Moving forward with the help of backward error analysis: improving symplectic and other numerical methods

Farkas Miklós Seminar on Applied Analysis, BME

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Overview

1. An introduction to backward error analysis (BEA) for ODEs
2. BEA-based compensation I. – Modifying system parameters
3. BEA-based compensation II. – Choosing a better coordinate system

Backward error analysis for ODEs

Notation, terminology

Autonomous, d-dimensional ODE (system), initial value problem:

$$\dot{\mathbf{y}}(t) = \mathbf{f}\big(\mathbf{y}(t)\big), \qquad \mathbf{y}(0) = \mathbf{y_0}, \tag{1}$$

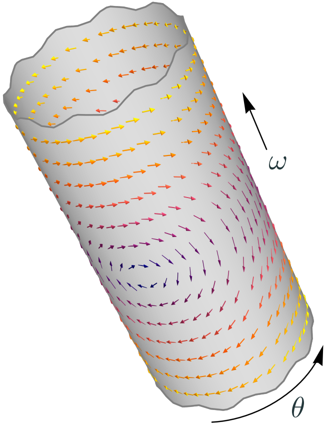
where $\mathbf{y} : \mathbb{R} \to \mathbb{R}^d$ is the (unknown) solution, $\mathbf{f} : \mathbb{R}^d \to \mathbb{R}^d$ is the (sufficiently smooth) generating vector field (the "system" being simulated), and $\mathbf{y_0} \in \mathbb{R}^d$ is the initial condition.

Explicit, one-step numerical *method* on a uniform grid with time step Δt:

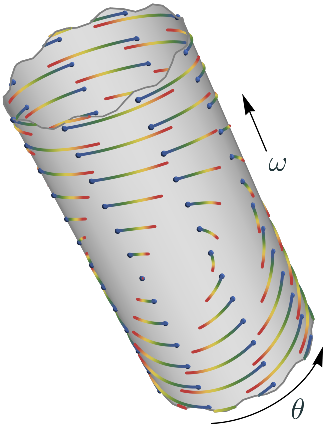
$$\mathbf{y}^{j+1} = \Phi_{\Delta t}(\mathbf{y}^j), \quad j = 0, 1, 2, \ldots \tag{2}$$

where $t^j := j\Delta t$, with $j = 0, 1, 2, \ldots$ as the index of the time step, $\mathbf{y}^j$ is the approximate solution at t^j. Designed to solve (1) approximately.

Flow of the vector field (integral curves at all points in state space, parametrised by t – a one-parameter map): $\varphi_t : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$



Vector field $\mathbf{f}$

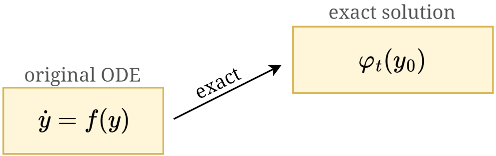


Flow φ_t

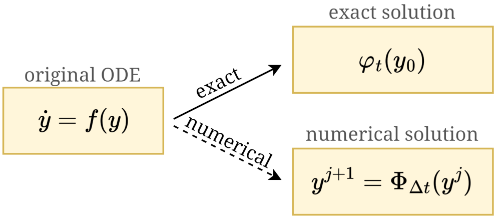
original ODE

$$\boxed{\dot{y} = f(y)}$$

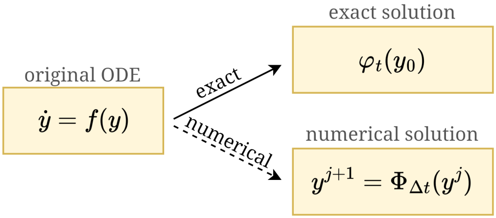
- The flow corresponds to the exact solution of the original problem



- The flow corresponds to the exact solution of the original problem
- The numerical solution is only approximate



- The flow corresponds to the exact solution of the original problem
- The numerical solution is only approximate
- *What is the numerical solution an exact solution of?*



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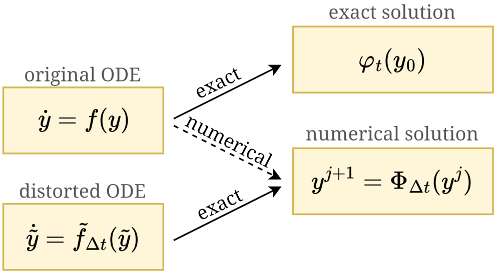
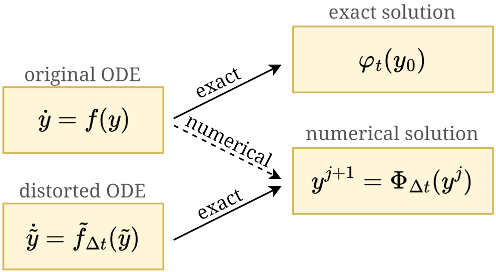
- The numerical solution is only approximate
- *What is the numerical solution an exact solution of?*
- BEA: constructing the *distorted* ODE



