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Stability, Accuracy, Conservation and Invariance Properties of a Predictor/Multi-corrector Method for Staggered Lagrangian Hydrodynamics

E. Love, G. Scovazzi*, W.J. Rider

1431 Computational Shock- and Multi-physics Department
Sandia National Laboratories, Albuquerque (NM), USA

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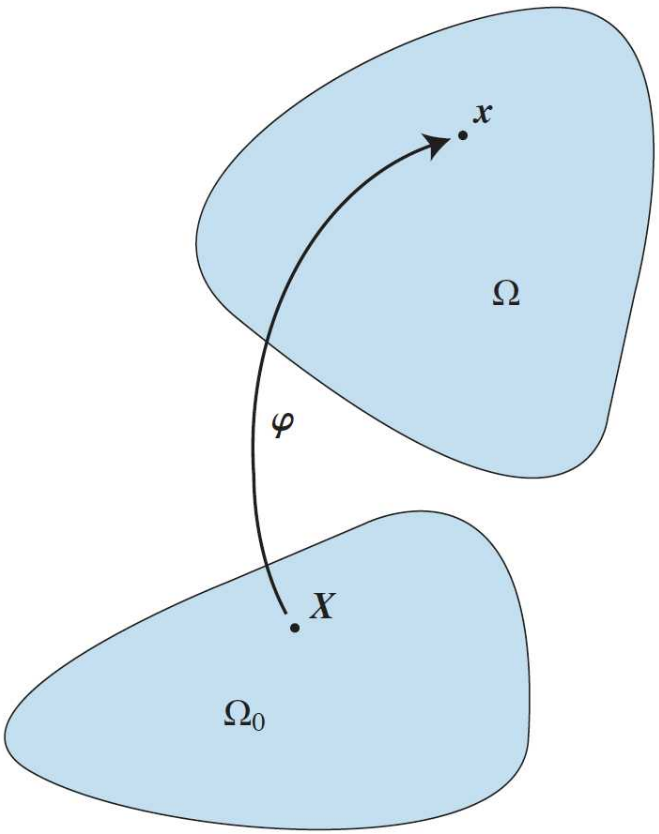
Overview

Analysis of a popular predictor/corrector method:

- Used by ALE-GRA (SNL)
- Identical in 1D to the compatible hydrodynamics time integrators at LANL, and the compatible FEM of Barlow at AWE
- Von Neumann analysis (1D) to understand stability and accuracy of the various P/C iterates
- Conservation of angular momentum
- Incremental objectivity

Lagrangian Shock Hydrodynamics Equations



$$\dot{\boldsymbol{u}} = \boldsymbol{v} \,,$$

$$\rho J = \rho_0 \,,$$

$$0 = \rho \dot{\boldsymbol{v}} + \nabla_x p - \nabla_x \cdot (\rho \, \nu \, \nabla_x^S \boldsymbol{v}) \,,$$

$$0 = \rho \dot{\epsilon} + p \nabla_x \cdot \boldsymbol{v} - \rho \, \nu \, \nabla_x^S \boldsymbol{v} : \nabla_x^S \boldsymbol{v} \,.$$

After some manipulations …

$$\rho \left. \frac{\partial \epsilon}{\partial p} \right|_{\rho} \left(\dot{p} + \rho c_s^2 \nabla_x \cdot \boldsymbol{v} \right) = \rho \, \nu \, \nabla_x^S \boldsymbol{v} : \nabla_x^S \boldsymbol{v} \,.$$

Structure of the Shock Hydrodynamics

A nonlinear wave equation in mixed form:

$$\rho \dot{\boldsymbol{v}} + \nabla_x p = \nabla_x \cdot (\rho \, \nu \, \nabla_x^S \boldsymbol{v}) \, ,$$

$$\dot{p} + \rho c_s^2 \nabla_x \cdot \boldsymbol{v} = \Gamma \, (\rho \nu \, \nabla_x^S \boldsymbol{v} : \nabla_x^S \boldsymbol{v}) \; .$$

Here, we consider only energy/momentum equations, and

$$\Gamma = \frac{1}{\rho \left. \dfrac{\partial \epsilon}{\partial p} \right|_\rho} = \frac{1}{\rho} \left. \frac{\partial p}{\partial \epsilon} \right|_\rho$$

is the Grüneisen parameter.

Linearization of the equations

Small strains/displacements:

$$\boldsymbol{v} = \boldsymbol{v}' << 1$$

$$\boldsymbol{u} = \boldsymbol{u}' << 1$$

Small thermodynamic perturbation of base state:

$$\rho = \bar{\rho} + \rho', \qquad \bar{\rho} = \text{const.}, \qquad \rho' << 1$$

$$p = \bar{p} + p', \qquad \bar{p} = \text{const.}, \qquad p' << 1$$

$$c_s = \bar{c}_s + c_s', \qquad \bar{c}_s = \text{const.}, \qquad c_s' << 1$$

Linearization of the equations

Linearized equations (momentum/energy):

$$\bar{\rho}\dot{\boldsymbol{v}}' + \nabla_X p' = \bar{\rho}\,\bar{\nu}\,\nabla_X \cdot (\nabla_X^s \boldsymbol{v}')\ ,$$

$$\dot{p}' + \bar{\rho}\,\bar{c}_s^2\,\nabla_X \cdot \boldsymbol{v}' = 0\ ,$$

Viscosity term is second-order, hence negligible

Displacement/mass conservation eqs. decouple:

$$\dot{\boldsymbol{u}}' = \boldsymbol{v}'\ ,$$

$$\dot{\rho}' + \bar{\rho}\nabla_X \cdot \boldsymbol{v}' = 0\ .$$

We will consider just the momentum and energy equations and drop the notation with “primes” and “bars”.

