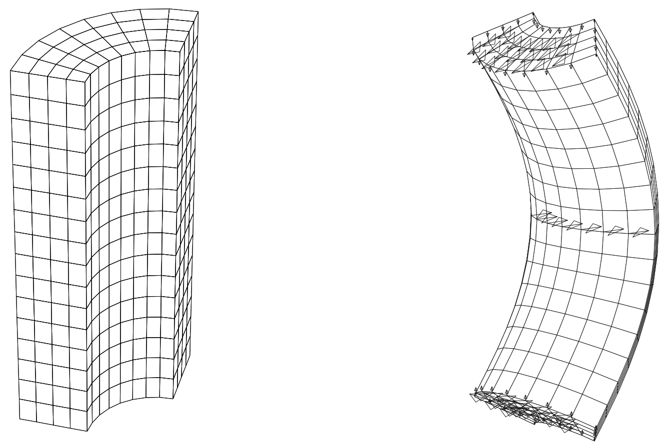
$$
\begin{aligned}
&\frac{\boldsymbol{\varphi}_{n+1} - \boldsymbol{\varphi}_n}{\Delta t} = \rho^{-1} \boldsymbol{\pi}_{n+\frac{1}{2}} && \text{in} \quad \Omega \\
&\frac{\boldsymbol{\pi}_{n+1} - \boldsymbol{\pi}_n}{\Delta t} = \nabla \cdot [\boldsymbol{F}(\boldsymbol{\varphi}_{n+\frac{1}{2}}) \boldsymbol{\Sigma}(\boldsymbol{\varphi}_{n+\frac{1}{2}})] + \boldsymbol{b} && \text{in} \quad \Omega \\
&\boldsymbol{\varphi}_{n+\frac{1}{2}} = \boldsymbol{g} && \text{on} \quad \Gamma_{\varphi} \\
&\boldsymbol{F}(\boldsymbol{\varphi}_{n+\frac{1}{2}}) \boldsymbol{\Sigma}(\boldsymbol{\varphi}_{n+\frac{1}{2}}) \boldsymbol{N} = \boldsymbol{h} && \text{on} \quad \Gamma_{\Sigma}
\end{aligned}
$$

where $(\cdot)_{n+\frac{1}{2}} = \frac{1}{2}[(\cdot)_n + (\cdot)_{n+1}]$ and $\Delta t > 0$ is the time step.

- time discretization reduces the IBVP to a sequence of BVPs for $\boldsymbol{\varphi}_{n+1}, \boldsymbol{\pi}_{n+1}$ $(n = 0, 1, 2, \ldots)$
- each BVP may be solved using a finite-element method
- scheme preserves $\boldsymbol{l}$ and $\boldsymbol{j}$, but in general not H

Numerical Example

Pinched Rubber Quarter-Cylinder



Initial Pinched

- Stored Energy Function: three-term Ogden model

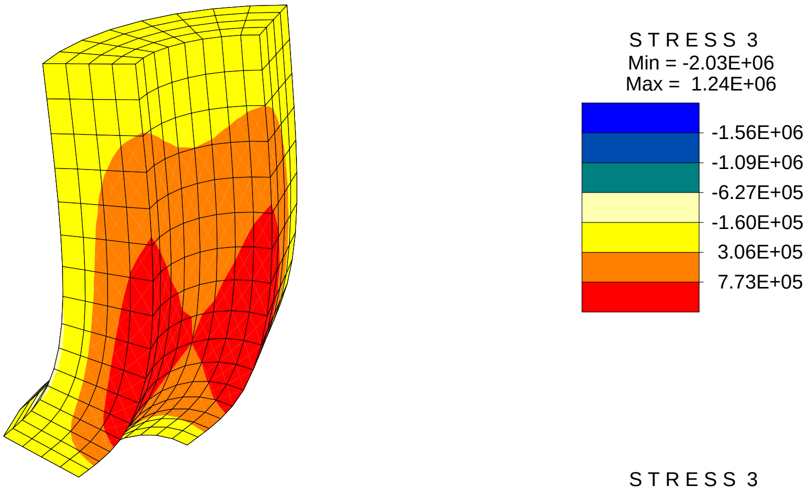
$$W(\boldsymbol{C}) = \sum_{A=1}^{3} \sum_{m=1}^{3} \frac{\mu_m}{\alpha_m} [\lambda_A^{\alpha_m}(\boldsymbol{C}) - 1] - \mu_m \ln[\lambda_A(\boldsymbol{C})]$$

where $\lambda_A^2(\boldsymbol{C}) > 0$ $\big(A = 1, 2, 3\big)$ are the eigenvalues of $\boldsymbol{C} \in \mathsf{S}^3_{\text{PD}}$.