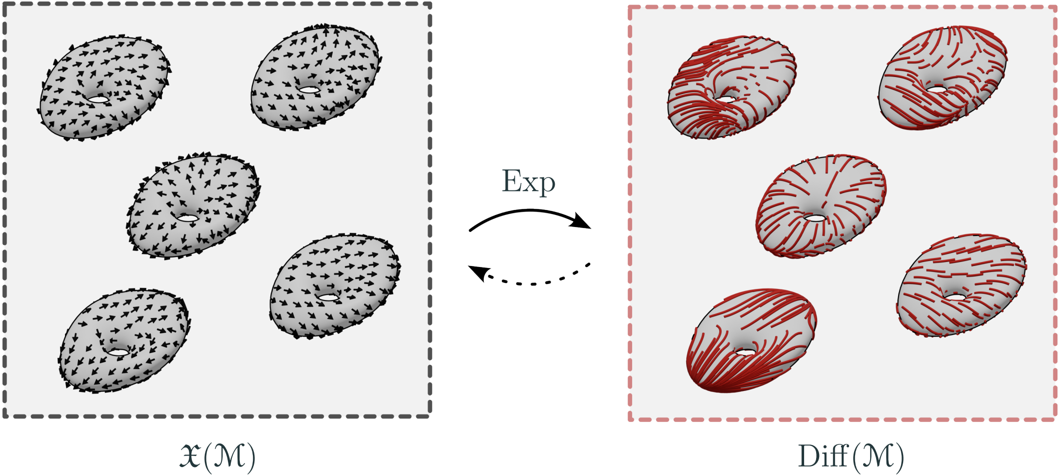
Backward error analysis for ODEs

- Backward error analysis: treating the approximate solution of $\mathbf{f}$ by $\Phi_{\Delta t}$ as an *exact solution* of a certain system nearby to the original one, i.e. $\tilde{\mathbf{y}}\left(t^j\right) = \mathbf{y}^j$.
- This other system is described by its so-called *modified equations* or *distorted equations*.
- Corresponding distorted vector field (DVF): $\tilde{\mathbf{f}}$
- $\tilde{\mathbf{f}}$ is an underlying, continuous-time counterpart of the discrete-time numerical method



Correspondence between the Lie algebra and the Lie group

Lie algebra of vector fields with Lie derivative $\overset{?}{\Leftrightarrow}$ Lie group of smooth maps?



The distorted vector field

The distorted vector field (DVF) $\tilde{\mathbf{f}}$:

- ...Does it exist?

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- usually, it does [1], but...
- it is not autonomous: $\tilde{\mathbf{f}}(\mathbf{y}, t)$
- or, it can be approximated via an asymptotic series of an autonomous $\tilde{\mathbf{f}}(\mathbf{y})$ as:

$$\tilde{\mathbf{f}}(\tilde{\mathbf{y}}) = \mathbf{f}(\tilde{\mathbf{y}}) + \Delta t\, \mathbf{f}_1(\tilde{\mathbf{y}}) + \Delta t^2\, \mathbf{f}_2(\tilde{\mathbf{y}}) + \Delta t^3\, \mathbf{f}_3(\tilde{\mathbf{y}}) + \cdots \tag{3}$$

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- Truncated version is “good enough” for “long enough”

Nice properties of the DVF

$$\tilde{\mathbf{f}}(\tilde{\mathbf{y}}) = \mathbf{f}(\tilde{\mathbf{y}}) + \Delta t\, \mathbf{f}_1(\tilde{\mathbf{y}}) + \Delta t^2\, \mathbf{f}_2(\tilde{\mathbf{y}}) + \Delta t^3\, \mathbf{f}_3(\tilde{\mathbf{y}}) + \cdots \tag{3}$$

Nice properties of the DVF include:

- If $\Phi_{\Delta t}$ has order p, then $\mathbf{f}_j(\mathbf{y}) \equiv \mathbf{0}$ for $j = 1, \ldots, p-1$
- If $\Phi_{\Delta t}$ is a symmetric method, then $\mathbf{f}_j(\mathbf{y}) \equiv \mathbf{0}$ for all odd j
- Transfer of structure-preserving properties:
  - If $\Phi_{\Delta t}$ exactly conserves a first integral $I(\mathbf{y})$, then the distorted equation also has $I(\mathbf{y})$ as a first integral
  - If $\Phi_{\Delta t}$ is symplectic when applied to a Hamiltonian system of the form $\mathbf{f} = \mathcal{J}_\mathrm{c}\, \mathbf{D}H(\mathbf{y})$, then the distorted equation is also Hamiltonian
    $\rightarrow$ with a *distorted Hamiltonian*: $\tilde{\mathbf{f}} = \mathcal{J}_\mathrm{c}\, \mathbf{D}\tilde{H}(\mathbf{y})$
    Central result for symplectic methods: [2]
  - etc.

Fruitful for the analysis of structure-preserving numerical methods

Example

Example: explicit Euler (EE) method, system: $\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y}(t))$

Numerical method:

$$\mathbf{y}^{j+1} = \mathbf{y}^{j} + \Delta t \, \mathbf{f}\big(\mathbf{y}^{j}\big) =: \Phi_{\Delta t}\big(\mathbf{y}^{j}\big) \tag{4}$$

Looking for the DVF in the form (ansatz):

$$\tilde{\mathbf{f}}(\tilde{\mathbf{y}}) = \mathbf{f}(\tilde{\mathbf{y}}) + \Delta t \, \mathbf{f}_1(\tilde{\mathbf{y}}) + \Delta t^2 \, \mathbf{f}_2(\tilde{\mathbf{y}}) + \cdots \tag{3}$$

Taylor expansion of the distorted solution $\tilde{\mathbf{y}}$ around t:

$$\tilde{\mathbf{y}}(t + \Delta t) = \tilde{\mathbf{y}}(t) + \Delta t \frac{\mathrm{d}\mathbf{y}}{\mathrm{d}t}(t) + \frac{\Delta t^2}{2!} \frac{\mathrm{d}^2\mathbf{y}}{\mathrm{d}t^2}(t) + \cdots \tag{5}$$

Expressing this via $\tilde{\mathbf{f}}(\tilde{\mathbf{y}})$ (chain rule):

$$\tilde{\mathbf{y}}(t + \Delta t) = \tilde{\mathbf{y}}(t) + \Delta t \, \tilde{\mathbf{f}}\big(\tilde{\mathbf{y}}(t)\big) + \frac{\Delta t^2}{2!} \Big(\mathbf{D}\tilde{\mathbf{f}}\tilde{\mathbf{f}}\Big)\big(\tilde{\mathbf{y}}(t)\big) + \cdots \tag{6}$$

Example (cont.)