Linearization of the equations

Galerkin FEM formulation on a periodic 1D-torus:

$$0 = \int_{\mathbb{T}} \psi \, \dot{V} - \int_{\mathbb{T}} \psi_{,X} P + \int_{\mathbb{T}} \psi_{,X} \nu V_{,X} \,,$$

$$0 = \int_{\mathbb{T}} \phi \, \dot{P} + \int_{\mathbb{T}} \phi \, c_s^2 V_{,X} \,,$$

$$V = \rho v$$

Time discretization with mid-point P/C method:

$$0 = \int_{\mathbb{T}} \psi \left(V_{n+1}^{(i+1)} - V_n \right) - \Delta t \int_{\mathbb{T}} \psi_{,X} P_{n+1/2}^{(i)} + \Delta t \int_{\mathbb{T}} \psi_{,X} \nu (V_{,X})_{n+1/2}^{(i)} \,,$$

$$0 = \int_{\mathbb{T}} \phi \left(P_{n+1}^{(i+1)} - P_n \right) + \Delta t \int_{\mathbb{T}} \phi \, c_s^2 (V_{,X})_{n+1/2}^{(i+1)} \,,$$

Linearization of the equations

Discrete equations:

$$0 = V^{(i+1)}_{j,n+1} - V_{j,n} + \frac{\sigma}{2c_s}\left(P^{(i)}_{j+1/2,n+1} + P_{j+1/2,n} - P^{(i)}_{j-1/2,n+1} - P_{j-1/2,n}\right)$$
$$+ \frac{\kappa}{2}\left(-V^{(i)}_{j+1,n+1} - V_{j+1,n} + 2V^{(i)}_{j,n+1} + 2V_{j,n} - V^{(i)}_{j-1,n+1} - V_{j-1,n}\right) \, ,$$

$$0 = P^{(i+1)}_{j+1/2,n+1} - P_{j+1/2,n} + \frac{c_s\sigma}{2}\left(V^{(i+1)}_{j+1,n+1} + V_{j+1,n} - V^{(i+1)}_{j-1,n+1} - V_{j-1,n}\right) \, ,$$

$$\sigma = \frac{c_s \Delta t}{h} \qquad \kappa = \frac{\nu \Delta t}{h^2}$$

These equations are identical to the FD scheme in:

-*Bauer-Burton-Caramana-Loubère-Shaskov-Whalen*, JCP **218** (2006),

-*Bauer-Loubère-Wendroff*, SINUM **46** (2008),

and the FEM scheme in

-Barlow, IJNMF **56** (2008).

Von Neumann Analysis

Discrete Fourier Transform:

$$V_{j,n}^{(i)} = \sum_{k=-N/2+1}^{N/2} \hat{V}_{k,n}^{(i)} e^{\mathrm{i}\beta_k j} ,$$

$$P_{j+1/2,n}^{(i)} = \sum_{k=-N/2+1}^{N/2} \hat{P}_{k,n}^{(i)} e^{\mathrm{i}\beta_k (j+1/2)} ,$$

$$\hat{\mathbf{Z}}_{k,n}^{(i)} = \left\{ \begin{array}{c} \hat{V}_{k,n}^{(i)} \\ \hat{P}_{k,n}^{(i)} \end{array} \right\}$$

$$(\boldsymbol{I} + \boldsymbol{A}_0)\hat{\mathbf{Z}}_{k,n+1}^{(i+1)} = \boldsymbol{A}_1 \hat{\mathbf{Z}}_{k,n+1}^{(i)} + (\boldsymbol{I} + \boldsymbol{A}_2)\hat{\mathbf{Z}}_{k,n} ,$$

$$\boldsymbol{I} = \left[\begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right], \qquad \boldsymbol{A}_1 = \left[\begin{array}{cc} \kappa\,(\cos(\beta_k) - 1) & -\mathrm{i}\frac{1}{2c_s}\sigma \sin\left(\frac{\beta_k}{2}\right) \\ 0 & 0 \end{array} \right],$$

$$\boldsymbol{A}_0 = \left[\begin{array}{cc} 0 & 0 \\ \mathrm{i}\frac{c_s}{2}\sigma \sin\left(\frac{\beta_k}{2}\right) & 0 \end{array} \right], \qquad \boldsymbol{A}_2 = \left[\begin{array}{cc} \kappa\,(\cos(\beta_k) - 1) & -\mathrm{i}\frac{1}{2c_s}\sigma \sin\left(\frac{\beta_k}{2}\right) \\ -\mathrm{i}\frac{c_s}{2}\sigma \sin\left(\frac{\beta_k}{2}\right) & 0 \end{array} \right].$$

Von Neumann Analysis

Modal conditions (real solution):

$$\hat{\mathbf{Z}}^{(i)}_{-k,n} = \left(\hat{\mathbf{Z}}^{(i)}_{k,n}\right)^{*} , \quad \text{for } 0 \leq k \leq N/2 - 1 , \; \hat{\mathbf{Z}}^{(i)}_{N/2,n} = \mathbf{0} .$$

First and (i+1)-th iterates:

$$\begin{aligned} \hat{\mathbf{Z}}^{(1)}_{k,n+1} &= \boldsymbol{B}_1 \hat{\mathbf{Z}}^{(0)}_{k,n+1} + \boldsymbol{B}_0 \hat{\mathbf{Z}}_{k,n} \\ &= (\boldsymbol{B}_0 + \boldsymbol{B}_1) \hat{\mathbf{Z}}_{k,n} \\ &= \boldsymbol{G}^{(1)} \hat{\mathbf{Z}}_{k,n} , \end{aligned}$$

$$\begin{aligned} \hat{\mathbf{Z}}^{(i+1)}_{k,n+1} &= \boldsymbol{B}_1 \hat{\mathbf{Z}}^{(i)}_{k,n+1} + \boldsymbol{B}_0 \hat{\mathbf{Z}}_{k,n} \\ &= \left(\boldsymbol{B}_1 \boldsymbol{G}^{(i)} + \boldsymbol{B}_0\right) \hat{\mathbf{Z}}_{k,n} \\ &= \boldsymbol{G}^{(i+1)} \hat{\mathbf{Z}}_{k,n} . \end{aligned}$$

Implicit (infinite iteration) limit:

$$\hat{\mathbf{Z}}_{k,n+1} = (\boldsymbol{I} + \boldsymbol{A}_0 - \boldsymbol{A}_1)^{-1} (\boldsymbol{I} + \boldsymbol{A}_2) \, \hat{\mathbf{Z}}_{k,n} = \boldsymbol{G}^{(\infty)} \hat{\mathbf{Z}}_{k,n} .$$

Von Neumann Analysis

Stability conditions:

Define $||\mathbf{G}^{(i)}|| = \max_{\mathbf{s}\in\mathbb{R}^2\backslash\mathbf{0}} \dfrac{||\mathbf{G}^{(i)}\mathbf{s}||}{||\mathbf{s}||} \leq 1$

and the spectral radius $\rho(\mathbf{G}^{(i)}) = \max\{|\lambda(\mathbf{G}^{(i)})|\} \leq ||\mathbf{G}^{(i)}||$

Theorem *Let* $\mathbf{A} \in \mathbb{C}^{m\times m}$, *where* $\mathbb{C}$ *is the complex field. Then:* $\lim_{n\to\infty} \mathbf{A}^n = \mathbf{0}$ *if and only if* $\rho(\mathbf{A}) < 1$.

