Dirichlet-Neumann waveform iteration with the coupling library preCICE

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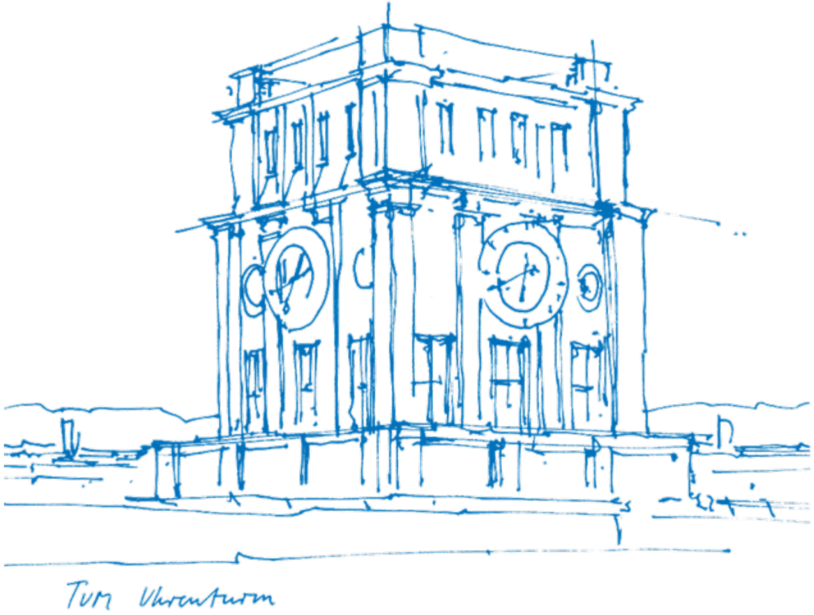
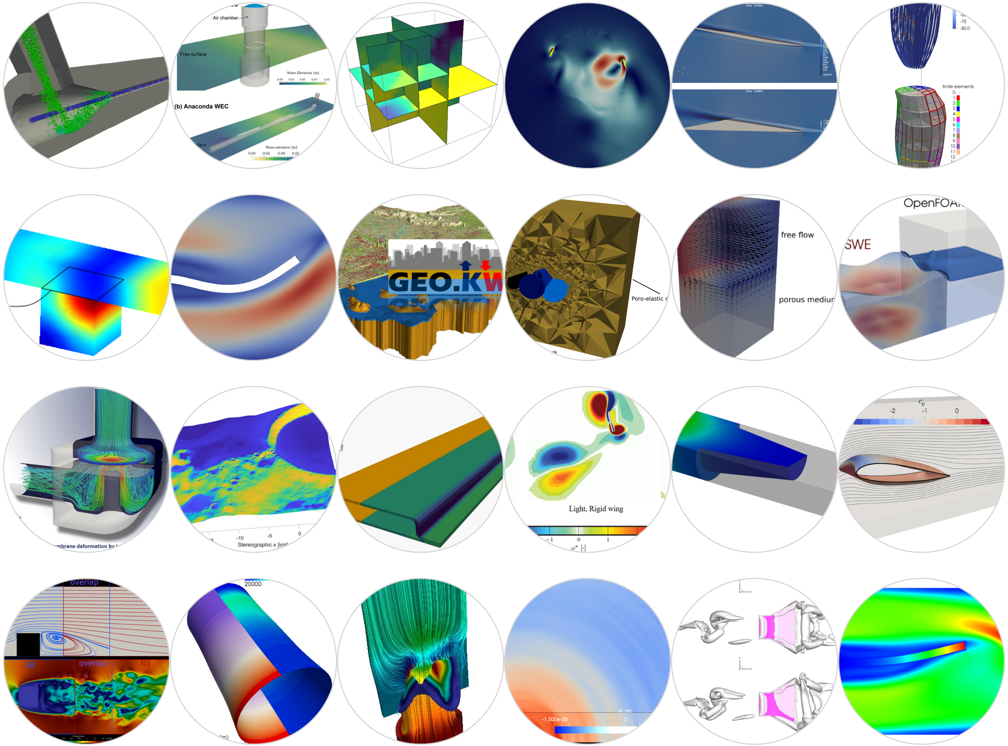
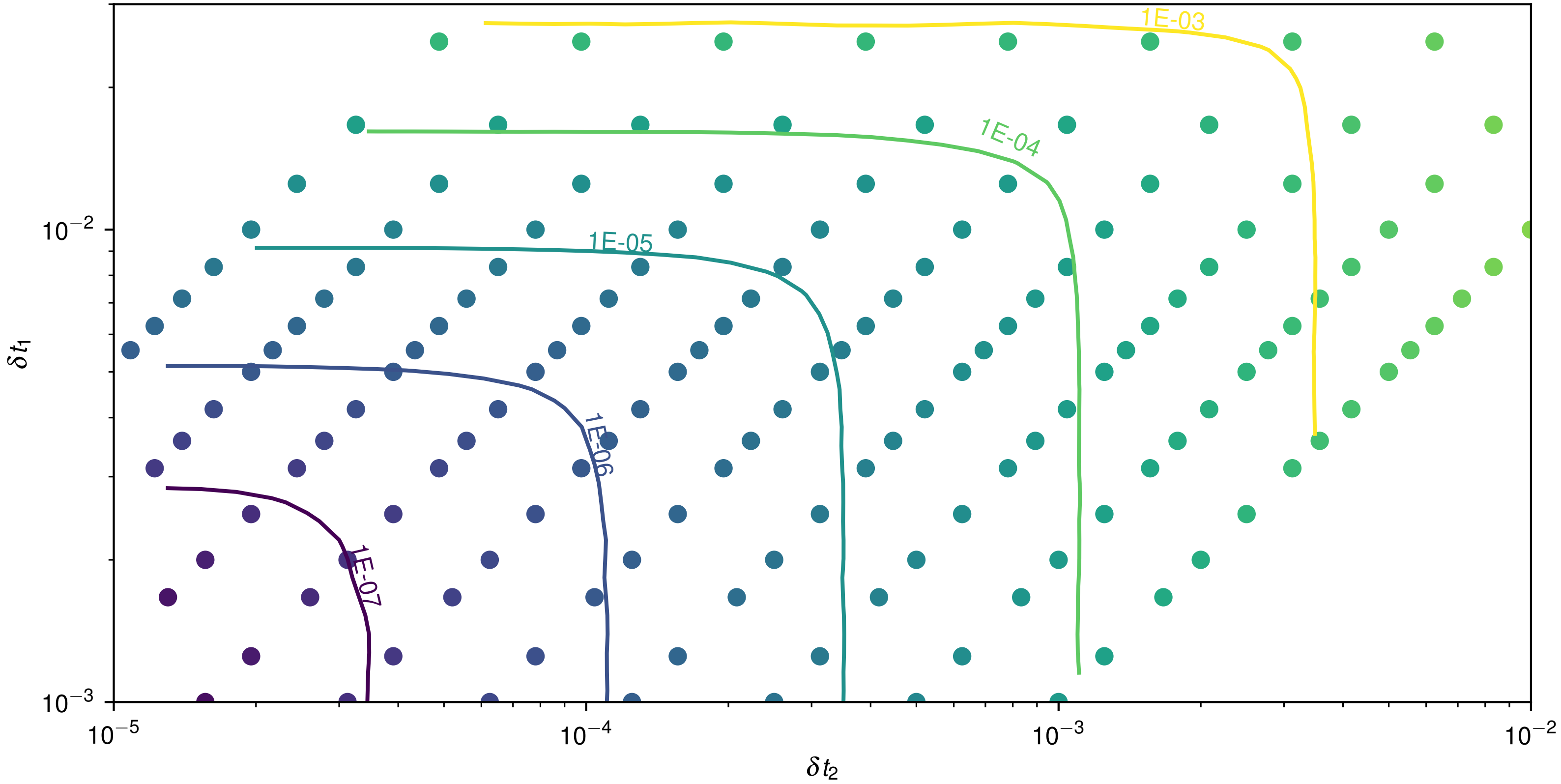
DD28, Jan. 31, 2024