$$\tilde{\mathbf{y}}(t+\Delta t) = \tilde{\mathbf{y}}(t) + \Delta t\,\tilde{\mathbf{f}}\big(\tilde{\mathbf{y}}(t)\big) + \frac{\Delta t^2}{2!}\Big(\mathbf{D}\tilde{\mathbf{f}}\tilde{\mathbf{f}}\Big)\big(\tilde{\mathbf{y}}(t)\big) + \cdots \tag{6}$$

Substituting the ansatz:

$$\tilde{\mathbf{y}}(t+\Delta t) = \tilde{\mathbf{y}}(t) + \Delta t\,\mathbf{f}\big(\tilde{\mathbf{y}}(t)\big) + \Delta t^2\left(\mathbf{f}_1 + \frac{1}{2}\mathbf{D}\mathbf{f}\mathbf{f}\right)\big(\tilde{\mathbf{y}}(t)\big) + \cdots \tag{7}$$

Set $t = t^j$, apply the defining condition $\tilde{\mathbf{y}}\big(t^j\big) = \mathbf{y}^j$, $\forall j$,

$$\mathbf{y}^{j+1} = \mathbf{y}^j + \Delta t\,\mathbf{f}\big(\mathbf{y}^j\big) + \Delta t^2\left(\mathbf{f}_1 + \frac{1}{2}\mathbf{D}\mathbf{f}\mathbf{f}\right)\big(\mathbf{y}^j\big) + \cdots \tag{8}$$

and compare with the formula for the EE method:

$$\mathbf{y}^{j+1} = \mathbf{y}^j + \Delta t\,\mathbf{f}\big(\mathbf{y}^j\big) \tag{4}$$

$\Rightarrow \mathbf{f}_1 = -\frac{1}{2}\mathbf{D}\mathbf{f}\mathbf{f}$, $\mathbf{f}_2 = \ldots$, etc.

Example (cont.)

DVF of the EE method in general (consistent, first-order):

$$\tilde{\mathbf{f}} = \mathbf{f} - \frac{\Delta t}{2}\mathbf{D}\mathbf{f}\mathbf{f} + \frac{\Delta t^2}{12}\mathbf{D}^2(\mathbf{f},\mathbf{f}) + \frac{\Delta t^2}{3}\mathbf{D}\mathbf{f}\mathbf{D}\mathbf{f}\mathbf{f} + \cdots \tag{9}$$

Mass-spring system (harmonic oscillator):

$$m\ddot{x}(t) + kx(t) = 0 \quad \Leftrightarrow \quad \underbrace{\begin{pmatrix}\dot{x}\\ \dot{v}\end{pmatrix}}_{\dot{\mathbf{y}}} = \underbrace{\begin{pmatrix}0 & 1\\ -\omega^2 & 0\end{pmatrix}}_{\mathbf{A}}\underbrace{\begin{pmatrix}x\\ v\end{pmatrix}}_{\mathbf{y}}, \quad \text{with } \omega := \sqrt{\frac{k}{m}} \tag{10}$$

DVF of this system simulated via the EE method:

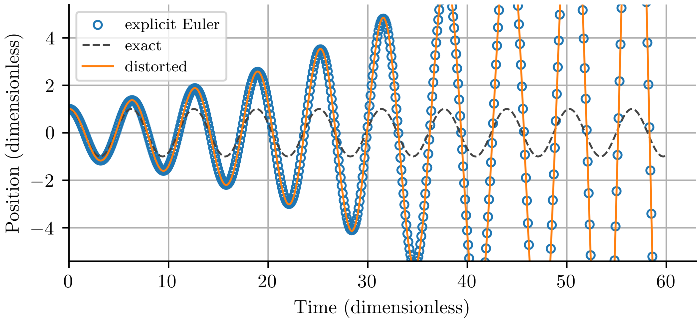
$$\dot{\tilde{x}} = \tilde{v} + \frac{\Delta t}{2}\omega^2\tilde{x} - \frac{\Delta t^2}{3}\omega^2\tilde{v} + \mathcal{O}\big(\Delta t^3\big), \tag{11}$$

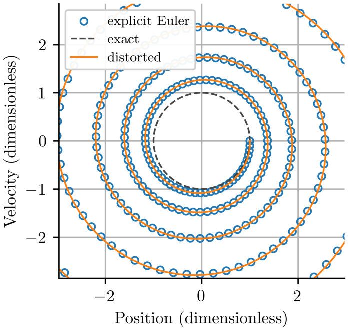
$$\dot{\tilde{v}} = -\omega^2\tilde{x} + \frac{\Delta t}{2}\omega^2\tilde{v} + \frac{\Delta t^2}{3}\omega^4\tilde{x} + \mathcal{O}\big(\Delta t^3\big). \tag{12}$$

Example (cont.)

Solution of DVF truncated up to $\mathcal{O}\left(\Delta t^2\right)$, position:

$$\tilde{x}(t) = C_1\, \mathrm{e}^{\frac{\Delta t}{2}\omega^2 t} \cos\left[\left(\omega - \frac{\Delta t^2}{3}\omega^3\right)t\right] + C_2\, \mathrm{e}^{\frac{\Delta t}{2}\omega^2 t} \sin\left[\left(\omega - \frac{\Delta t^2}{3}\omega^3\right)t\right], \qquad (13)$$





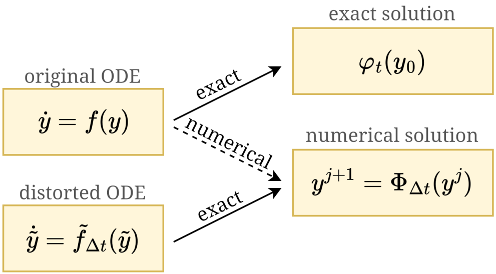
→ notice: numerical anti-dissipation, shift in frequency (dispersion error)

BEA in practice: how to do it?

