Innovative Time Integration 2012

Higher order time integration of wave equations

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Content

Wave equations

Acoustic (scalar)

System of first order equations

$$\begin{cases} \kappa \dot{p} = -\nabla \cdot \underline{\mathbf{v}} \\ \rho \dot{\underline{\mathbf{v}}} = -\nabla p + \underline{\mathbf{f}} \end{cases}$$

Second order equation

$$\rho \kappa \ddot{p} - \nabla^2 p = -\nabla \cdot \underline{\mathbf{f}}$$

Wave equations

Electromagnetic (vectorial)

System of first order equations

$$\begin{cases} \mu \underline{\dot{\mathbf{H}}} = -\nabla \times \underline{\mathbf{E}} \\ \varepsilon \underline{\dot{\mathbf{E}}} = \nabla \times \underline{\mathbf{H}} - \sigma \underline{\mathbf{E}} - \underline{\mathbf{J}}_s \end{cases}$$

Second order equation

$$\nabla \times \left(\frac{1}{\mu} \nabla \times \underline{\mathbf{E}} \right) + \sigma \underline{\dot{\mathbf{E}}} + \varepsilon \underline{\ddot{\mathbf{E}}} = -\underline{\dot{\mathbf{J}}}_s$$

Wave equations

Elastodynamic (tensorial)

System of first order equations

$$\begin{cases} \underline{\underline{\underline{\underline{\mathbf{S}}}}} : \dot{\underline{\underline{\mathbf{T}}}} = \frac{1}{2}\left(\nabla \underline{\mathbf{v}} + (\nabla \underline{\mathbf{v}})^T\right) = \nabla_s \underline{\mathbf{v}} \\ \underline{\underline{\rho}} \cdot \dot{\underline{\mathbf{v}}} = \nabla \cdot \underline{\underline{\mathbf{T}}} + \underline{\mathbf{f}} \end{cases}$$

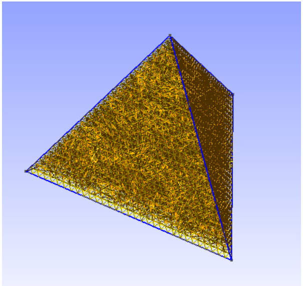
Second order equation

$$\underline{\underline{\rho}} \cdot \underline{\underline{\underline{\underline{\mathbf{S}}}}} : \ddot{\underline{\underline{\mathbf{T}}}} - \nabla_s \left(\nabla \cdot \dot{\underline{\underline{\mathbf{T}}}}\right) = \nabla_s \underline{\mathbf{f}}$$

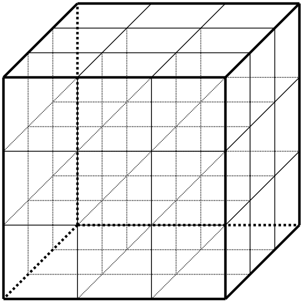
Spatial discretization

Methods

[Gedney & Navsariwala 1995, Marklein 1997]



Finite Element Method (FEM)



Finite Integration Technique (FIT)

Spatial discretization

semi-discrete problem

$$\begin{pmatrix} \mathbf{M}_u & 0 \\ 0 & \mathbf{M}_v \end{pmatrix} \begin{pmatrix} \dot{\mathbf{u}} \\ \dot{\mathbf{v}} \end{pmatrix} = \begin{pmatrix} 0 & -\mathbf{K}^T \\ \mathbf{K} & -\mathbf{M}_\sigma \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} + \begin{pmatrix} 0 \\ \mathbf{j} \end{pmatrix},$$

with

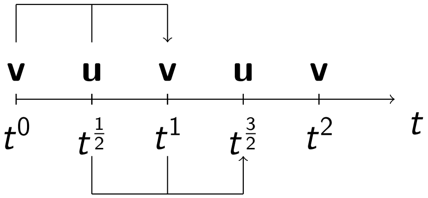
- $\mathbf{u}$, $\mathbf{v}$ vectors containing the unknowns (degrees of freedom)
- $\mathbf{M}_u$, $\mathbf{M}_v$ and $\mathbf{M}_\sigma$ discrete Hodge operators
- $\mathbf{K}$, $\mathbf{K}^T$ topological operators (div, grad, curl)
- $\mathbf{j}$ a vector containing the source information

Time integration

Leapfrog (LF2)

