

A Simple Test Case for Error Reduction of Black-Box Coupling Schemes

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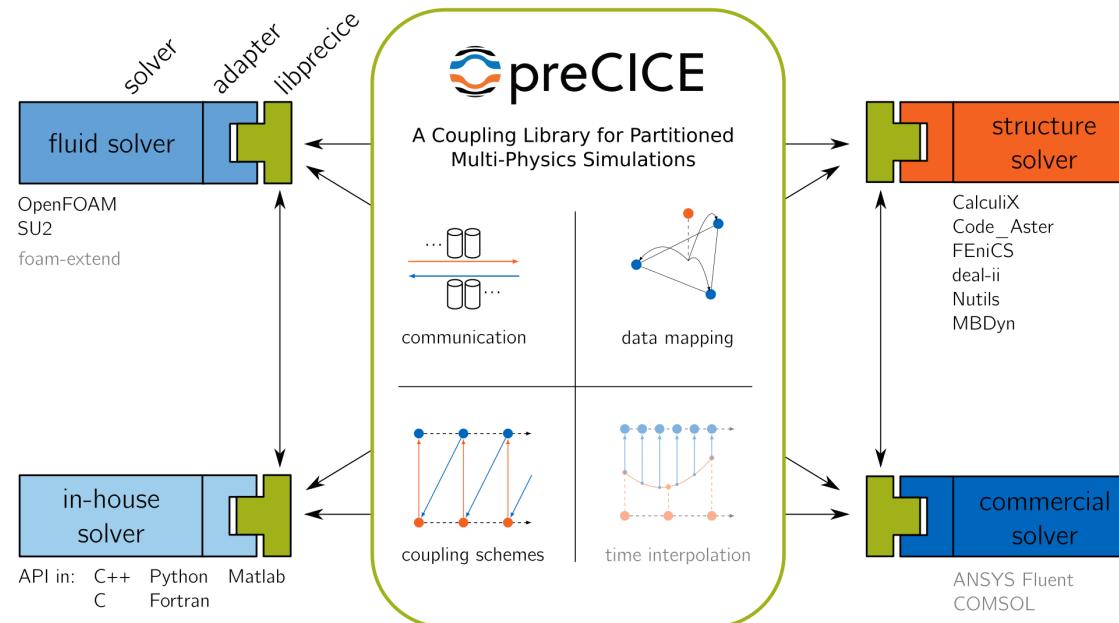
²University of Stuttgart, Usability and Sustainability of Simulation Software

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Essen, September 22, 2022



Why black-box coupling?



Why study the numerics of coupling schemes?

- **order degradation:** the coupling scheme can decrease the achievable convergence order in time
- additional impacts on stability, **energy conservation**

⇒ isolate and study these phenomena systematically (this talk)

⇒ support more sophisticated black-box coupling schemes in preCICE (→ Outlook)

The oscillator example

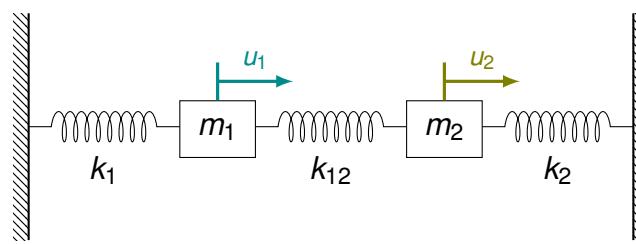
$$\begin{bmatrix} m_1 & 0 \\ 0 & m_2 \end{bmatrix} \begin{pmatrix} \ddot{u}_1 \\ \ddot{u}_2 \end{pmatrix} + \begin{bmatrix} k_1 + k_{12} & -k_{12} \\ -k_{12} & k_2 + k_{12} \end{bmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = 0$$

or, in shorthand notation,

$$M\ddot{\mathbf{u}} + K\mathbf{u} = 0$$

some properties of this system:

- analytical solution simple to compute
- energy conservation



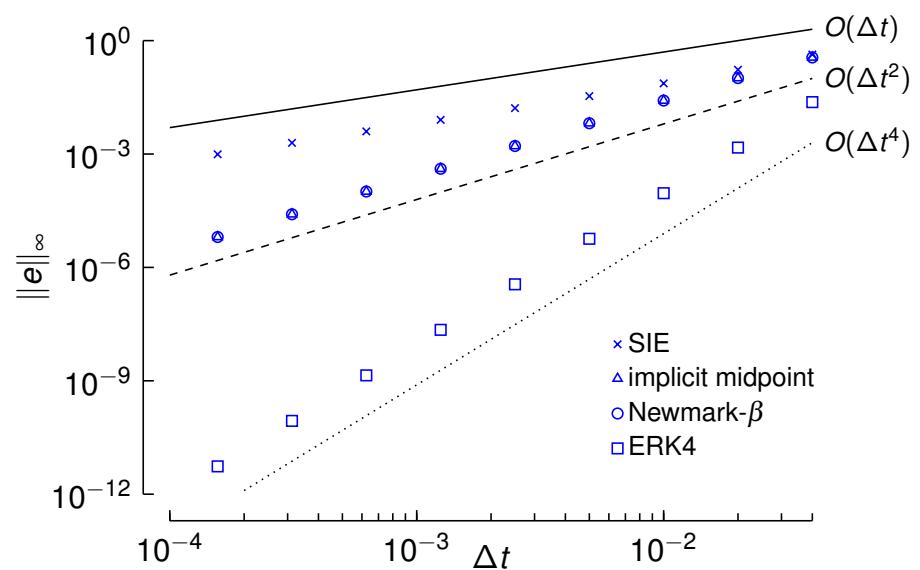
The oscillator example: Convergence study

4 time integration methods:

- $O(\Delta t)$: semi-implicit Euler (SIE)
- $O(\Delta t^2)$: implicit midpoint
- $O(\Delta t^2)$: Newmark- β
- $O(\Delta t^4)$: classical Runge-Kutta (ERK4)

decreasing time step sizes Δt

measure error w.r.t. analytical solution $\|e\|_\infty$



The oscillator example: Partitioned system

$$\begin{bmatrix} m_1 & 0 \\ 0 & m_2 \end{bmatrix} \begin{pmatrix} \ddot{u}_1 \\ \ddot{u}_2 \end{pmatrix} + \begin{bmatrix} k_1 + k_{12} & -k_{12} \\ -k_{12} & k_2 + k_{12} \end{bmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = 0$$

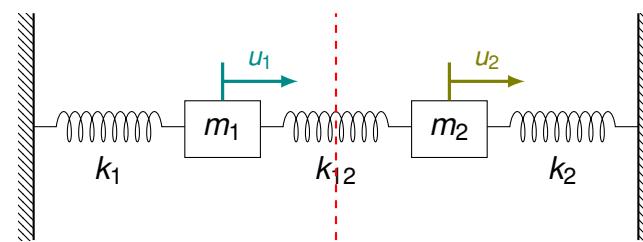
Idea: cut through the connecting spring k_{12}

⇒ interface forces and two decoupled initial value problems:

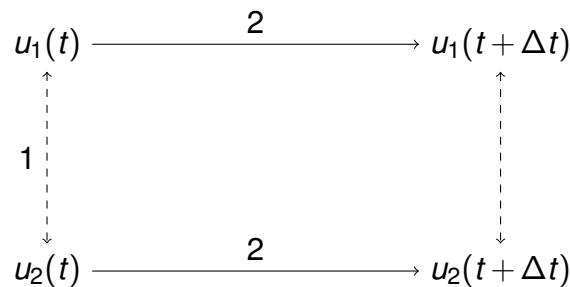
$$m_1 \ddot{u}_1 = -(k_1 + k_{12})u_1 + F_2(t)$$