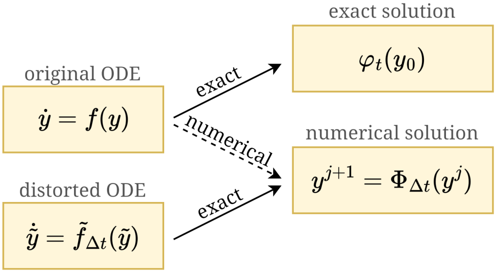
- Some more examples of this approach based on Taylor series: [3]
- Equivalent, but different approaches also exist [4, 5, 6] $\rightarrow$ sometimes better suited for proofs
- Usually, the calculation quickly becomes tedious
- Quite algorithmic: original computer algebra implementation [3], extended in [7]

BEA-based compensation I. – Modifying system parameters

- BEA: tool for the analysis of structure-preserving numerical methods



- BEA: tool for the analysis of structure-preserving numerical methods
- Can it also be applied constructively?



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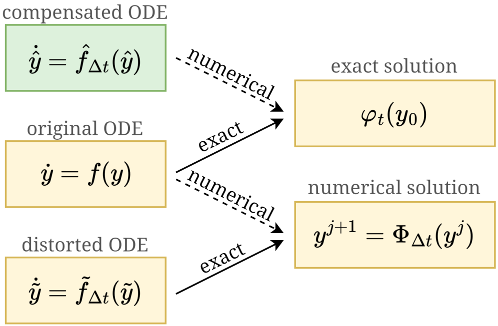
- *Compensating the system being simulated*



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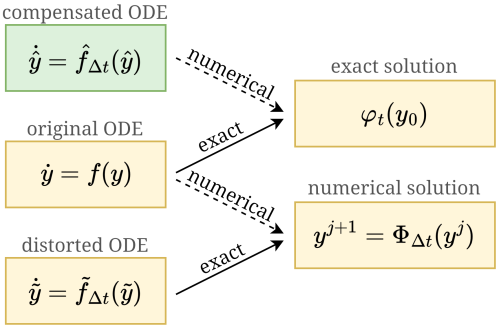

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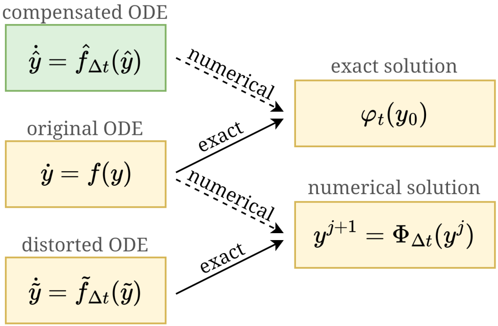
- Potential advantages:
    - Rectification of existing methods
    - No need to modify existing software implementations



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- Potential advantages:
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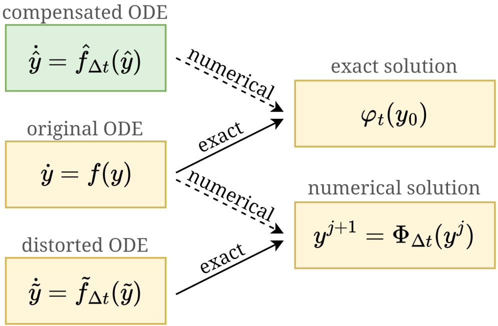
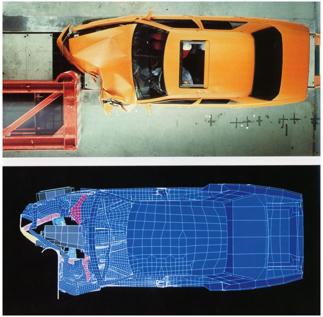
    - No need to modify existing software implementations
- Existing similar approaches [8, 9, 10] modify the vector field directly, not the parameters



Analysis and improvement of the Newmark method

- Demonstration: compensating the Newmark method [7]
- Newmark method: widely used time integration method for dynamics, available in commercial engineering software (ANSYS, Abaqus)
- Time-dependent finite element method (FEM) simulations for dynamics (*direct time integration*)
  - Wave propagation, crash simulations...
- Generally, numerical dissipation is present (absent only in special cases) – can be a (dis)advantage
- BEA-based compensation: opportunity to achieve better results with existing software

→ More accurate / less computationally intensive, more reliable numerical simulations



Analysis and improvement of the Newmark method

ODE: second-order linear system, corresponding to the semi-discrete equation of motion from the FEM model, with time-dependent external excitation

$$\mathbf{M}\ddot{\mathbf{q}}(t) + \mathbf{C}\dot{\mathbf{q}}(t) + \mathbf{K}\mathbf{q}(t) = \mathbf{F}(t), \quad \mathbf{q}(0) = \mathbf{q}_0, \, \dot{\mathbf{q}}(0) = \mathbf{v}_0. \tag{14}$$

To solve this numerically, the Newmark method is applied:

$$\mathbf{M}\mathbf{a}^{j+1} + \mathbf{C}\mathbf{v}^{j+1} + \mathbf{K}\mathbf{q}^{j+1} = \mathbf{F}^{j+1}, \tag{15}$$

$$\mathbf{q}^{j+1} = \mathbf{q}^{j} + \Delta t \mathbf{v}^{j} + \frac{\Delta t^2}{2}\left[(1-2\beta)\,\mathbf{a}^{j} + 2\beta\mathbf{a}^{j+1}\right], \tag{16}$$

$$\mathbf{v}^{j+1} = \mathbf{v}^{j} + \Delta t\left[(1-\gamma)\,\mathbf{a}^{j} + \gamma\mathbf{a}^{j+1}\right], \tag{17}$$

where γ, β are parameters of the Newmark method. $\gamma = 1/2 \to$ symmetric, second-order