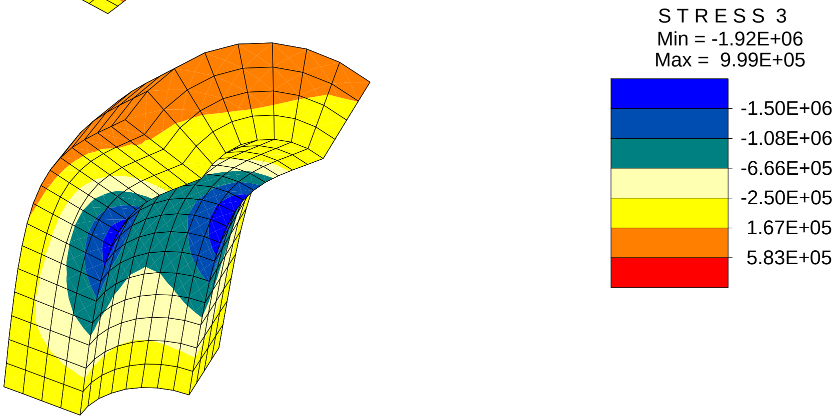
- Spatial Discretization: FEM with 512 trilinear bricks (2295 dof).

Implicit Mid-Point Rule with Time Step $\Delta t = 0.0005s$

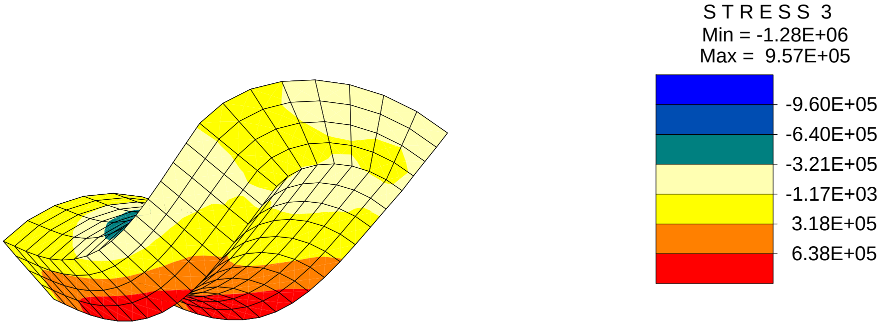
$t = 0.0035s$