[Yee 1966]

$$\begin{cases} \mathbf{M}_u \dfrac{\mathbf{u}^{n+1/2} - \mathbf{u}^{n-1/2}}{\Delta t} = -\mathbf{K}^T \mathbf{v}^n \\ \mathbf{M}_v \dfrac{\mathbf{v}^{n+1} - \mathbf{v}^{n}}{\Delta t} = \mathbf{K}\mathbf{u}^{n+1/2} - \mathbf{M}_\sigma \dfrac{1}{2}\left(\mathbf{v}^{n+1} + \mathbf{v}^n\right) + \mathbf{j}^{n+1/2} \end{cases}$$



Time integration

Composition schemes (CO2)

[Verwer/Botchev 2008, Hairer/Lubich/Wanner 2002]

Consider a system of the following form:

$$\begin{cases} \dot{\mathbf{u}} &= f(t, \mathbf{v}) \\ \dot{\mathbf{v}} &= g(t, \mathbf{u}, \mathbf{v}) \end{cases} . \tag{1}$$

We apply subsequently the integration rule $\Phi_{\Delta t/2}$, with

$$\Phi_{\Delta t} = \begin{cases} \mathbf{u}^{n+1} &= \mathbf{u}^n + \Delta t f(t^{n+1}, \mathbf{v}^{n+1}) \\ \mathbf{v}^{n+1} &= \mathbf{v}^n + \Delta t g(t^{n+1}, \mathbf{u}^n, \mathbf{v}^{n+1}) \end{cases} , \tag{2}$$

and its adjoint $\Phi^*_{\Delta t/2}$, with

$$\Phi^*_{\Delta t} = \begin{cases} \mathbf{u}^{n+1} &= \mathbf{u}^n + \Delta t f(t^n, \mathbf{v}^n) \\ \mathbf{v}^{n+1} &= \mathbf{v}^n + \Delta t g(t^n, \mathbf{u}^{n+1}, \mathbf{v}^n) \end{cases} . \tag{3}$$

Time integration

Composition schemes (CO2)

[Verwer/Botchev 2008, Hairer/Lubich/Wanner 2002]

We now have a *three* equations to solver per timestep:

$$\begin{cases} \mathbf{M}_u \dfrac{\mathbf{u}^{n+1/2} - \mathbf{u}^n}{\Delta t/2} = -\mathbf{K}^T \mathbf{v}^n \\ \mathbf{M}_v \dfrac{\mathbf{v}^{n+1} - \mathbf{v}^n}{\Delta t} = \mathbf{K}\mathbf{u}^{n+1/2} - \mathbf{M}_\sigma \dfrac{1}{2}\left(\mathbf{v}^{n+1} + \mathbf{v}^n\right) \\ \qquad\qquad + \dfrac{1}{2}\left(\mathbf{j}^n + \mathbf{j}^{n+1}\right) \\ \mathbf{M}_u \dfrac{\mathbf{u}^{n+1} - \mathbf{u}^{n+1/2}}{\Delta t/2} = -\mathbf{K}^T \mathbf{v}^{n+1} \end{cases} .$$

Time integration

Leapfrog ⇔ CO2

Leapfrog

$$\begin{cases} \mathbf{M}_u \dfrac{\mathbf{u}^{n+1/2} - \mathbf{u}^{n-1/2}}{\Delta t} = -\mathbf{K}^T \mathbf{v}^n \\ \mathbf{M}_v \dfrac{\mathbf{v}^{n+1} - \mathbf{v}^n}{\Delta t} = \mathbf{K}\mathbf{u}^{n+1/2} - \mathbf{M}_\sigma \dfrac{1}{2}\left(\mathbf{v}^{n+1} + \mathbf{v}^n\right) + \mathbf{j}^{n+1/2} \end{cases}$$

CO2

$$\begin{cases} \mathbf{M}_u \dfrac{\mathbf{u}^{n+1/2} - \mathbf{u}^{n}}{\Delta t/2} = -\mathbf{K}^T \mathbf{v}^n \\ \mathbf{M}_v \dfrac{\mathbf{v}^{n+1} - \mathbf{v}^n}{\Delta t} = \mathbf{K}\mathbf{u}^{n+1/2} - \mathbf{M}_\sigma \dfrac{1}{2}\left(\mathbf{v}^{n+1} + \mathbf{v}^n\right) + \dfrac{1}{2}\left(\mathbf{j}^{n} + \mathbf{j}^{n+1}\right) \\ \mathbf{M}_u \dfrac{\mathbf{u}^{n+1} - \mathbf{u}^{n+1/2}}{\Delta t/2} = -\mathbf{K}^T \mathbf{v}^{n+1} \end{cases}$$

Time integration

Composition schemes (CO4, CO6, CO8)

[Verwer/Botchev 2008, Hairer/Lubich/Wanner 2002]