$$m_2 \ddot{u}_2 = -(k_2 + k_{12})u_2 + F_1(t)$$

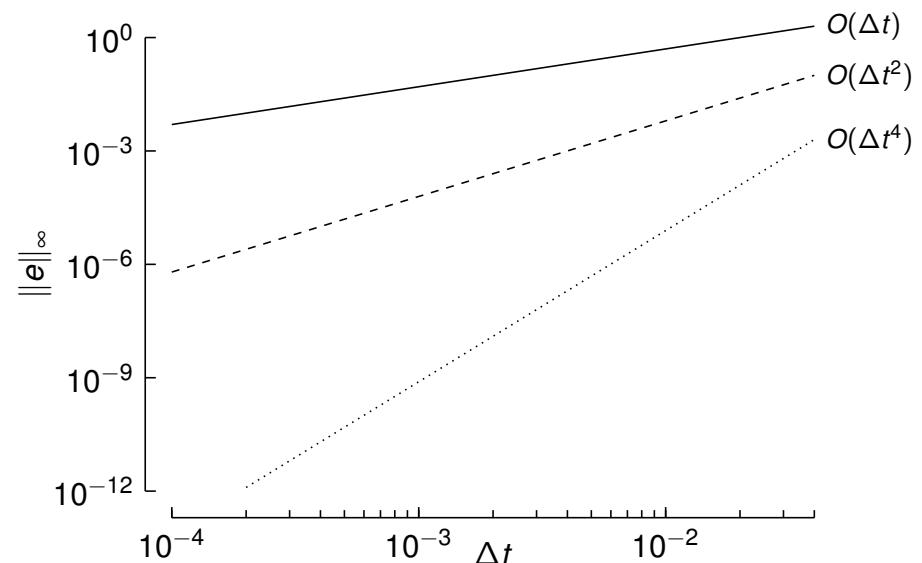
with $F_i(t) = k_{12}u_i(t)$



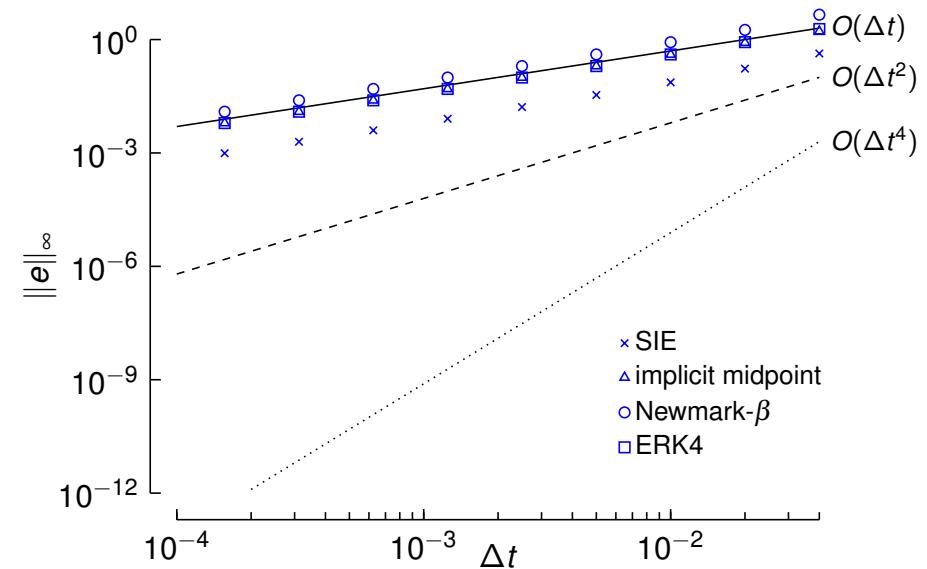
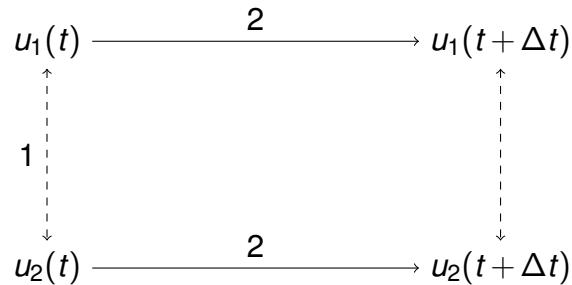
Naive coupling: A parallel scheme



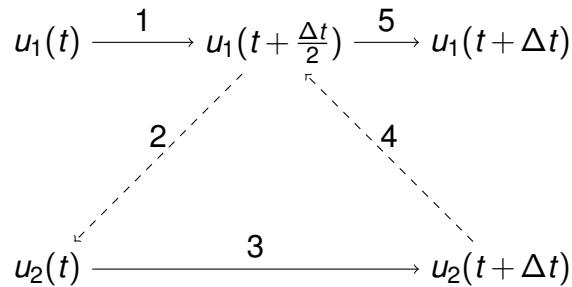
conventional parallel staggered (CPS) scheme
(Farhat and Lesoinne 1998)
achievable convergence order: $O(\Delta t)$