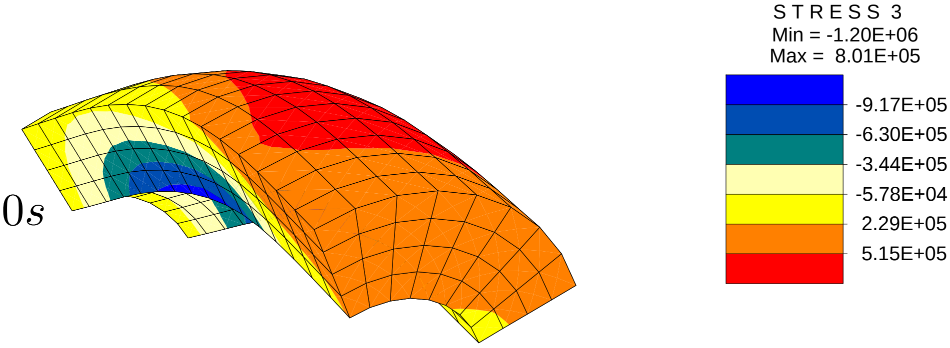
$t = 0.0050s$



$t = 0.0070s$

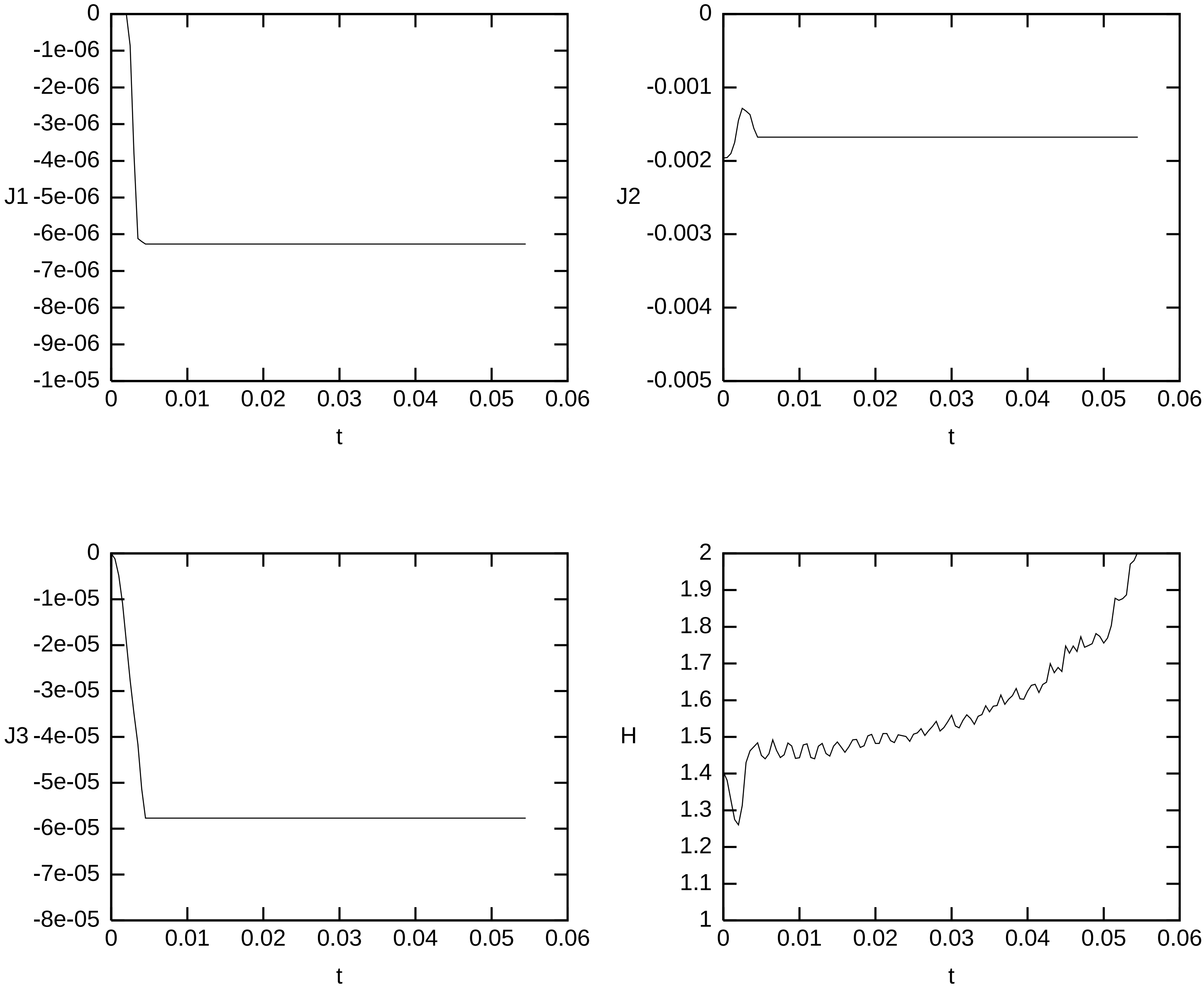


$t = 0.0090s$



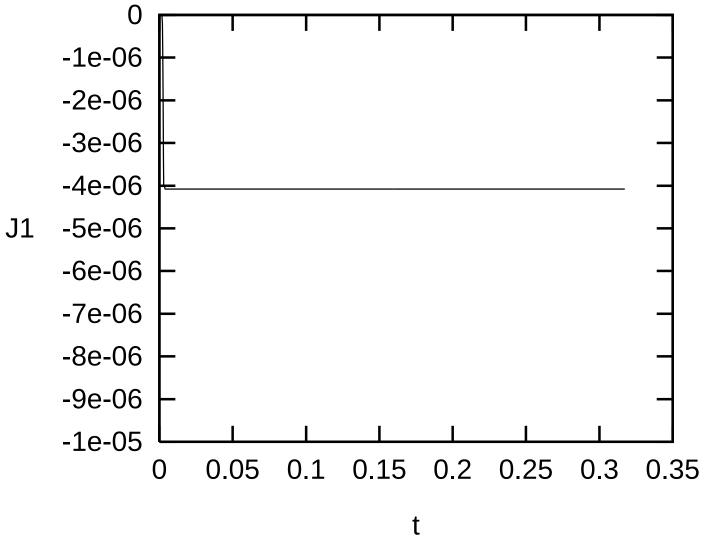
Implicit Mid-Point Rule with Time Step $\Delta t = 0.0005s$