Analysis and improvement of the Newmark method

Rewriting (14) to an autonomous, first-order form is needed for BEA:

$$\underbrace{\begin{pmatrix} \dot{\tau} \\ \dot{\mathbf{q}} \\ \dot{\mathbf{v}} \end{pmatrix}}_{\dot{\mathbf{y}}} = \underbrace{\begin{pmatrix} 1 \\ \mathbf{v} \\ -\mathbf{M}^{-1}\left(\mathbf{C}\mathbf{v} + \mathbf{K}\mathbf{q} - \mathbf{F}(\tau)\right) \end{pmatrix}}_{\mathbf{f}(\mathbf{y})}, \tag{18}$$

$\Rightarrow$ the corresponding DVF $\tilde{\mathbf{f}}$ has been derived (margin on this slide too narrow)

$\Rightarrow$ remarkably, the resulting DVF can be re-written in a second-order form with *distorted matrices*

$$\mathbf{M}\ddot{\mathbf{q}}(t) + \tilde{\mathbf{C}}\dot{\mathbf{q}}(t) + \tilde{\mathbf{K}}\mathbf{q}(t) = \tilde{\mathbf{F}}(t), \tag{19}$$

$\Rightarrow$ this means that the Newmark method simulates a very similar system with different parameters: opportunity for compensation!

Distorted matrices

$$\tilde{\mathbf{C}} = \mathbf{C} + \mathbf{W}(\Delta t, \gamma)\left(\mathbf{M}^{-1}\mathbf{K} - \mathbf{M}^{-1}\mathbf{C}\mathbf{M}^{-1}\mathbf{C}\right) + \Delta t^2\left(\eta - \tfrac{1}{12}\right)\mathbf{K}\mathbf{M}^{-1}\mathbf{C}, \qquad (20)$$

$$\tilde{\mathbf{K}} = \mathbf{K} - \mathbf{W}(\Delta t, \gamma)\mathbf{M}^{-1}\mathbf{C}\mathbf{M}^{-1}\mathbf{K} + \Delta t^2\left(\eta - \tfrac{1}{12}\right)\mathbf{K}\mathbf{M}^{-1}\mathbf{K}, \qquad (21)$$

$$\begin{aligned}\tilde{\mathbf{F}}(t) = \mathbf{F}(t) - \mathbf{W}(\Delta t, \gamma)\left(\mathbf{M}^{-1}\mathbf{C}\mathbf{M}^{-1}\mathbf{F}(t) - \mathbf{M}^{-1}\mathbf{F}'(t)\right) + \\ + \Delta t^2\left(\eta - \tfrac{1}{12}\right)\left(\mathbf{K}\mathbf{M}^{-1}\mathbf{F}(t) - \mathbf{F}''(t)\right),\end{aligned} \qquad (22)$$

up to $\mathcal{O}\left(\Delta t^2\right)$, with

$$\eta = \tfrac{1}{2}\gamma - \beta - \tfrac{1}{12}, \quad \mathbf{W}(\Delta t, \gamma) = \Delta t\left(\gamma - \tfrac{1}{2}\right)\mathbf{M} - \Delta t^2\left(\left(\gamma - \tfrac{1}{2}\right)^2 + \tfrac{1}{12}\right)\mathbf{C}, \qquad (23)$$

and distorted initial conditions

$$\mathbf{q}(0) = \mathbf{q}_0, \qquad (24)$$

$$\begin{aligned}\dot{\mathbf{q}}(0) = \mathbf{v}_0 + \Delta t^2\eta\left(-\mathbf{M}^{-1}\mathbf{C}\mathbf{M}^{-1}\mathbf{K}\mathbf{q}_0 + \left(\mathbf{M}^{-1}\mathbf{K} - \mathbf{M}^{-1}\mathbf{C}\mathbf{M}^{-1}\mathbf{C}\right)\mathbf{v}_0 + \right. \\ \left. + \mathbf{M}^{-1}\mathbf{C}\mathbf{M}^{-1}\mathbf{F}(0) - \mathbf{M}^{-1}\mathbf{F}'(0)\right).\end{aligned} \qquad (25)$$

Compensated system:

$$\mathbf{M}\ddot{\mathbf{q}}(t) + \widehat{\mathbf{C}}\dot{\mathbf{q}}(t) + \widehat{\mathbf{K}}\mathbf{q}(t) = \widehat{\mathbf{F}}(t), \qquad \mathbf{q}(0) = \mathbf{q}_0, \quad \dot{\mathbf{q}}(0) = \mathbf{v}_0, \tag{26}$$

Two compensations introduced:

- Eliminating numerical damping (not shown here)
- **Achieving fourth-order accuracy**
  - for $\gamma = 1/2$, only the $\mathcal{O}\left(\Delta t^2\right)$ terms need to be eliminated

Fourth-order compensation of the Newmark method

Result of derivation for the fourth-order compensation:

$$\widehat{\mathbf{C}} = \mathbf{C} + \frac{1}{12}\Delta t^2 \left(\mathbf{C}\mathbf{M}^{-1}\mathbf{K} + \mathbf{K}\mathbf{M}^{-1}\mathbf{C} - \mathbf{C}\mathbf{M}^{-1}\mathbf{C}\mathbf{M}^{-1}\mathbf{C}\right), \tag{27}$$

$$\widehat{\mathbf{K}} = \mathbf{K} + \frac{1}{12}\Delta t^2 \left(\mathbf{K}\mathbf{M}^{-1}\mathbf{K} - \mathbf{C}\mathbf{M}^{-1}\mathbf{C}\mathbf{M}^{-1}\mathbf{K}\right), \tag{28}$$