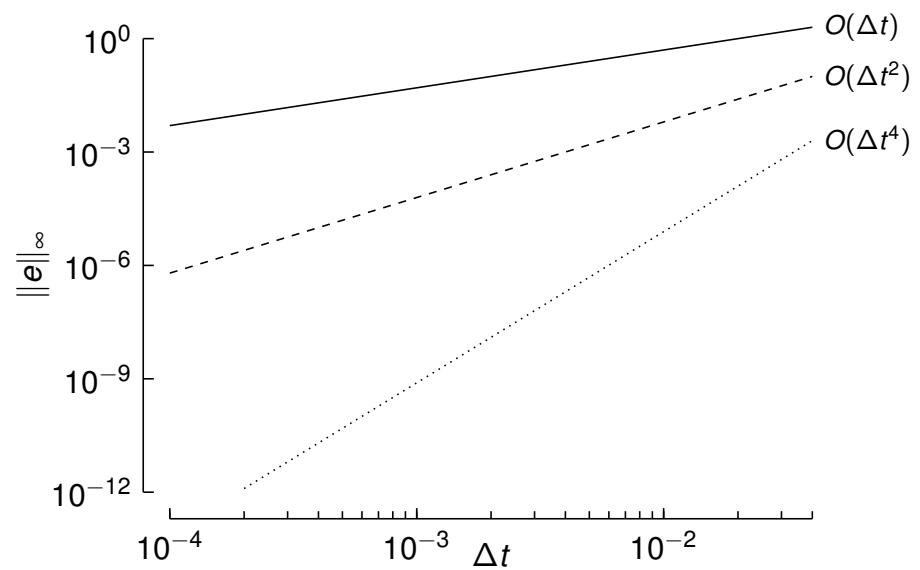
Naive coupling: A parallel scheme



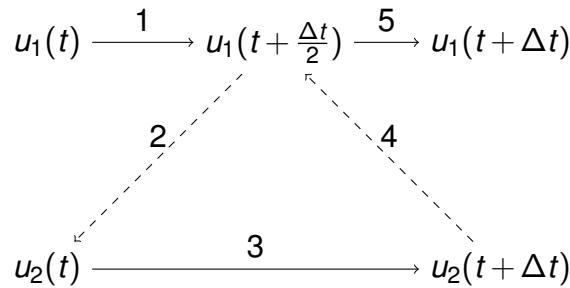
Strang splitting



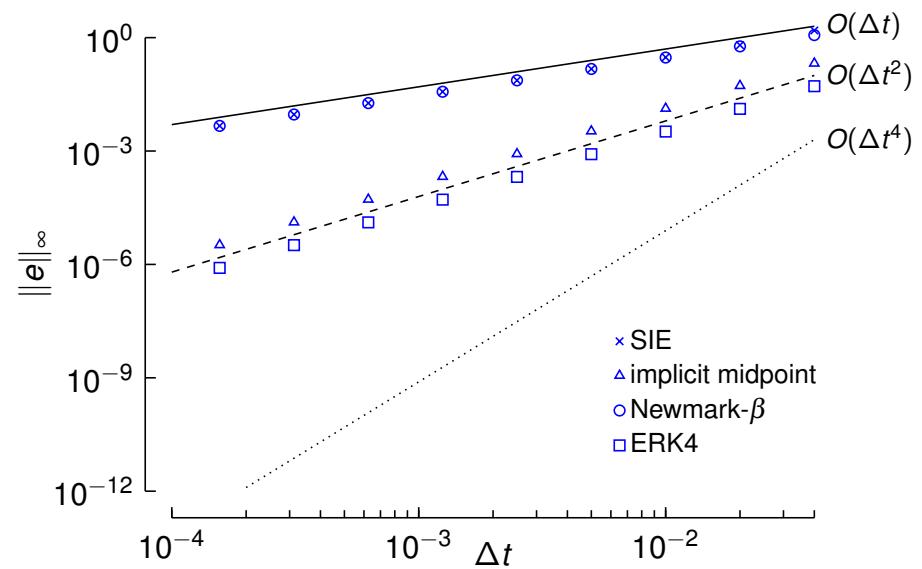
achievable convergence order: $O(\Delta t^2)$ (Strang 1968)



Strang splitting



achievable convergence order: $O(\Delta t^2)$ (Strang 1968)
⇒ What is surprising?