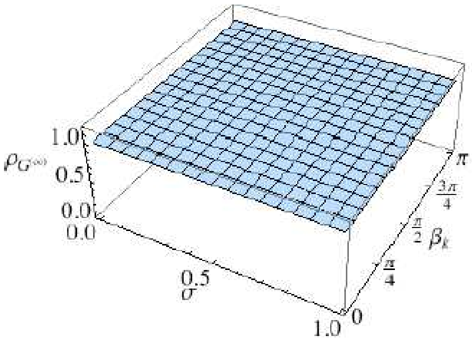
$\rho(\mathbf{G}^{(i)}) < 1 \Rightarrow$ stability ,

$\rho(\mathbf{G}^{(i)}) > 1 \Rightarrow$ instability .

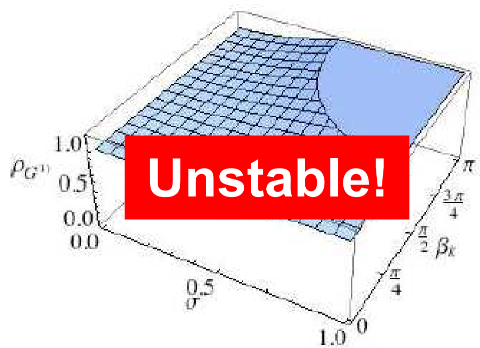
One can treat the case when the spectral radius is equal to unity as a limit case.

Von Neumann Analysis

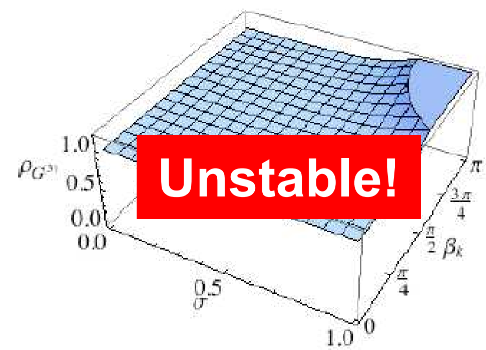
Spectral radii of various iterates (no viscosity):



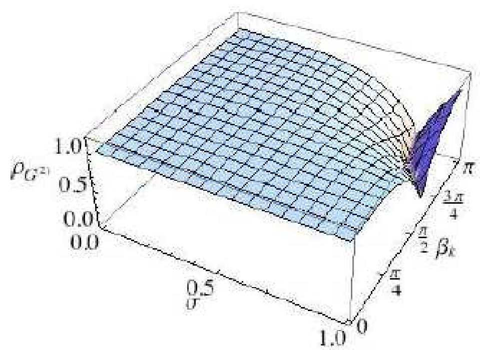
(a) Implicit. $\kappa = 0$.



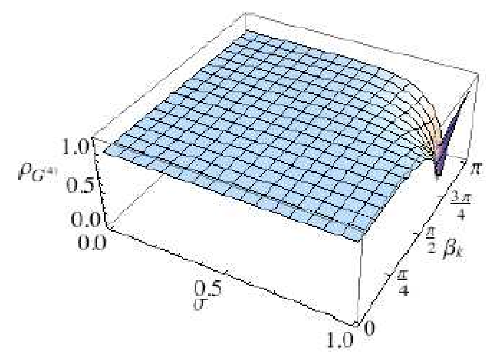
(d) 1st iterate. $\kappa = 0$. (C)



(j) 3rd iterate. $\kappa = 0$. (C)



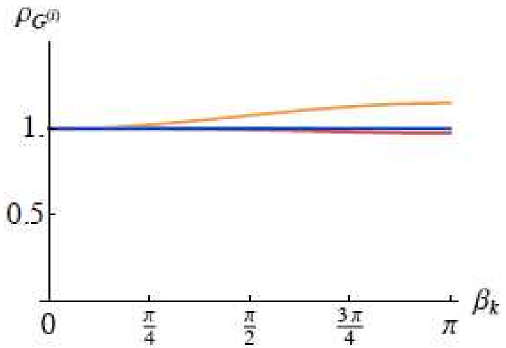
(g) 2nd iterate. $\kappa = 0$. (C)



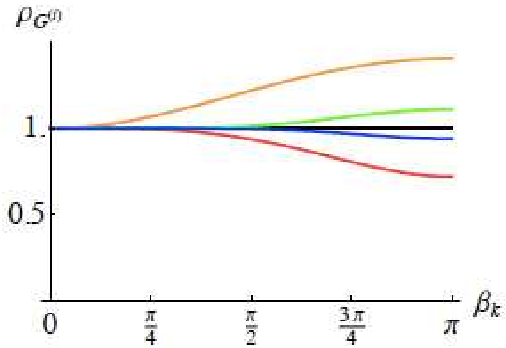
(m) 4th iterate. $\kappa = 0$. (C)

Von Neumann Analysis

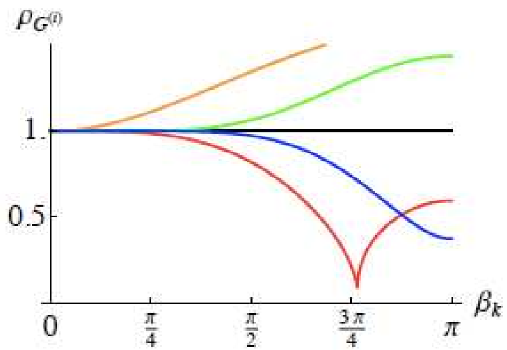
Spectral radii of various iterates (no viscosity):