Set $U_0 = \mathbf{u}^n$ en $V_0 = \mathbf{v}^n$
for k from 1 to s (= number of steps)

$$\mathbf{M}_u \frac{U_k - U_{k-1}}{\Delta t} = -\left(\beta_k + \alpha_{k-1}\right) \mathbf{K} V_{k-1}$$

$$\mathbf{M}_v \frac{V_k - V_{k-1}}{\Delta t} = \left(\beta_k + \alpha_k\right) \mathbf{K}^T U_k - \mathbf{M}_\sigma \left(\beta_k V_{k-1} + \alpha_k V_k\right) - \left(\mathbf{j}(t^v_{k-1}) + \mathbf{j}(t^v_k)\right)$$

final step

$$\mathbf{M}_u \frac{\mathbf{u}^{n+1} - U_s}{\Delta t} = -\alpha_s \mathbf{K} \mathbf{v}^{n+1}; \qquad \mathbf{v}^{n+1} = V_s$$

Time integration

Explicit Runge-Kutta methods (RK4)

[Verwer/Botchev 2008]

$$
\begin{array}{c|cccc}
0 & & & & \\
1/2 & 1/2 & & & \\
1/2 & 0 & 1/2 & & \\
1 & 0 & 0 & 1 & \\
\hline
 & 1/6 & 1/3 & 1/3 & 1/6
\end{array}
$$

Time integration

Richardson extrapolation (GEX4, LEX4)

[Hairer/Wanner 2010]

The used extrapolation rule for symmetric methods

$$T_{j,k+1} = T_{j,k} + \frac{T_{j,k} - T_{j-1,k}}{(n_j/n_{j-k})^2 - 1}.$$

Global

$n_1 = 1$ and $n_2 = 2$

Local

$n_1 = 1$ and $n_2 = 2$ or $n_2 = 3$

Error criteria

$$\epsilon_t^u = \frac{\left\| \mathbf{u}_t - \mathbf{u}_t^* \right\|}{\left\| \mathbf{u}_t^* \right\|}, \qquad \epsilon_t^v = \frac{\left\| \mathbf{v}_t - \mathbf{v}_t^* \right\|}{\left\| \mathbf{v}_t^* \right\|}$$

PDE error

Where $\mathbf{u}_t^*$ and $\mathbf{v}_t^*$ are the exact solutions of the PDE.
$\rightarrow$ Requires an analytical solution

ODE error

Where $\mathbf{u}_t^*$ and $\mathbf{v}_t^*$ are the exact solutions of the ODE.
$\rightarrow$ Requires a numerical solution with a smaller time step

Results

Model (elastodynamic)

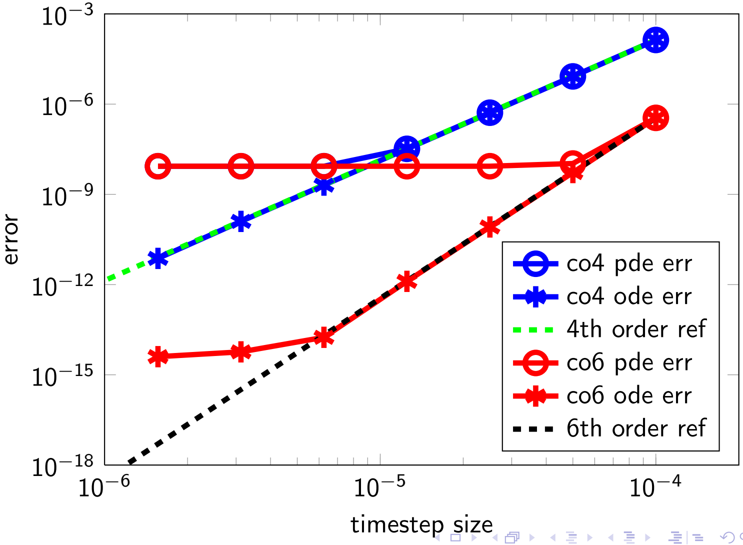
- $2\text{m} \times 2\text{m} \times 2\text{m}$ cube
- Velocity & source