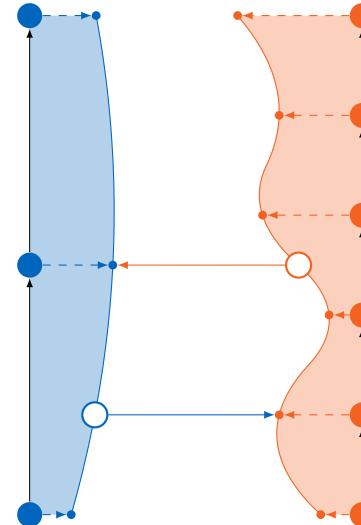


Waveform iterations

$$\begin{aligned}m_1 \ddot{u}_1 &= -(k_1 + k_{12}) u_1 + \mathbf{F}_2(t) \\m_2 \ddot{u}_2 &= -(k_2 + k_{12}) u_2 + \mathbf{F}_1(t)\end{aligned}$$

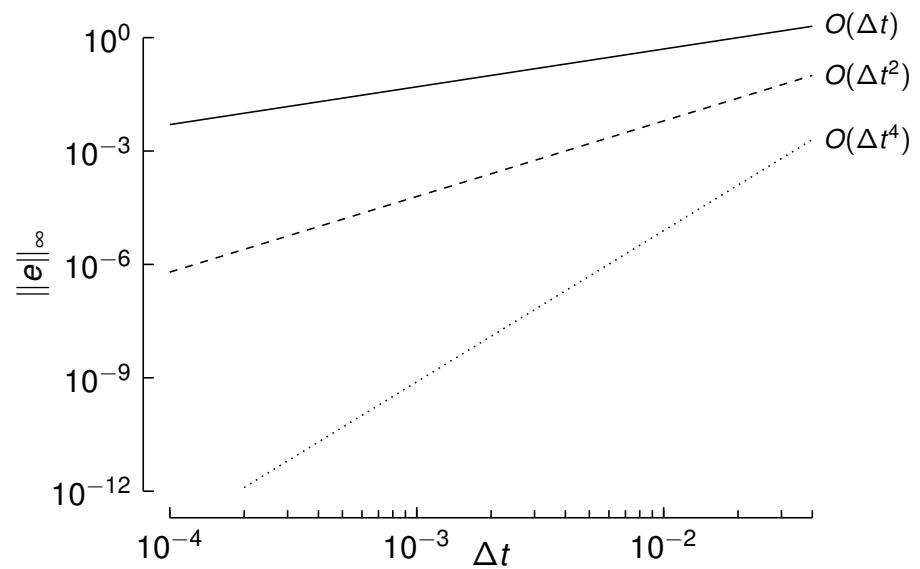
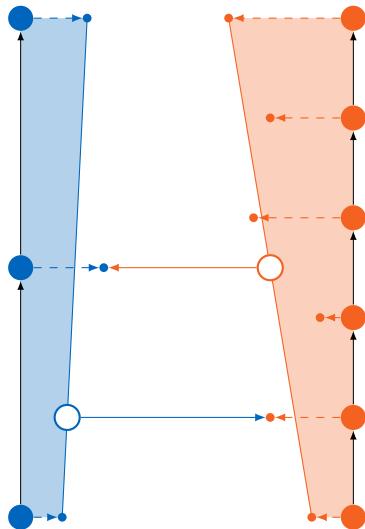
new approach: (Rüth et al. 2018, 2021)

- exchange **polynomial interpolants** of boundary terms $(\mathbf{F}_1, \mathbf{F}_2)$ instead of single values
- initial guess: constant interpolation
- *iterate* until convergence