(a) $\sigma = 0.4$. (C)



(b) $\sigma = 0.7$. (C)



(d) $\sigma = 0.9$. (C)

- Implicit
- First iterate
- Second iterate
- Third iterate
- Fourth iterate

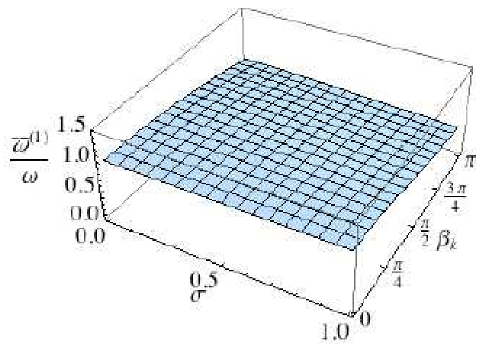
Von Neumann Analysis

Dispersion error:

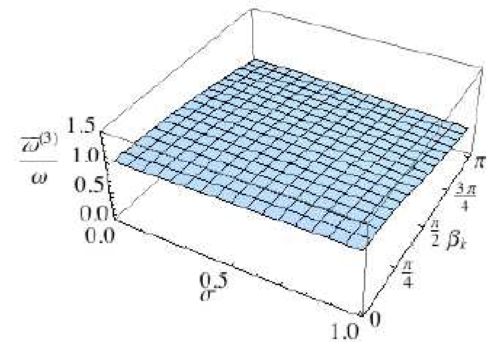
$$\lambda(\mathbf{G}^{(i)}) = |\lambda(\mathbf{G}^{(i)})| e^{\mathrm{i}\bar{\omega}\Delta t}$$

$$\omega \Delta t = \sigma \beta_k$$

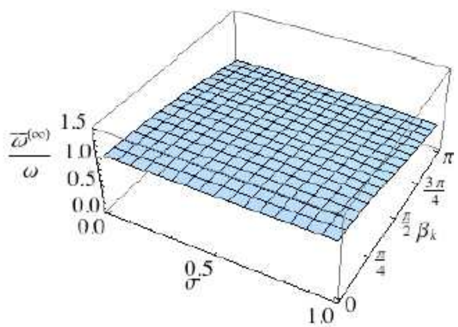
$$\frac{\bar{\omega}}{\omega} = \frac{\arg(\lambda(\sigma, \beta_k))}{\sigma \beta_k}$$



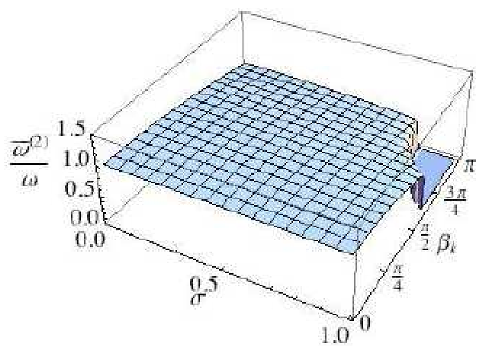
(c) 1st iterate. (C)



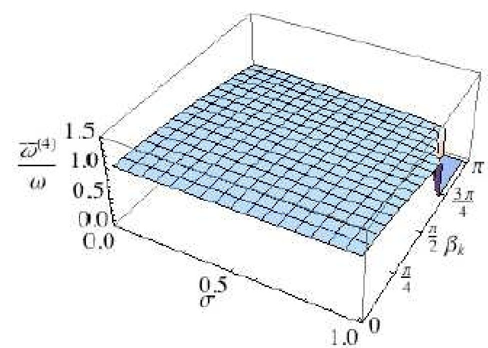
(g) 3rd iterate. (C)



(a) Implicit.



(e) 2nd iterate. (C)



(i) 4th iterate. (C)

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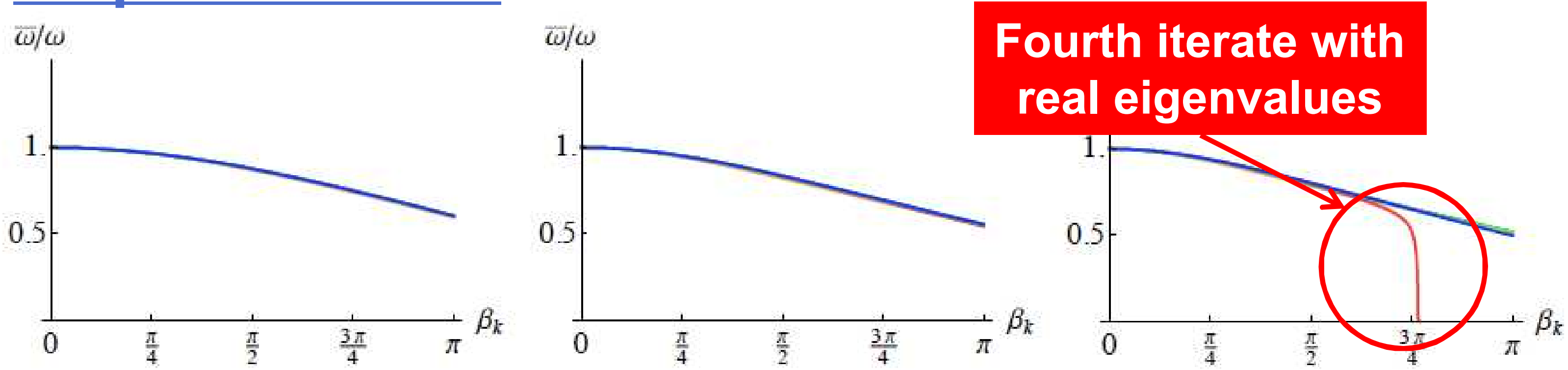
Von Neumann Analysis

Dispersion error:



(a) $\sigma = 0.4(C)$. (b) $\sigma = 0.7(C)$. (d) $\sigma = 0.9(C)$.