Technical University of Munich, Department of Informatics


Air chamber
Free surface
(b) Anaconda WEC
finite elements
free flow
SWE
Light, Rigid wing
overlap
overlap
NS
20000

Partitioned = heterogeneous



Outline

What is preCICE?

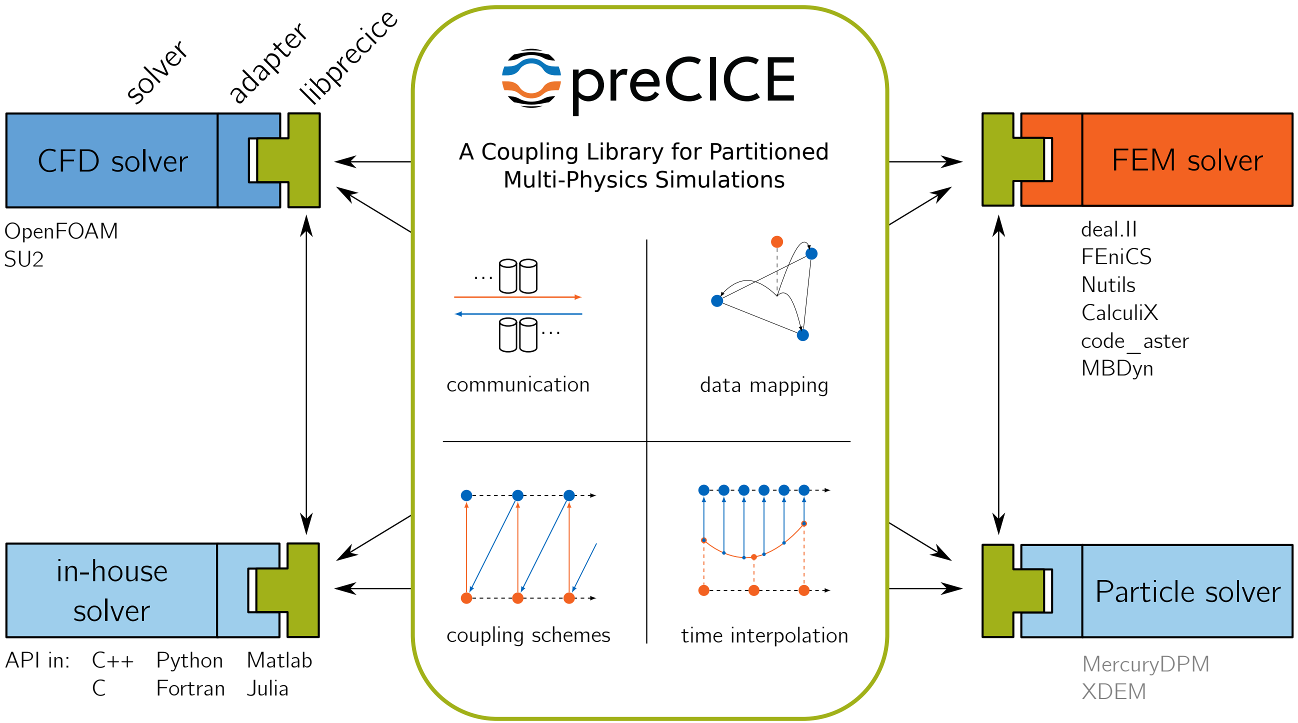
Why preCICE relies on domain decomposition

preCICE v3: waveform iteration ($=$ PinT)

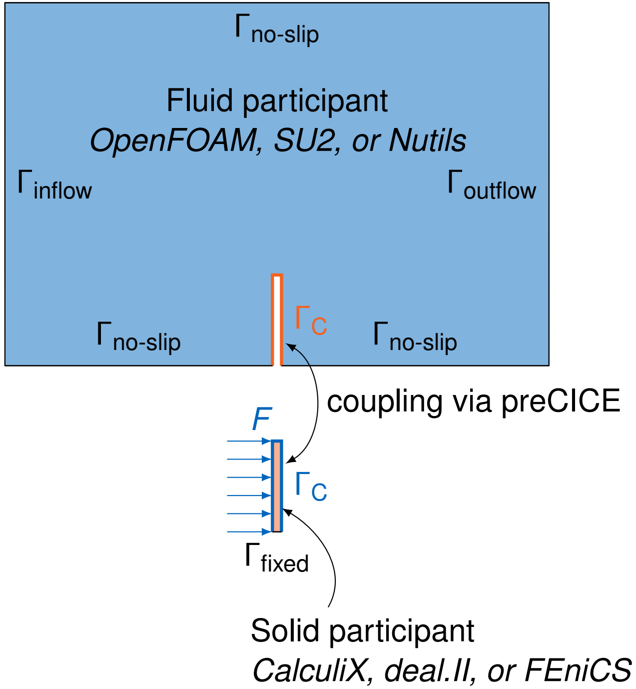
Partitioned heat equation

preCICE user interface + waveform iteration

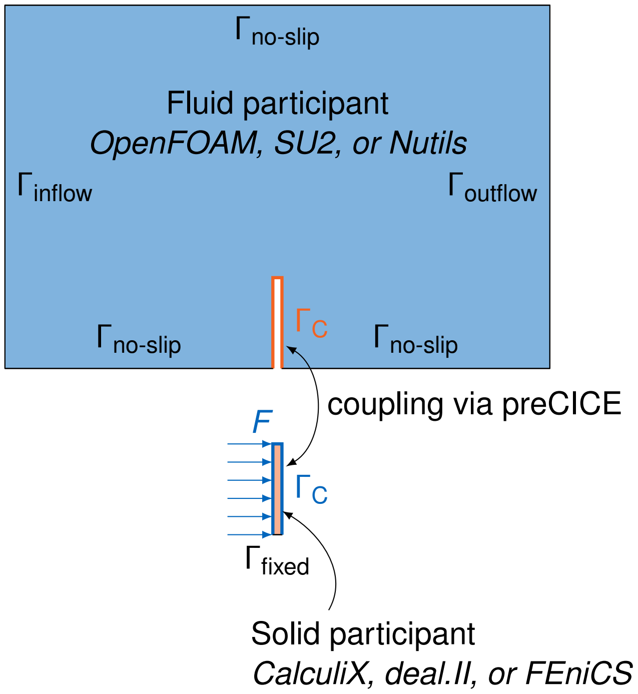
What is preCICE?