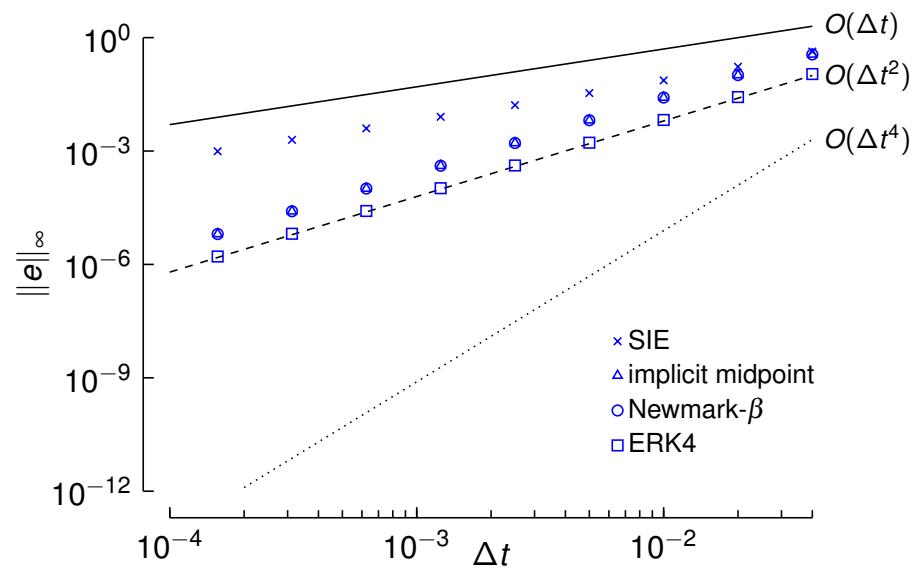
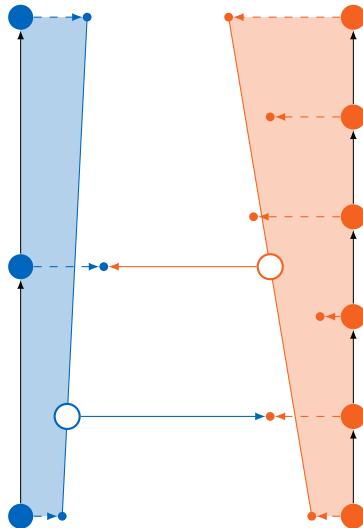
Waveform iterations: Convergence study

here: implementation with linear interpolant



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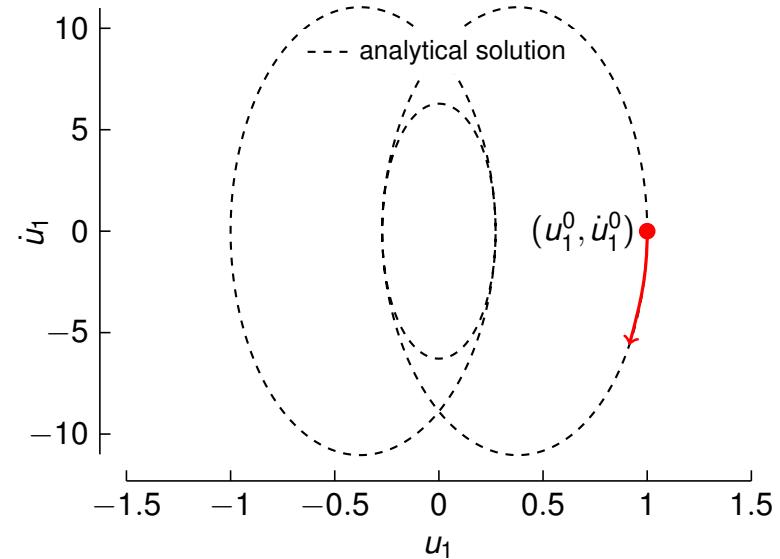


Energy Conservation

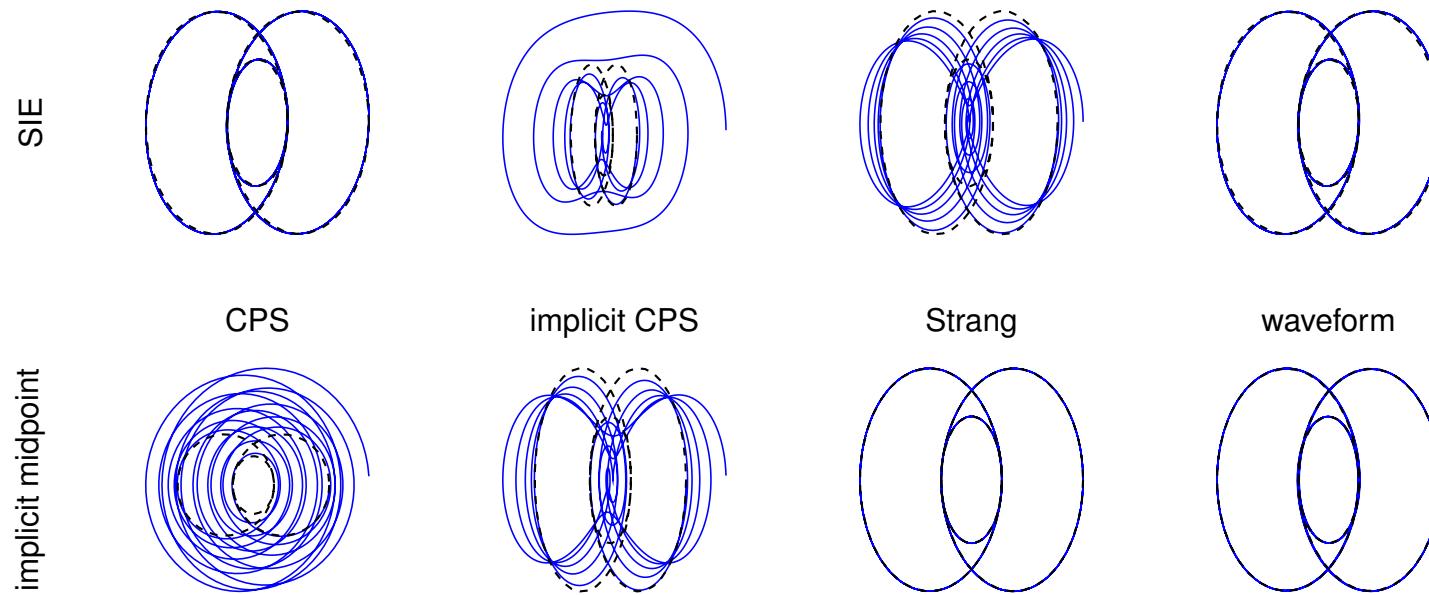
$$E = \frac{1}{2} \dot{\mathbf{u}}^T M \dot{\mathbf{u}} + \frac{1}{2} \mathbf{u}^T K \mathbf{u}$$