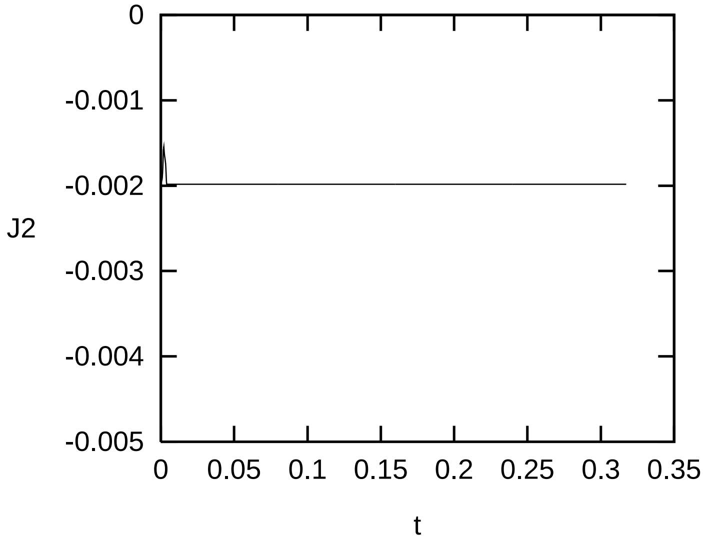
Angular Momentum and Energy Histories

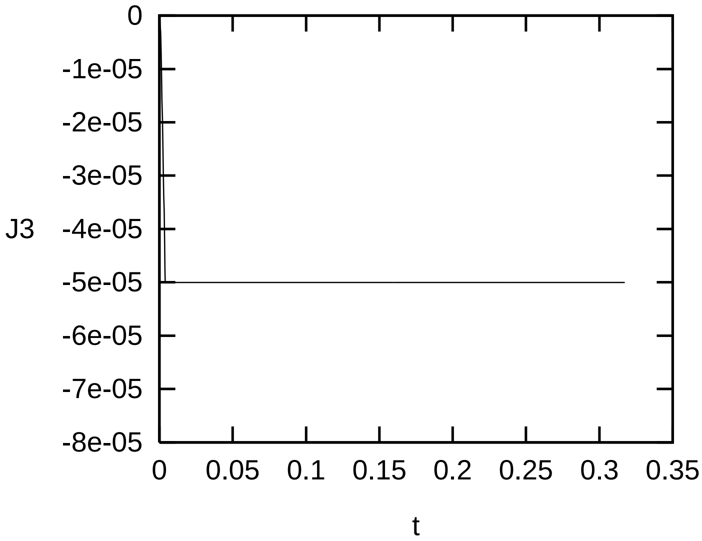


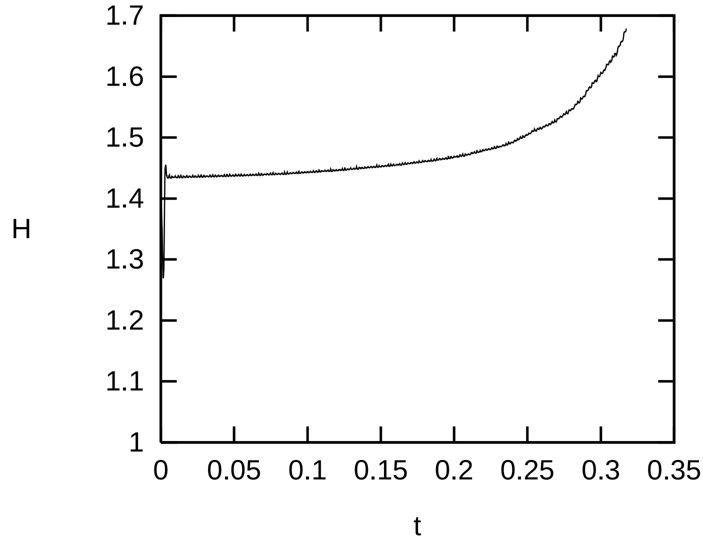
Implicit Mid-Point Rule with Time Step $\Delta t = 0.0002s$