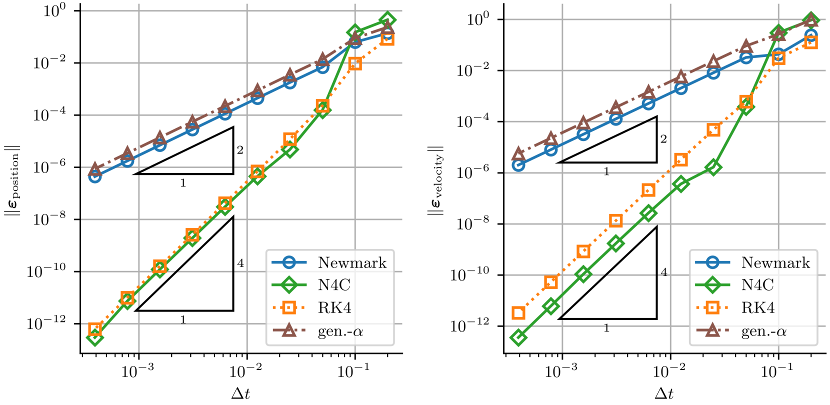
$$\widehat{\mathbf{F}}(t) = \mathbf{F}(t) + \frac{1}{12}\Delta t^2 \left(\mathbf{C}\mathbf{M}^{-1}\left(\mathbf{C}\mathbf{M}^{-1}\mathbf{F}(t) - \mathbf{F}'(t)\right) - \mathbf{K}\mathbf{M}^{-1}\mathbf{F}(t) + \mathbf{F}''(t)\right), \tag{29}$$

and $\gamma = 1/2$, $\beta = 1/6$ is required.

Once calculated, these can be used through the entire computation.

Fourth-order compensation of the Newmark method

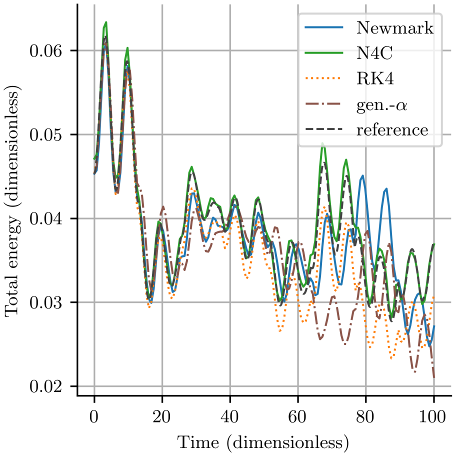
Convergence with Δt is indeed fourth-order:



Derivatives of $\mathbf{F}(t)$ can also be calculated/estimated numerically with an at least second-order accurate formula.

Fourth-order compensation of the Newmark method

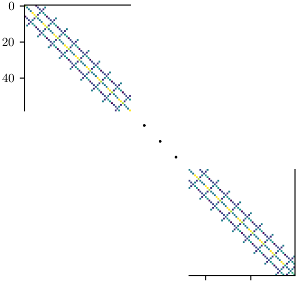
Non-continuous excitation (square wave), total energy of the system:



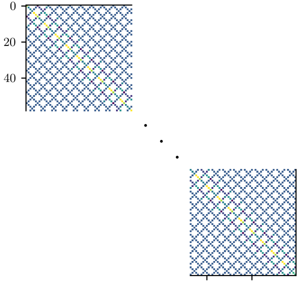
Structure of the compensated matrices

$\mathbf{M}$ does not change in the compensated system, but $\mathbf{K} \to \widehat{\mathbf{K}}$ does – how does this change the sparsity structure of the FEM matrices?

$\mathbf{K}$



$\widehat{\mathbf{K}}$



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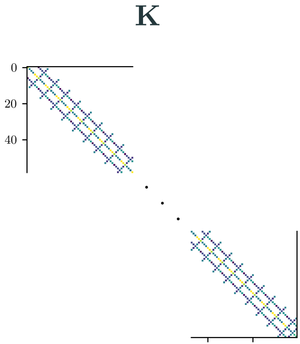
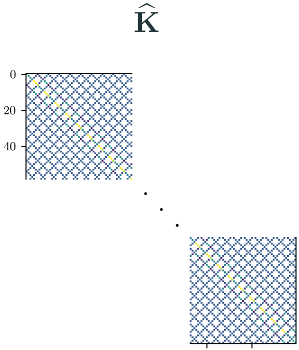
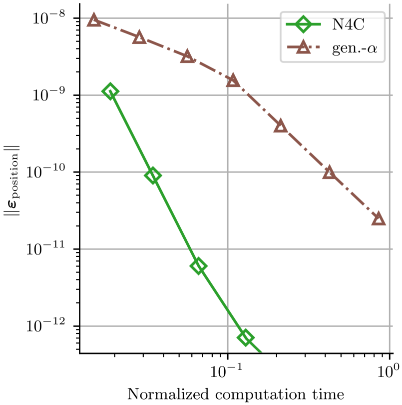


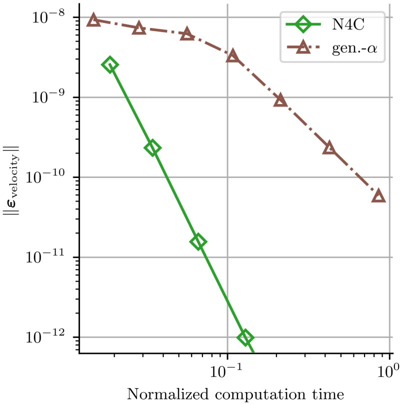


The derived DVF is underdetermined up to a matrix multiplier of $\mathbf{M}$
$\to$ opportunity for a better structure

Structure of the compensated matrices

Computation time vs. accuracy (~ 750 DoF)





Open questions, future work

- How does the computational time / accuracy tradeoff scale with the number of DoFs? (ongoing work with D. Borza)
- How do the eigenfrequencies change from $\mathbf{K}$ to $\widehat{\mathbf{K}}$?
- Can this approach be extended for more complex (nonlinear) excitation?
- Can a more favourable rewriting into second-order form be achieved with respect to the sparsity structure?
- Extension of this approach to extensions of the Newmark method: HHT-α, generalised-α

More details on this topic: [7] D. M. Takács and T. Fülöp. **"Improving the accuracy of the Newmark method through backward error analysis".** In: *Computational Mechanics* 75.5 (2025), pp. 1585–1606.