Second-order accurate for 2 or more iterations

$$\lambda(\mathbf{G}^{(i)}) = e^{(-\bar{\xi}+\mathrm{i}\bar{\omega})\Delta t}$$

$$\bar{\xi}(\mathbf{G}^{(1)}) = -\frac{1}{4}c_s^2\tilde{k}^2\Delta t + O(h^2\Delta t) ,$$

$$\bar{\omega}(\mathbf{G}^{(1)}) = \omega - \frac{1}{24}c_s h^2\tilde{k}^3 - \frac{11}{96}c_s^3\tilde{k}^3\Delta t^2 + O(\Delta t^2 h^2) ,$$

$$\bar{\xi}(\mathbf{G}^{(2)}) = \frac{1}{16}c_s^4\tilde{k}^4\Delta t^3 + O(h^2\Delta t^3) ,$$

$$\bar{\omega}(\mathbf{G}^{(2)}) = \omega - \frac{1}{24}c_s h^2\tilde{k}^3 - \frac{1}{12}c_s^3\tilde{k}^3\Delta t^2 + O(\Delta t^2 h^2) ,$$

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Von Neumann Analysis

Stable time-step limit:

Analyzing the highest wave number

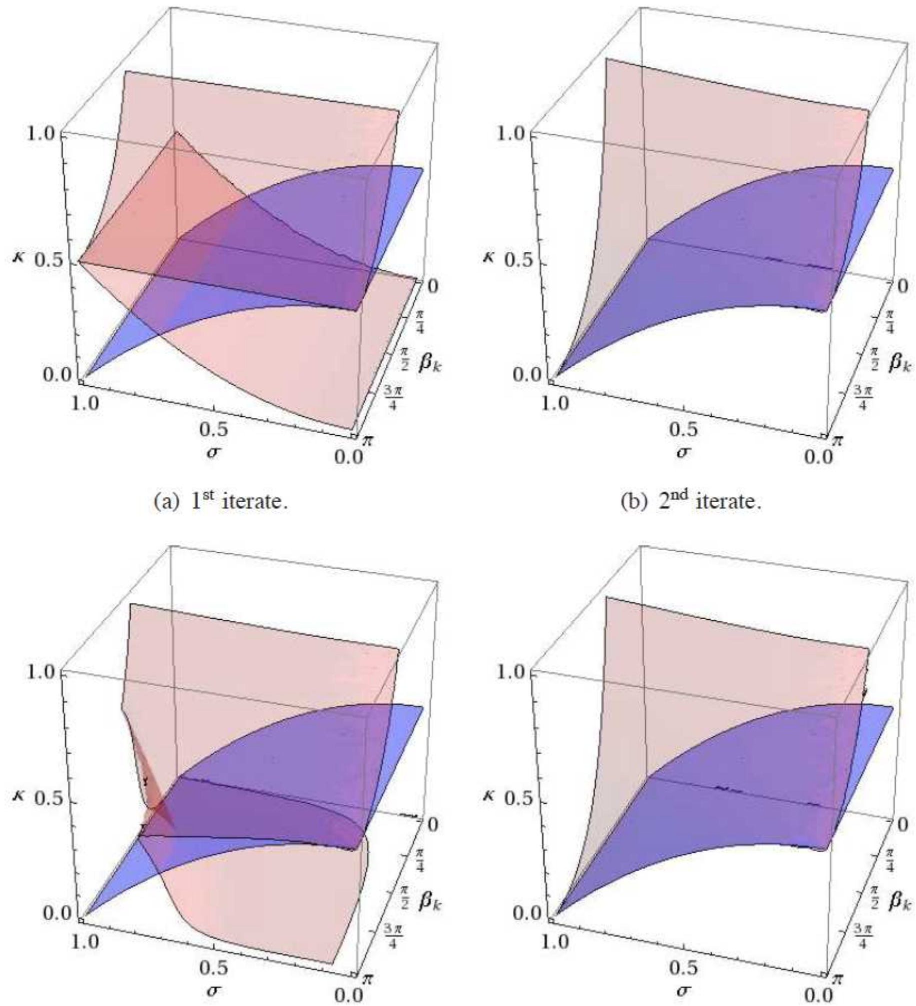
$$\Delta t \leq \frac{h^2}{\nu + \sqrt{\nu^2 + c_s^2 h^2}}$$

Acoustic case:

$$\Delta t \leq \frac{h}{c_s}$$

Diffusive case:

$$\Delta t \leq \frac{h^2}{2\nu}$$



(a) 1st iterate. (b) 2nd iterate. (c) 3rd iterate. (d) 4th iterate.

Numerical tests (no art. viscosity)

Euler equations: Periodic breaking wave

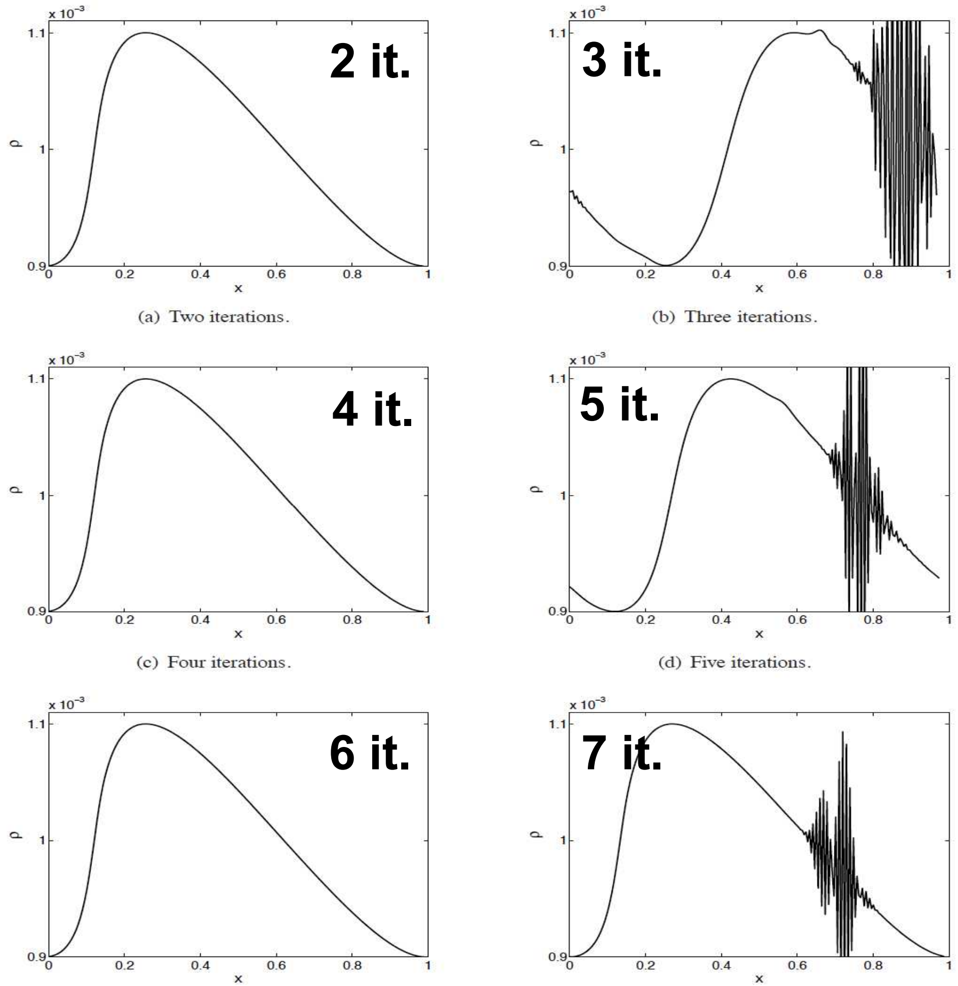
Initial conditions:

$$\rho(x,0) = 0.001\,(1.0 + 0.1\sin(2\pi x))$$

$$p(x,0) = 10^6\left(\frac{\rho(x,0)}{0.001}\right)^{\gamma},$$

$$v(x,0) = 2\frac{(c_{s_0} - c_s)}{\gamma - 1},$$

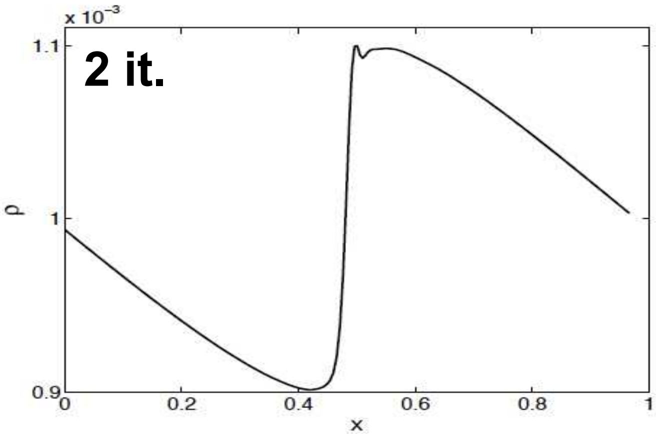
$$c_s = \left(\gamma\frac{p(x,0)}{\rho(x,0)}\right)^{1/2},$$



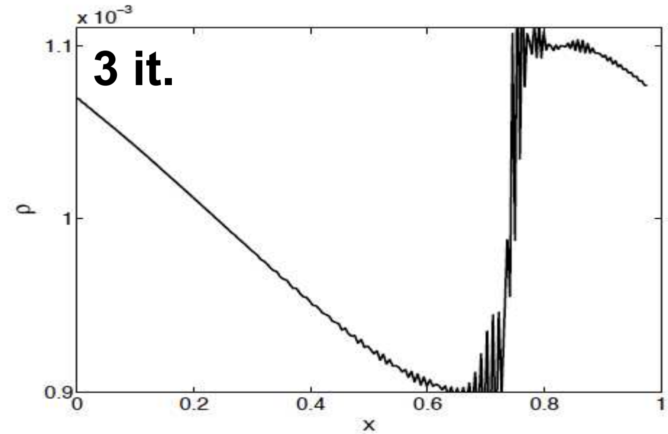
(a) Two iterations. (b) Three iterations. (c) Four iterations. (d) Five iterations. (e) Six iterations. (f) Seven iterations.

Numerical tests (with art. viscosity)

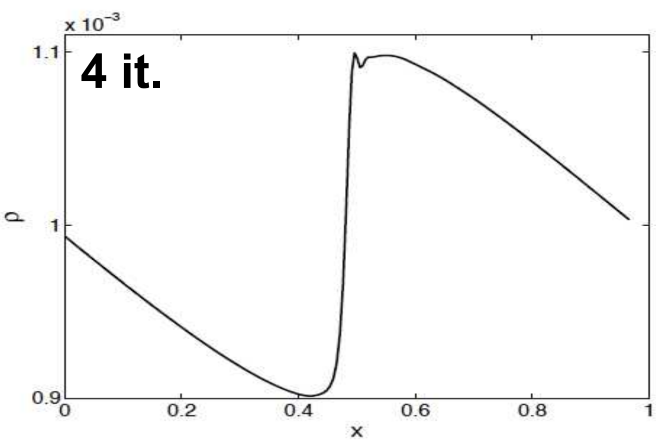
Periodic breaking wave:



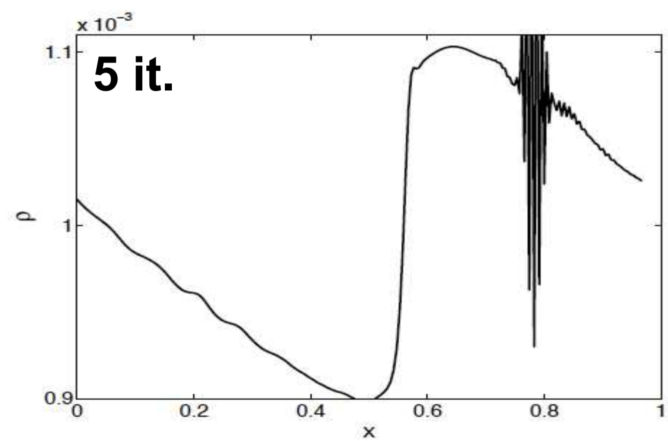
(a) Two iterations.



(b) Three iterations.



(c) Four iterations.



(d) Five iterations.