Angular Momentum and Energy Histories

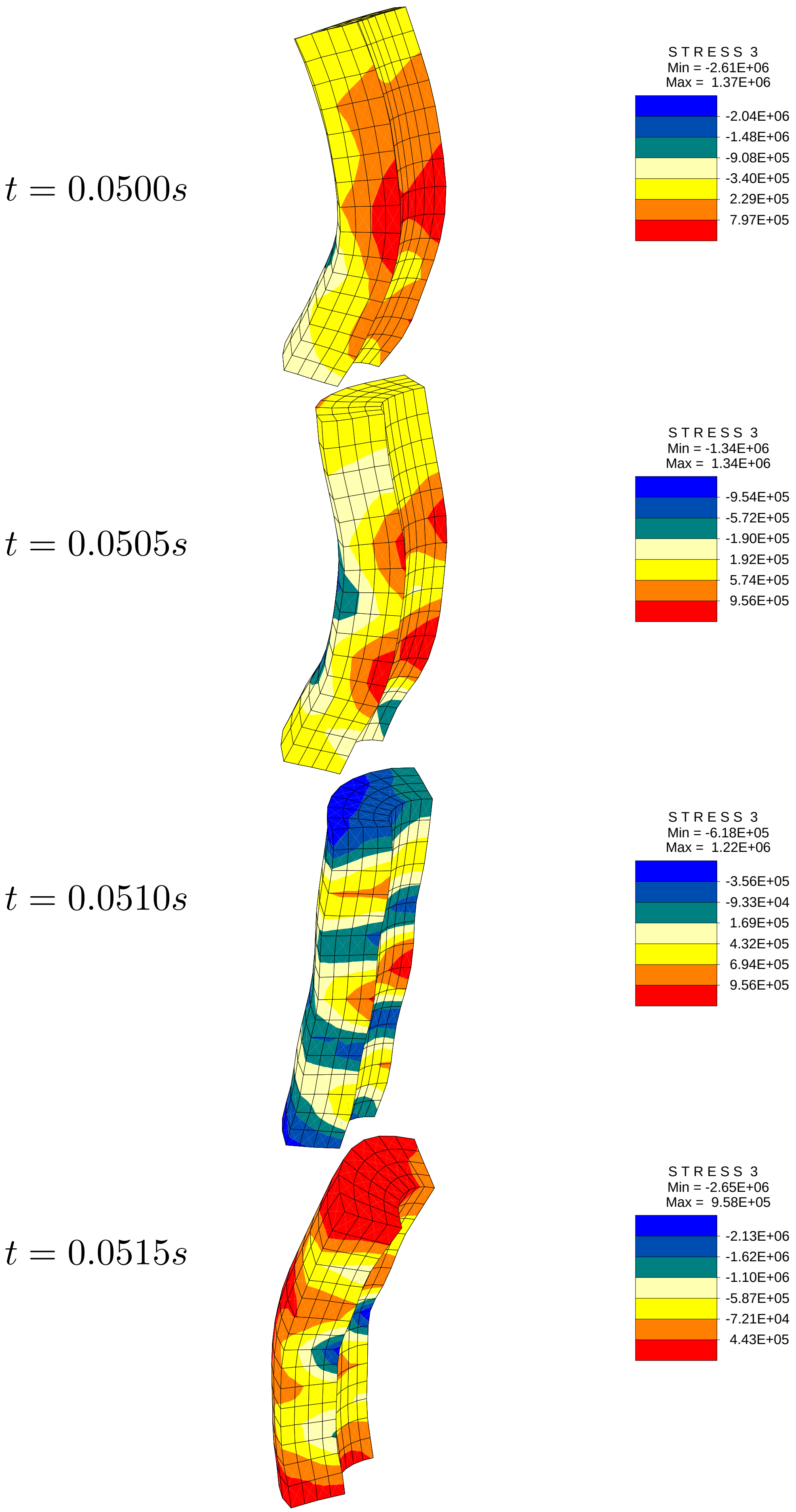








Character of Solution During Energy Growth



A Familiar Difficulty

Exact Problem:

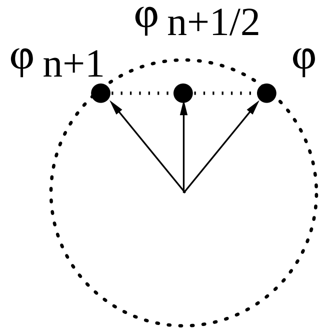
$$\boldsymbol{\Sigma}(\boldsymbol{\varphi}) = 2\, DW(\boldsymbol{C}(\boldsymbol{\varphi}))$$

invariant when $\quad \boldsymbol{\varphi} = \boldsymbol{\Lambda}(t)\boldsymbol{\varphi}_0$

Mid-point discretization:

$$\boldsymbol{\Sigma}(\boldsymbol{\varphi}_{n+\frac{1}{2}}) = 2\, DW(\boldsymbol{C}(\boldsymbol{\varphi}_{n+\frac{1}{2}}))$$

not invariant when $\quad \boldsymbol{\varphi}_{n+1} = \boldsymbol{\Lambda}\boldsymbol{\varphi}_n$



A Remedy

replace $\quad DW(\boldsymbol{C}(\boldsymbol{\varphi}_{n+\frac{1}{2}}))$

by $\quad dW(\boldsymbol{C}_n, \boldsymbol{C}_{n+1}) \approx DW(\boldsymbol{C}(\boldsymbol{\varphi}_{n+\frac{1}{2}}))$ where $\quad \boldsymbol{C}_n = \boldsymbol{C}(\boldsymbol{\varphi}_n)$

A Conserving Scheme

$$
\begin{aligned}
&\frac{\boldsymbol{\varphi}_{n+1} - \boldsymbol{\varphi}_n}{\Delta t} = \rho^{-1} \boldsymbol{\pi}_{n+\frac{1}{2}} && \text{in} \quad \Omega \\
&\frac{\boldsymbol{\pi}_{n+1} - \boldsymbol{\pi}_n}{\Delta t} = \nabla \cdot [\boldsymbol{F}(\boldsymbol{\varphi}_{n+\frac{1}{2}}) \widetilde{\boldsymbol{\Sigma}}] + \boldsymbol{b} && \text{in} \quad \Omega \\
&\boldsymbol{\varphi}_{n+\frac{1}{2}} = \boldsymbol{g} && \text{on} \quad \Gamma_{\varphi} \\
&\boldsymbol{F}(\boldsymbol{\varphi}_{n+\frac{1}{2}}) \widetilde{\boldsymbol{\Sigma}} \boldsymbol{N} = \boldsymbol{h} && \text{on} \quad \Gamma_{\Sigma}
\end{aligned}
$$

where

$$\widetilde{\boldsymbol{\Sigma}} \triangleq 2\, dW(\boldsymbol{C}_n, \boldsymbol{C}_{n+1})$$

$$dW(\boldsymbol{C}_n, \boldsymbol{C}_{n+1}) \triangleq DW(\boldsymbol{C}_{n+\frac{1}{2}})$$