→ visualize the solution in phase space

→ use methods with good energy conservation properties
(semi-implicit Euler, implicit midpoint)



Energy Conservation



Summary & Outlook

- coupling schemes and time integration methods *interact*
- simple coupling schemes lead to order degradation and worse behavior regarding energy conservation *most of the time*
- Strang splitting is a cheap way to get a better solution in both aspects *most of the time*
- waveform iterations are an expensive way to get a better solution *reliably*
 - more potential for applications with multiscale characteristics (cf. slide 17)

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 - more potential for applications with multiscale characteristics (cf. slide 17)

⇒ experimental linear waveform iterations are already part of preCICE v2.4

⇒ quadratic, cubic,... waveform iterations will be part of preCICE v3 (\sim start of 2023)

more info + tutorials: <https://precice.org/>, or talk to me!

Full paper

"A Simple Test Case for Convergence Order in Time and Energy Conservation of Black-Box Coupling Schemes."
Schüller et al. 2022, DOI: 10.23967/wccm-apcom.2022.038.

Thank you!

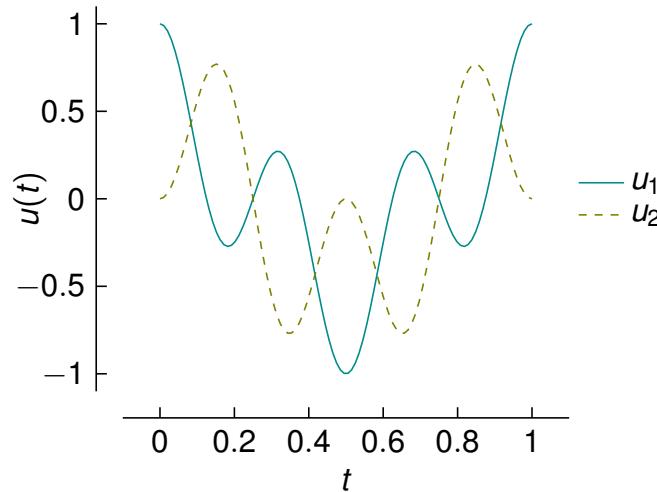
Questions?