BEA-based compensation II. – Choosing a better coordinate system

Accuracy of a numerical method and the applied coordinate system

- We have seen so far that, through BEA, the DVF corresponding to a numerical method as applied to a system can be constructed
- For structure-preserving methods: the DVF is associated with a system of the same structure (detailed above)
- Specifically, for symplectic numerical methods: the DVF is Hamiltonian; there is a distorted Hamiltonian $\tilde{H}$ associated
- But: is the DVF invariant to a coordinate transformation of the original system?
  - Is the distorted Hamiltonian?
- Can this be exploited to achieve better accuracy?

Hamiltonian system (autonomous): described by the *Hamiltonian* $H(\mathbf{q}, \mathbf{p})$, $H : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$

Equations of motion:

$$\underbrace{\begin{pmatrix} \dot{\mathbf{q}} \\ \dot{\mathbf{p}} \end{pmatrix}}_{\dot{\mathbf{y}}} = \underbrace{\begin{pmatrix} \mathbf{0} & \mathbf{I} \\ -\mathbf{I} & \mathbf{0} \end{pmatrix}}_{\mathcal{J}_{\mathrm{c}}} \underbrace{\begin{pmatrix} H_q(\mathbf{q}, \mathbf{p}) \\ H_p(\mathbf{q}, \mathbf{p}) \end{pmatrix}}_{\mathbf{D}H(\mathbf{y})}, \tag{30}$$

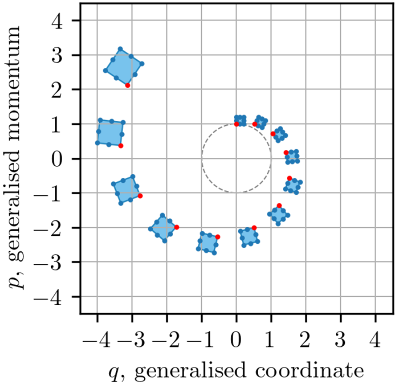
Symplectic property:

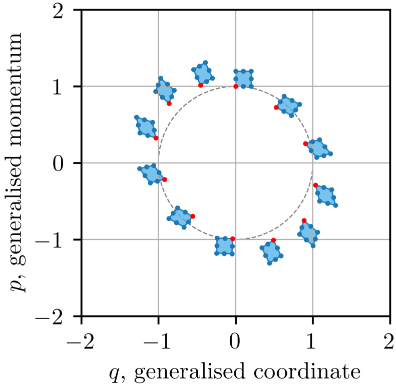
$$\left(\frac{\partial \varphi_t}{\partial \mathbf{y}}\right)^{\mathsf{T}} \mathcal{J}_{\mathrm{c}}^{-1} \left(\frac{\partial \varphi_t}{\partial \mathbf{y}}\right) = \mathcal{J}_{\mathrm{c}}^{-1} \tag{31}$$

For a numerical method:

$$\left(\frac{\partial \Phi_{\Delta t}}{\partial \mathbf{y}}\right)^{\mathsf{T}} \mathcal{J}_{\mathrm{c}}^{-1} \left(\frac{\partial \Phi_{\Delta t}}{\partial \mathbf{y}}\right) = \mathcal{J}_{\mathrm{c}}^{-1} \tag{32}$$

Explicit Euler vs. Symplectic Euler method, harmonic oscillator:





To canonical transformations

$$\begin{pmatrix}\mathbf{q}\\ \mathbf{p}\end{pmatrix} \mapsto \begin{pmatrix}\bar{\mathbf{q}}\\ \bar{\mathbf{p}}\end{pmatrix} = \begin{pmatrix}\mathbf{Q}(\mathbf{q},\mathbf{p})\\ \mathbf{P}(\mathbf{q},\mathbf{p})\end{pmatrix}, \tag{33}$$

the Hamiltonian is invariant, i.e.

$$\bar{H}\big(\bar{\mathbf{q}},\bar{\mathbf{p}}\big) := H\big(\mathbf{Q}^{-1}(\bar{\mathbf{q}},\bar{\mathbf{p}}),\mathbf{P}^{-1}(\bar{\mathbf{q}},\bar{\mathbf{p}})\big); \qquad \bar{H} = H \tag{34}$$

From here on, we restrict ourselves to the subset of canonical transformations induced by a coordinate transformation $\bar{\mathbf{q}} = \mathbf{Q}(\mathbf{q})$:

$$\bar{q}^\alpha = Q^\alpha(\mathbf{q}); \quad \bar{p}_\alpha = p_i \left(\frac{\partial \left(Q^{-1}\right)^i}{\partial \bar{q}^\alpha}\right) \circ \mathbf{Q}(\mathbf{q}) \tag{35}$$

Does this change of coordinates change the numerical results in a meaningful way?

Distorted Hamiltonian of a symplectic method

Symplectic Euler (SE) method (first-order):

$$\begin{aligned} \mathbf{q}^{j+1} &= \mathbf{q}^{j} + \Delta t H_p\left(\mathbf{q}^{j+1}, \mathbf{p}^{j}\right), \\ \mathbf{p}^{j+1} &= \mathbf{p}^{j} - \Delta t H_q\left(\mathbf{q}^{j+1}, \mathbf{p}^{j}\right). \end{aligned} \tag{36}$$

Distorted Hamiltonian from BEA:

$$\tilde{H} = H - \frac{\Delta t}{2} H_p H_q + \mathcal{O}\left(\Delta t^2\right), \tag{37}$$

Similarly, in the transformed coordinate system:

$$\tilde{\bar{H}} = \bar{H} - \frac{\Delta t}{2} \bar{H}_{\bar{p}} \bar{H}_{\bar{q}} + \mathcal{O}\left(\Delta t^2\right). \tag{38}$$

$\rightarrow$ are these actually the same, i.e., is $\tilde{H}$ invariant to coordinate transformations?