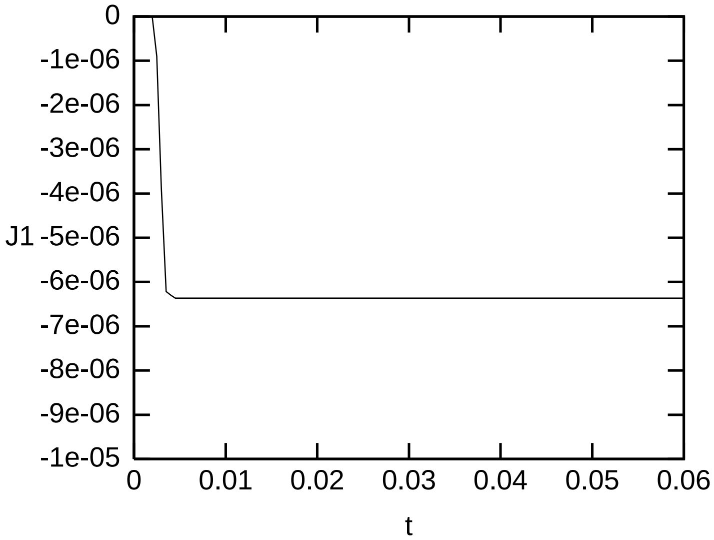
$$+ \left[\frac{W(\boldsymbol{C}_{n+1}) - W(\boldsymbol{C}_n) - DW(\boldsymbol{C}_{n+\frac{1}{2}}) : \boldsymbol{M}}{||\boldsymbol{M}||^2} \right] \boldsymbol{M}$$

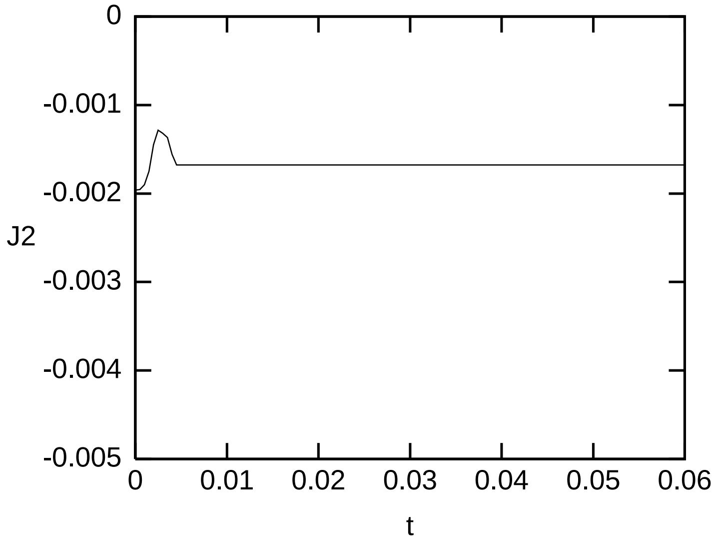
and $\boldsymbol{M} \triangleq \boldsymbol{C}_{n+1} - \boldsymbol{C}_n$.

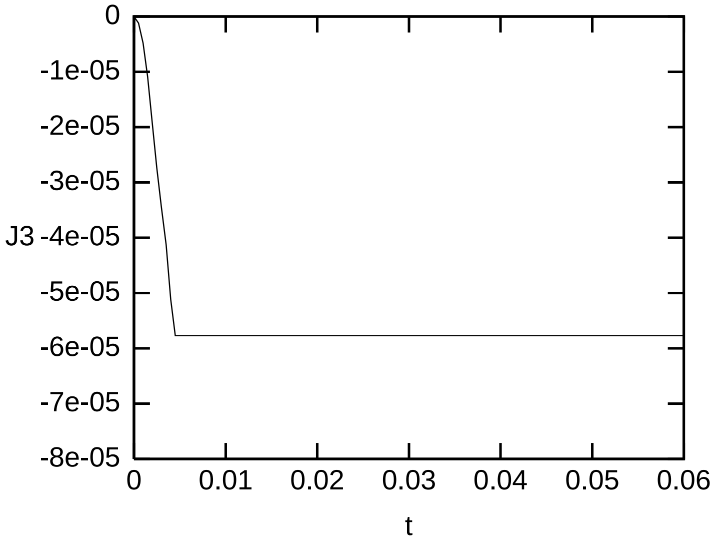
- $dW(\boldsymbol{C}_n, \boldsymbol{C}_{n+1})$ is a "discrete gradient"
- conserves $\boldsymbol{l}$, $\boldsymbol{j}$ and H

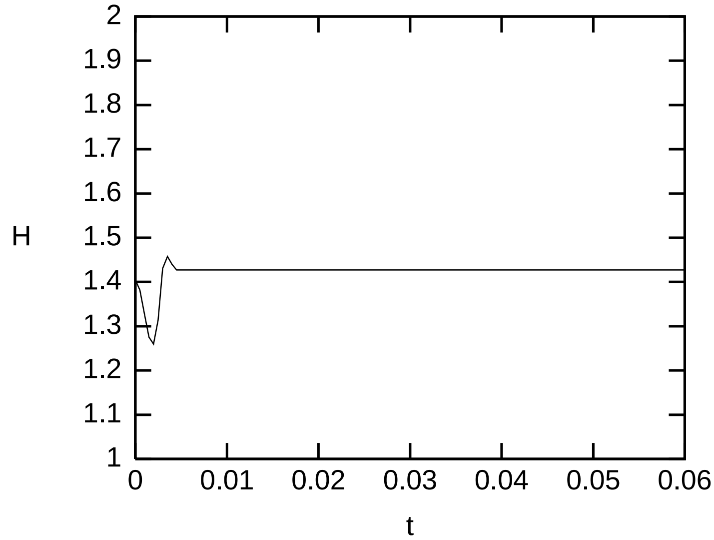
Conserving Scheme with Time Step $\Delta t = 0.0005s$