$$\begin{cases} \underline{\mathbf{v}}_x = \sin\left(\frac{n_x * 2 * \pi}{D_z} z - \omega_x t\right) \\ \underline{\mathbf{v}}_y = \sin\left(\frac{n_y * 2 * \pi}{D_x} x - \omega_y t\right) \\ \underline{\mathbf{v}}_z = \sin\left(\frac{n_z * 2 * \pi}{D_y} y - \omega_z t\right) \end{cases} \quad \begin{cases} \underline{\mathbf{f}}_x = -\frac{\rho\omega_x^2 + \mu\left(\frac{n_x 2\pi}{D_z}\right)^2}{\omega_x} \cos\left(\left(\frac{n_x 2\pi}{D_z}\right) z - \omega_x t\right) \\ \underline{\mathbf{f}}_y = -\frac{\rho\omega_y^2 + \mu\left(\frac{n_y 2\pi}{D_x}\right)^2}{\omega_y} \cos\left(\left(\frac{n_y 2\pi}{D_x}\right) x - \omega_y t\right) \\ \underline{\mathbf{f}}_z = -\frac{\rho\omega_z^2 + \mu\left(\frac{n_z 2\pi}{D_y}\right)^2}{\omega_z} \cos\left(\left(\frac{n_z 2\pi}{D_y}\right) y - \omega_z t\right) \end{cases}$$

- Material: $\rho = 1$, $\lambda = 0.75$, $\mu = 0.375$
- Free boundaries
- $t \in [0,\ 2\ 10^{-4}]$
- ± 15 cells per wavelength

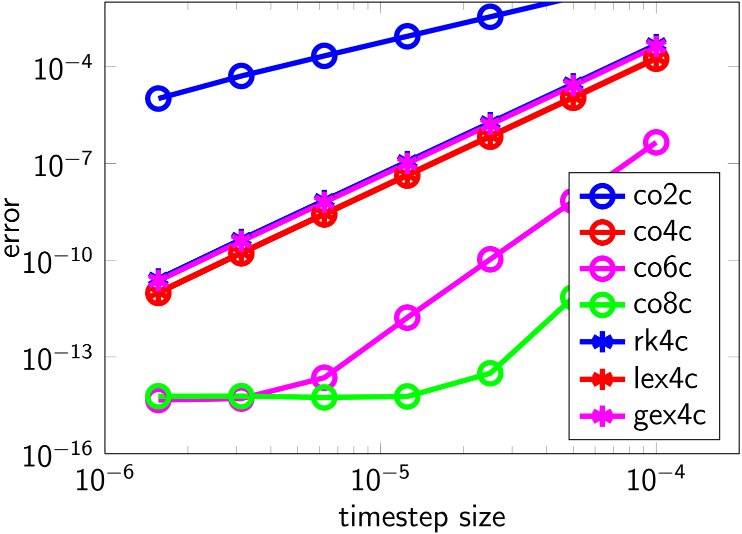
Results

PDE error vs ODE error



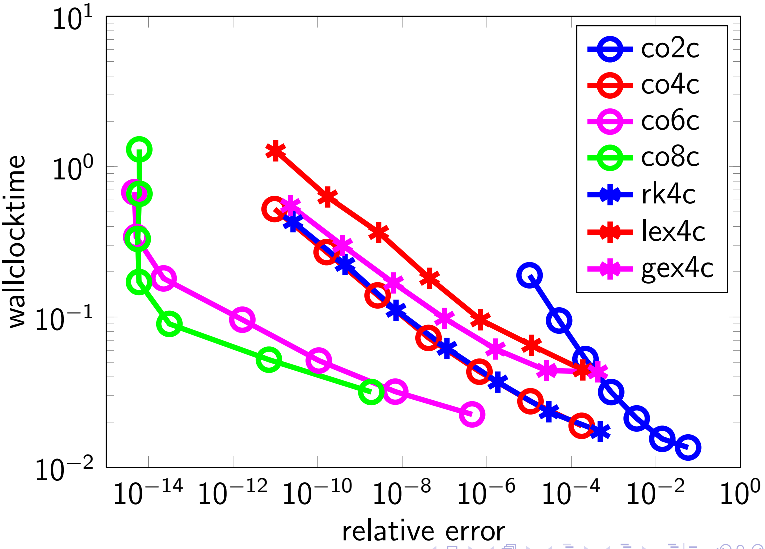
Results

Convergence orders



Results

Efficiency



Conclusion

Summary

Many wave propagation problems fit the same semi-discrete formulation. Higher order time integrators for this semi-discrete formulation were compared to the classical scheme for wave propagation problems.

Conclusion

In certain cases, higher order time stepping methods are more efficient than the classical second order method, even in combination with low order spatial discretization.

Outlook

Implementation of a fast (EFIT) solver.
Application of the solver for non-destructive testing.

Fin

Thank you!

Any questions, thoughts, suggestions?

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Appendix
CFL condition

$$\Delta t \leq \Delta t_{\max} = \frac{2}{\omega_{\max}}$$

$$\Delta t \leq \Delta t_{\max} \leq \frac{1}{v\sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}}$$