Distorted Hamiltonian of a symplectic method

$$
\begin{tikzcd}
H \arrow[r, dashed, "\text{discretisation}"] \arrow[d, shift right, "\mathbf{Q}"'] & \tilde{H} \arrow[d, dash, dashed, "?"] \\
\bar{H} \arrow[r, dashed, "\text{discretisation}"] \arrow[u, shift right, "\mathbf{Q^{-1}}"'] & \tilde{\bar{H}}
\end{tikzcd}
$$

Distorted Hamiltonian of a symplectic method

$$\tilde{\bar{H}} = \bar{H} - \frac{\Delta t}{2} \bar{H}_{\bar{p}} \bar{H}_{\bar{q}} + \mathcal{O}\left(\Delta t^2\right). \tag{38}$$

Let us consider the second term in (38), $H_p H_q$ (first elementary Hamiltonian):

$$\bar{H}_{\bar{p}} \bar{H}_{\bar{q}} \equiv \frac{\partial \bar{H}}{\partial \bar{p}_\alpha} \frac{\partial \bar{H}}{\partial \bar{q}^\alpha} = \ldots = \underbrace{\frac{\partial H}{\partial p_i} \frac{\partial H}{\partial p_k} p_l \frac{\partial \left(Q^{-1}\right)^l}{\partial \bar{q}^\beta} \frac{\partial^2 Q^\beta}{\partial q^k \, \partial q^i}}_{=: \Xi_{H_p H_q, \mathbf{Q}}} + \frac{\partial H}{\partial p_i} \frac{\partial H}{\partial q^i}. \tag{39}$$

$\rightarrow$ necessary condition for the invariance of the distorted Hamiltonian:

$$\Xi_{H_p H_q, \mathbf{Q}} = 0 \tag{40}$$

- trivially fulfilled for affine coordinate transformations, can also be fulfilled nontrivially
- non-invariant in general
- can this be exploited to eliminate the first-order term in $\tilde{H}$ to raise accuracy?

Second-order accuracy with the symplectic Euler method

Condition for second-order accuracy of SE in the transformed coordinate system:

$$\bar{H}_{\bar{p}}\bar{H}_{\bar{q}} \equiv 0 \quad \Leftrightarrow \quad \Xi_{H_p H_q,\mathbf{Q}} = -\frac{\partial H}{\partial p_i}\frac{\partial H}{\partial q^i} \tag{41}$$

- trivially fulfilled in fully cyclic (action-angle) coordinates.
  - achieving this is usually not possible
- are there any other, non-trivial $\mathbf{Q}$ coordinate transformations that achieve this?
  - not guaranteed, but sometimes possible

Demonstration: harmonic oscillator, symplectic Euler method

Harmonic oscillator:

$$H(q,p) = \frac{1}{2}p^2 + \frac{1}{2}q^2, \tag{42}$$

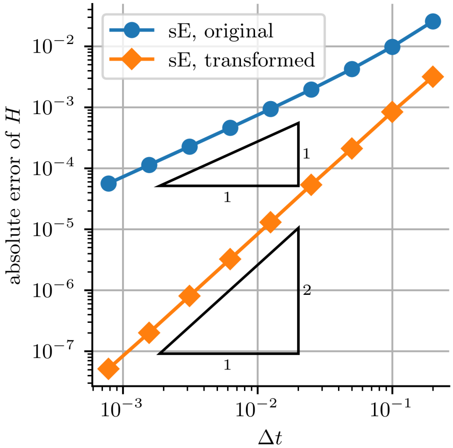
Condition (41) for second-order SE in this case, after calculations:

$$\left(1 - q^2\right)\left(\frac{\partial Q}{\partial q}\right)^{-1}\frac{\partial^2 Q}{\partial q^2} + q = 0. \tag{43}$$

Appropriate coordinate transformation fulfilling this condition:

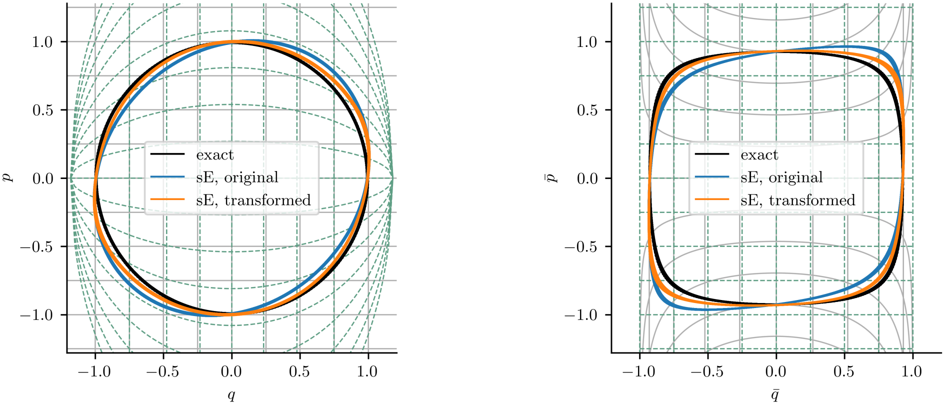
$$Q(q) = \frac{2}{\pi}\left(\hat{q}\sqrt{1-\hat{q}^2} + \arcsin(\hat{q})\right), \qquad \text{where } \hat{q} = \frac{q}{1+2\Delta t^2}, \tag{44}$$

Demonstration



Demonstration

Trajectory of the numerical results in the two coordinate systems:



Open questions, future work, other results

- When does a better coordinate system exist in general?
- Extension of this approach beyond the SE method? (Størmer–Verlet might be a good candidate)
- Extension to the entire class of canonical transformations?
- Additional result not explored here: preservation of first integrals in the SE method

More details on this topic: [11] D. M. Takács and T. Fülöp. **"On the coordinate system-dependence of the accuracy of symplectic methods".** In: *Journal of Numerical Analysis and Approximation Theory* (2025). In press.

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Thank you for your kind attention!

Non-invariance of the distorted Hamiltonian