Angular Momentum and Energy Histories

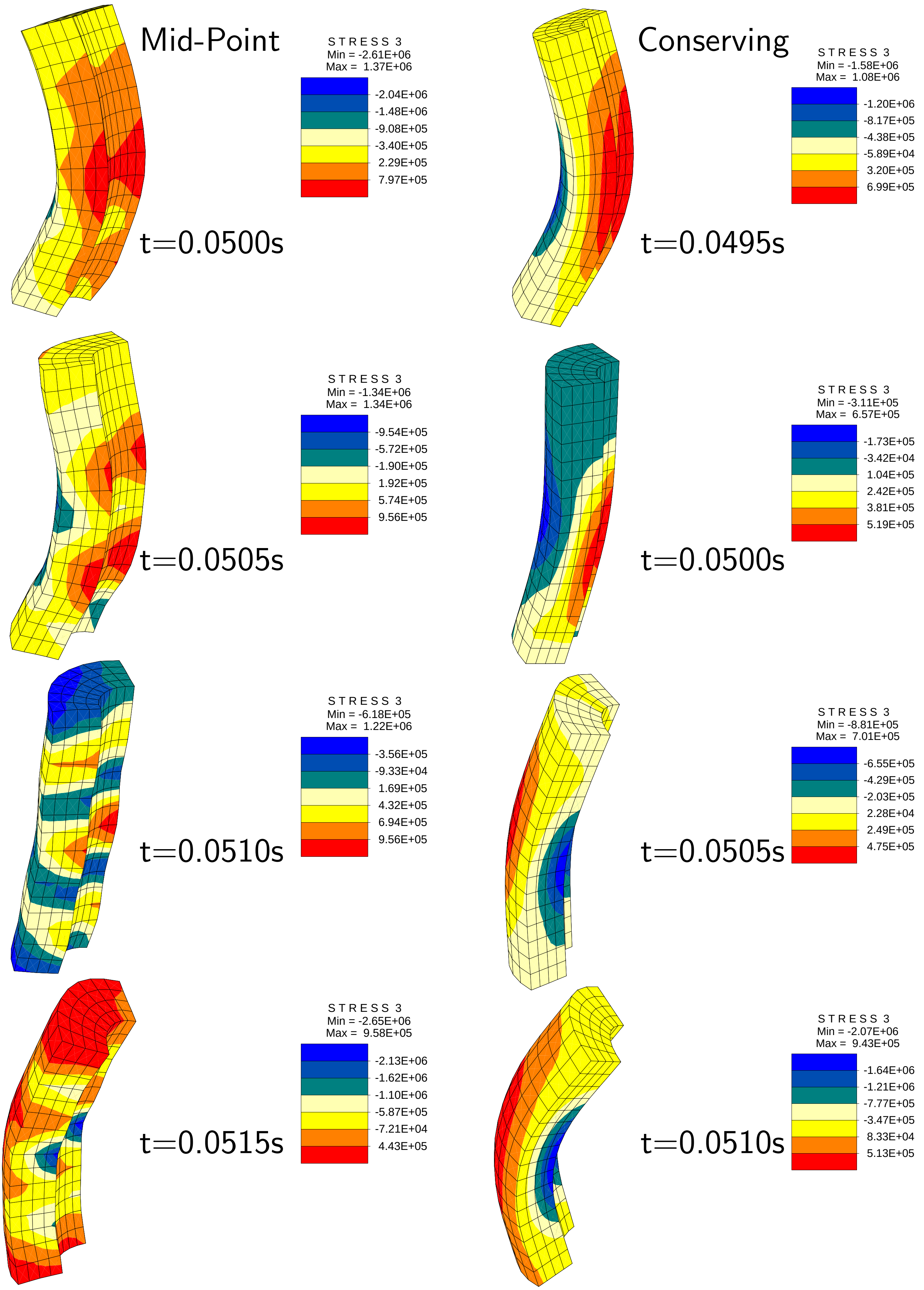








Comparison of Mid-Point and Conserving Schemes



Two remarks on conserving scheme:

- same formal order of accuracy as Mid-Point rule
- "conserving" modification cures coupling/stability problem

GENERAL CONSERVING SCHEMES

$$\dot{\boldsymbol{z}} = \boldsymbol{J}(\boldsymbol{z})\nabla H(\boldsymbol{z}) - \boldsymbol{D}(\boldsymbol{z})\nabla H(\boldsymbol{z})$$

$$\boldsymbol{z} \in \boldsymbol{R}^m, \qquad H : \boldsymbol{R}^m \to \boldsymbol{R},$$

$$\boldsymbol{J} = -\boldsymbol{J}^T \in \boldsymbol{R}^{m\times m}, \qquad \boldsymbol{D} = \boldsymbol{D}^T \geq 0 \in \boldsymbol{R}^{m\times m}$$