Angular Momentum Conservation

Abstract discussion (Homogeneous Neumann BCs)

$$0 = \int_{\Omega_0} \delta\boldsymbol{\varphi} \cdot \rho_0 \left(\boldsymbol{v}_{n+1}^{(i+1)} - \boldsymbol{v}_n \right) + \Delta t \int_{\Omega_{n+1/2}^{(i)}} (\nabla_x(\delta\boldsymbol{\varphi}))_{n+1/2}^{(i)} : \boldsymbol{\sigma}_{n+1/2}^{(i)}$$

Test with a variation $\delta\boldsymbol{\varphi} = \boldsymbol{\xi} \times \boldsymbol{\varphi}_{n+1/2}^{(j)}$, with $\boldsymbol{\xi} \in \mathbb{R}^3$

Define $\hat{\boldsymbol{\xi}}$, a *skew-symmetric* tensor s. t. $\hat{\boldsymbol{\xi}}\mathbf{a} = (\boldsymbol{\xi} \times \mathbf{a}), \forall \mathbf{a} \in \mathbb{R}^3$

Use $J_{n+1/2}^{(i)} \boldsymbol{\sigma}_{n+1/2}^{(i)} = \boldsymbol{F}_{n+1/2}^{(i)} \boldsymbol{S}_{n+1/2}^{(i)} \boldsymbol{F}_{n+1/2}^{(i)T}$, to obtain

$$0 = \boldsymbol{\xi} \cdot \int_{\Omega_0} \boldsymbol{\varphi}_{n+1/2}^{(j)} \times \rho_0 \left(\boldsymbol{v}_{n+1}^{(i+1)} - \boldsymbol{v}_n \right)$$

$$+ \Delta t \, \hat{\boldsymbol{\xi}} : \left(\int_{\Omega_0} J_{n+1/2}^{(i)} \boldsymbol{\sigma}_{n+1/2}^{(i)} \right),$$

Cancellation only if Cauchy stress is symmetric!

Angular Momentum Conservation

Mid-point integrator

$$0 = \boldsymbol{\xi} \cdot \left(\int_{\Omega_0} \boldsymbol{\varphi}^{(\infty)}_{n+1/2} \times \rho_0 \left(\boldsymbol{v}^{(\infty)}_{n+1} - \boldsymbol{v}_n \right) \right) + \Delta t \, \hat{\boldsymbol{\xi}} : \left(\int_{\Omega_0} J^{(\infty)}_{n+1/2} \, \boldsymbol{\sigma}^{(\infty)}_{n+1/2} \right) ,$$

Defining $\Pi_n := \int_{\Omega_n} \boldsymbol{\varphi}_n \times (\rho_n \boldsymbol{v}_n) = \int_{\Omega_0} \boldsymbol{\varphi}_n \times (\rho_0 \boldsymbol{v}_n)$,

We obtain, due to the symmetry of the stress tensor, *angular momentum conservation*, that is:

$$0 = \boldsymbol{\xi} \cdot (\Pi_{n+1} - \Pi_n)$$

Angular Momentum Conservation

Predictor/multi-corrector:

$$0 = \xi \cdot \left(\Pi_{n+1}^{(i+1)} - \Pi_n \right) - \xi \cdot \left(\frac{\Delta t}{4} \int_{\Omega_0} \rho_0 \left(\boldsymbol{v}_{n+1}^{(i+1)} - \boldsymbol{v}_{n+1}^{(i)} \right) \times \left(\boldsymbol{v}_{n+1}^{(i+1)} - \boldsymbol{v}_n \right) \right)$$

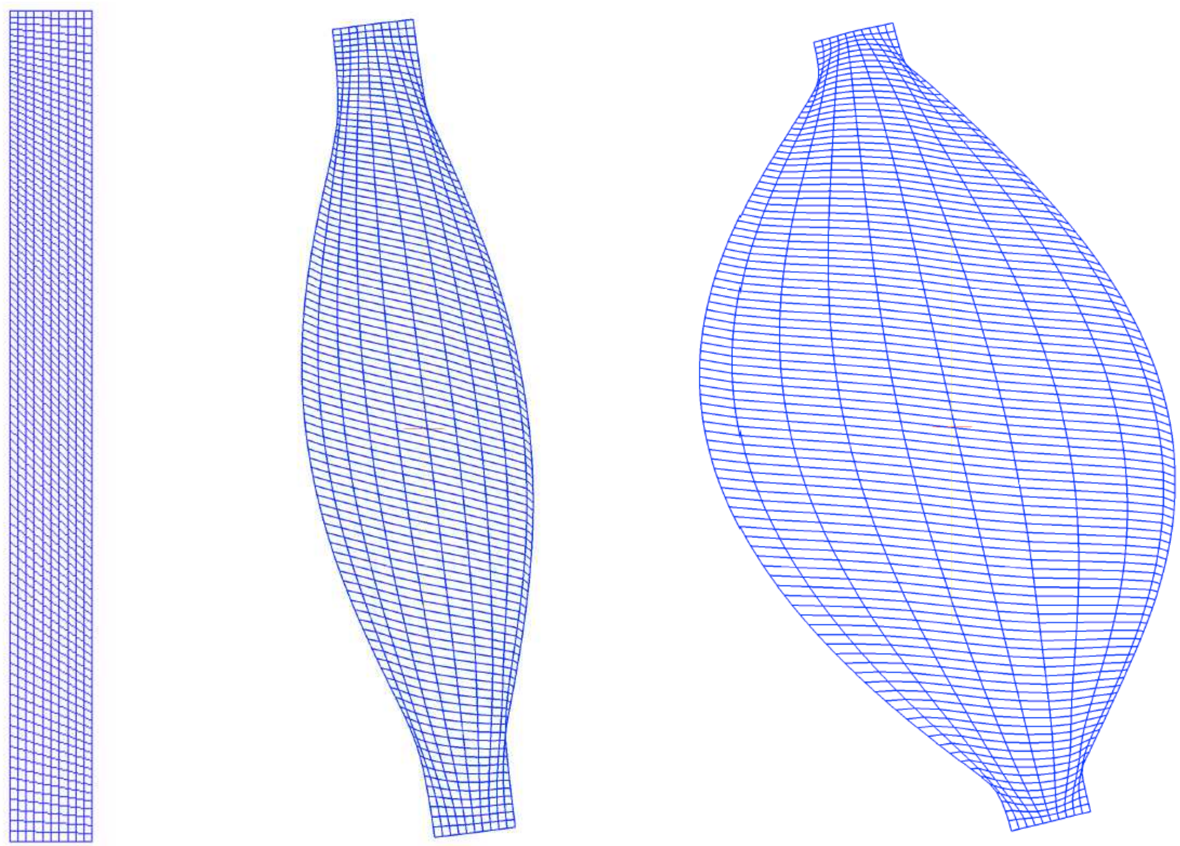
Different from zero in general, goes to zero for an infinite number of iterations