References / Further Reading

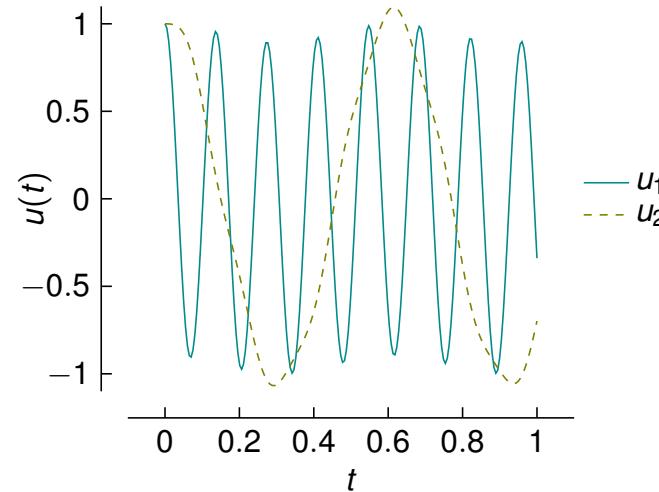
- Farhat, Charbel and Michel Lesoinne (Jan. 1998). "Higher-Order Staggered and Subiteration Free Algorithms for Coupled Dynamic Aeroelasticity Problems". In: *36th AIAA Aerospace Sciences Meeting and Exhibit*. Reno, NV, USA: American Institute of Aeronautics and Astronautics. DOI: [10.2514/6.1998-516](https://doi.org/10.2514/6.1998-516).
- Rüth, Benjamin et al. (2018). "Time Stepping Algorithms for Partitioned Multi-Scale Multi-Physics in preCICE". In: *ECCOMAS ECFD-ECCM 2018*. Glasgow, UK, p. 12.
- Rüth, Benjamin et al. (2021). "Quasi-Newton Waveform Iteration for Partitioned Surface-Coupled Multiphysics Applications". In: *International Journal for Numerical Methods in Engineering* 122.19, pp. 5236–5257. ISSN: 1097-0207. DOI: [10.1002/nme.6443](https://doi.org/10.1002/nme.6443).
- Schüller, Valentina et al. (July 2022). "A Simple Test Case for Convergence Order in Time and Energy Conservation of Black-Box Coupling Schemes". In: *WCCM-APCOM 2022*. Yokohama, Japan. DOI: [10.23967/wccm-apcom.2022.038](https://doi.org/10.23967/wccm-apcom.2022.038).
- Strang, Gilbert (Sept. 1968). "On the Construction and Comparison of Difference Schemes". In: *SIAM Journal on Numerical Analysis* 5.3, pp. 506–517. ISSN: 0036-1429, 1095-7170. DOI: [10.1137/0705041](https://doi.org/10.1137/0705041).

Appendix

The oscillator example: Analytical solutions



$$k_1 = k_2 = 4\pi^2, k_{12} = 16\pi^2 \text{ -- studied here}$$



$$k_1 = 2000, k_2 = 10, k_{12} = 100$$

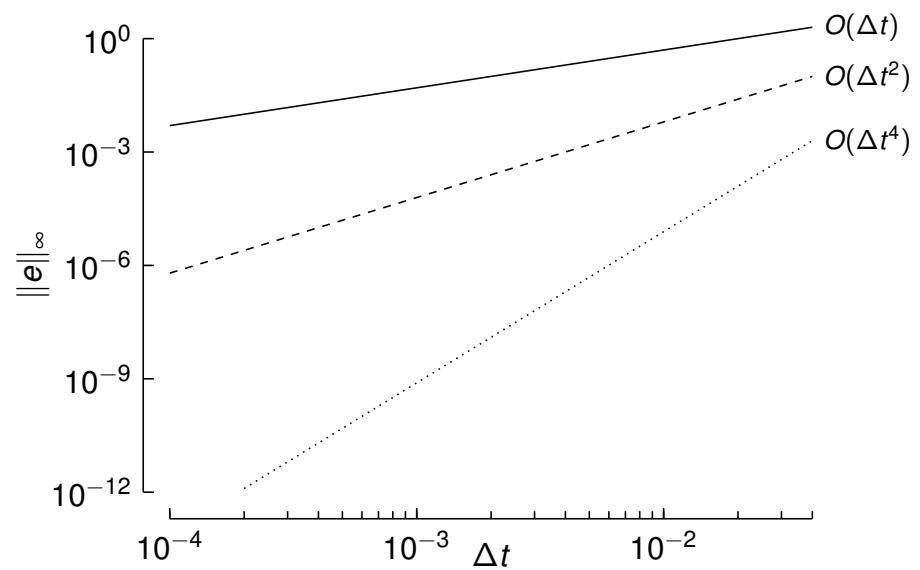
Naive coupling: A parallel scheme with iterations

Fixed-point iterations over the CPS scheme:

$$\left\| (u_i^{n+1})^{k+1} - (u_i^{n+1})^k \right\| \leq \varepsilon.$$

"implicit CPS" (Farhat and Lesoinne 1998)

Achievable convergence order: $O(\Delta t)$
(but higher stability)



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⇒ What happened here?