- Abstract framework based on "discrete gradients"
- can treat arbitrary integrals
- carries over to infinite-dimensions

Discrete Gradients

Definition

$dH : \boldsymbol{R}^m \times \boldsymbol{R}^m \to \boldsymbol{R}^m$ is a discrete gradient of H if

1) $dH(x,y) \cdot (y-x) = H(y) - H(x), \qquad \forall x, y \in \boldsymbol{R}^m$

2) $dH(x,x) = \nabla H(x), \qquad \forall x \in \boldsymbol{R}^m$

Example

$$dH(x,y)$$
$$= \nabla H(\frac{x+y}{2}) + \left[\frac{H(y) - H(x) - \nabla H(\frac{x+y}{2}) \cdot (y-x)}{|y-x|^2}\right](y-x)$$

General Conserving Scheme

To approximate

$$\dot{\boldsymbol{z}} = \boldsymbol{J}(\boldsymbol{z})\nabla H(\boldsymbol{z}) - \boldsymbol{D}(\boldsymbol{z})\nabla H(\boldsymbol{z})$$

consider

$$\boxed{\frac{\boldsymbol{z}_{n+1} - \boldsymbol{z}_n}{\Delta t} = \boldsymbol{J}(\boldsymbol{z}_{n+\frac{1}{2}})dH(\boldsymbol{z}_n, \boldsymbol{z}_{n+1}) - \boldsymbol{D}(\boldsymbol{z}_{n+\frac{1}{2}})dH(\boldsymbol{z}_n, \boldsymbol{z}_{n+1})}$$

where $\boldsymbol{z}_{n+\frac{1}{2}} = \frac{1}{2}(\boldsymbol{z}_{n+1} + \boldsymbol{z}_n)$.

Key Features

Energy decay/conservation

$$\begin{aligned} \frac{H(\boldsymbol{z}_{n+1}) - H(\boldsymbol{z}_n)}{\Delta t} &= \frac{dH(\boldsymbol{z}_n, \boldsymbol{z}_{n+1}) \cdot (\boldsymbol{z}_{n+1} - \boldsymbol{z}_n)}{\Delta t} \\ &= dH \cdot [\boldsymbol{J}dH - \boldsymbol{D}dH] \\ &= -dH \cdot \boldsymbol{D}dH \leq 0 \end{aligned}$$

and

$$\frac{H(\boldsymbol{z}_{n+1}) - H(\boldsymbol{z}_n)}{\Delta t} = 0 \quad \text{when} \quad \boldsymbol{D} \equiv \boldsymbol{O}.$$

Momentum conservation (linear/angular momentum)

Suppose

- $H = \widehat{H} \circ \boldsymbol{\zeta}$
- $\boldsymbol{\zeta} : \boldsymbol{R}^m \to \boldsymbol{R}^k$ invariants under a symmetry group, e.g.

$$\boldsymbol{\zeta}(\boldsymbol{z}) = (|\boldsymbol{q}|^2, \boldsymbol{q} \cdot \boldsymbol{p}, |\boldsymbol{p}|^2), \quad \boldsymbol{z} = (\boldsymbol{q}, \boldsymbol{p}) \in \boldsymbol{R}^6$$

"rotational invariants"

- $F(z)$ an integral associated with $\boldsymbol{\zeta}$, i.e. $\boldsymbol{J}\nabla F \in \ker[\nabla\boldsymbol{\zeta}]$

Result

$\boldsymbol{\zeta}(z)$, $F(z)$ at most quadratic
$\oplus$
"composed" discrete gradient $d^c H = d\widehat{H} \circ \nabla\boldsymbol{\zeta}$
$\Downarrow$
conservation of F, H when $\boldsymbol{D} \equiv \boldsymbol{O}$

Two remarks:

- internal force $d\widehat{H}(\boldsymbol{\zeta}_n, \boldsymbol{\zeta}_{n+1})$ depends only on invariants
- order of accuracy same as Mid-Point rule

Closing Remarks

- Why does the Mid-Point Rule fail?

  $\Rightarrow$ artificial coupling between internal forces/rotations

- Is there a cure?

  $\Rightarrow$ decoupled discretization $\oplus$ discrete gradients

- Why preserve decay inequalities and integrals?

  $\Rightarrow$ enhanced stability

  $\Rightarrow$ useful for constrained systems:

Lagrangian $\oplus$ config constraints	$\Rightarrow$	Hamiltonian $\oplus$ integrals

- Other application for discrete gradients:

  $\Rightarrow$ discrete gradient flow

$$\frac{\boldsymbol{z}_{n+1} - \boldsymbol{z}_n}{\Delta t} = -dF(\boldsymbol{z}_{n+1}, \boldsymbol{z}_n)$$

"generates strictly decreasing sequence"

$$F_{n+1} - F_n = -\Delta t \, |dF|^2 < 0$$

$$dF = \mathbf{0} \quad \Leftrightarrow \quad \nabla F = \mathbf{0}$$