With Taylor-series expansions, one has the estimate:

$$\Pi_{n+1}^{(i)} - \Pi_n = \Pi_{n+1}^{(i)} - \Pi_{n+1}^{(\infty)} = O(\Delta t^{2i}) \ .$$

Angular Momentum Conservation

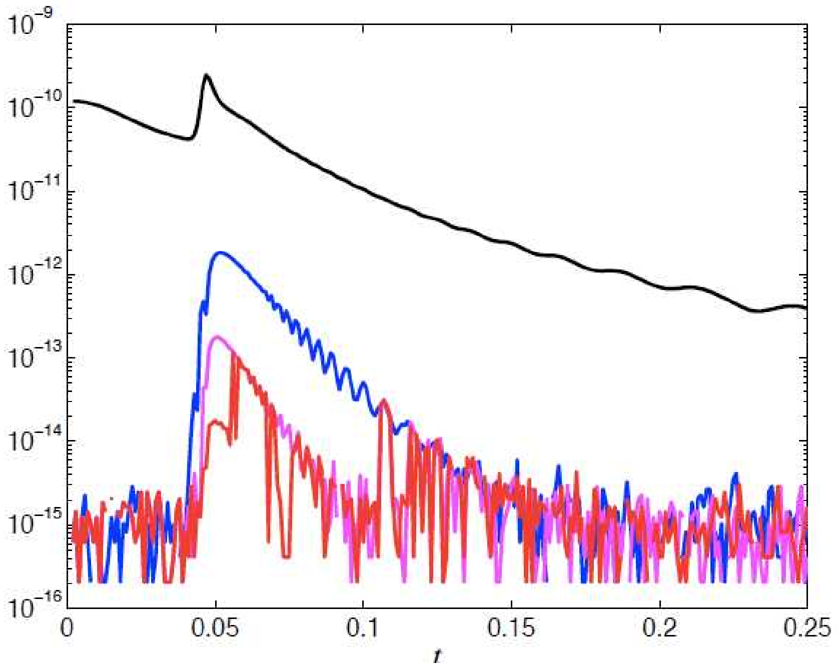
Numerical test: flow with expansion + rotation



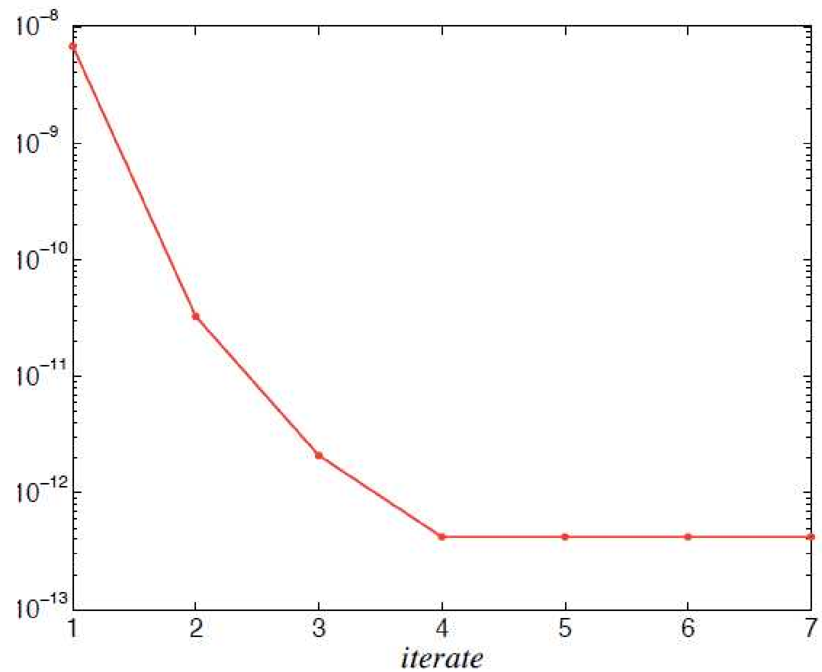
(a) $t = 0.$ (b) $t = 0.125.$ (c) $t = 0.25$

Angular Momentum Conservation

Numerical test: flow with expansion + rotation



(b) $\Delta_n \Pi$, various iterates.



(c) Semi-logarithmic plot, $\Delta\Pi(t = 0.25)$.

Incremental objectivity

Definition:

“Internal energy must be preserved under orthogonal rotations, that is $\boldsymbol{F}_{n+1} = \mathbf{Q}\boldsymbol{F}_n$ for some $\mathbf{Q} \in SO(3)$”

$$\rho_0 \left(\varepsilon_n^{(i+1)} - \varepsilon_n \right) = \Delta t \left((\nabla_x)_{n+1/2}^{(i)} \boldsymbol{v}_{n+1/2}^{(i+1)} \right) : \left(J_{n+1/2}^{(i)} \boldsymbol{\sigma}_{n+1/2}^{(i)} \right) .$$

Mid-point integrator is incrementally objective, but for the predictor/multi-corrector we have:

$$\varepsilon_{n+1}^{(i)} - \varepsilon_n = \varepsilon_{n+1}^{(i)} - \varepsilon_{n+1}^{(\infty)} = O(\Delta t^{2i}) .$$

References

Preprints available at: *www.cs.sandia.gov/~gscovaz*

1. E. Love, W.J. Rider, G. Scovazzi, "Stability Analysis of a Predictor/Multi-corrector Method for Staggered-Grid Lagrangian Shock Hydrodynamics", SAND-2009-1525J. *(In press & early view, J. Comp. Physics)*

2. E. Love, G. Scovazzi, *"On the angular momentum conservation and incremental objectivity properties of a predictor/multi-corrector method for Lagrangian shock hydrodynamics"*, SAND-2009-5236J. *(In press & early view, Comp. Meth. in Appl. Mech. & Eng.)*