tutorials/perpendicular-flap



Why preCICE relies on domain decomposition



Divide

- OpenFOAM $\neq$ CalculiX
- preCICE $=$ *partitioned* multiphysics
- Dirichlet-Neumann $=$ black box

Conquer

- Fluid: $\mathscr{F}(d) = u$
- Solid: $\mathscr{S}(u) = d$

Boundary response maps

(= Poincaré-Steklov operator)

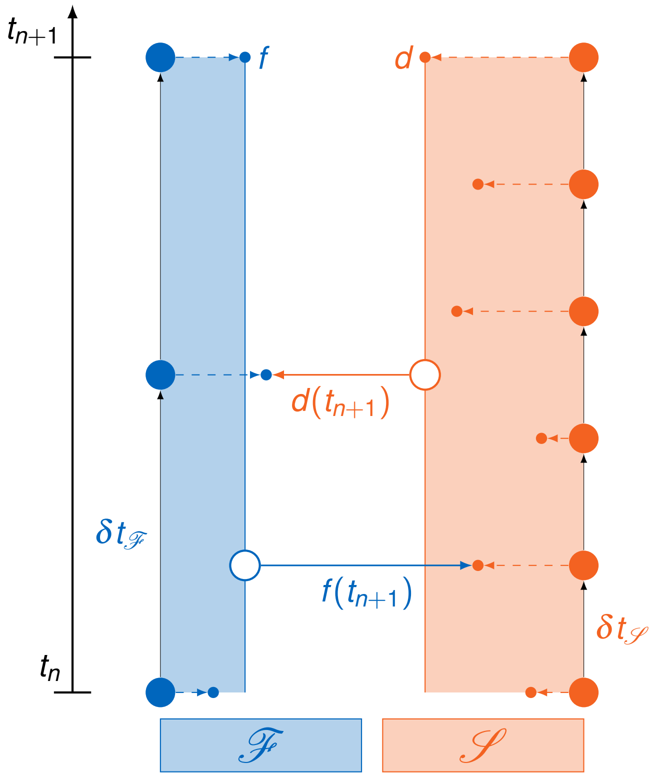
Combine

- $\mathscr{F}(\mathscr{S}(u^k)) = \tilde{u}^k$
- $\tilde{u}^k \xrightarrow{\mathscr{A}} u^{k+1}$

Picard iteration + acceleration

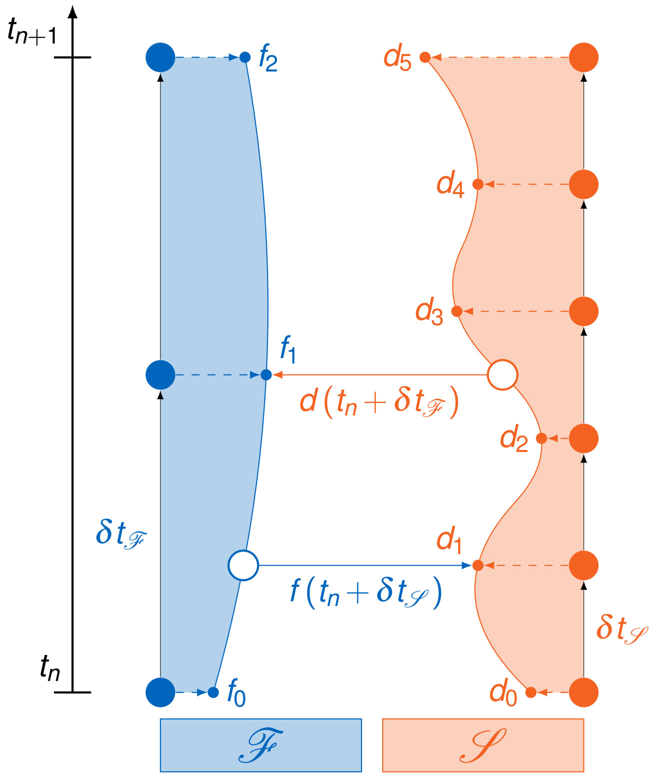
preCICE v2: single-value coupling

```
<data:vector name="Force" />
<data:vector name="Displ" />
...
<coupling-scheme:serial-implicit>
  <participants first="Fluid" second="Solid" />
  <exchange
    data="Force"
    from="Fluid"
    to="Solid" />
  <exchange
    data="Displ"
    from="Solid"
    to="Fluid" />
  ...
</coupling-scheme:serial-implicit>
```

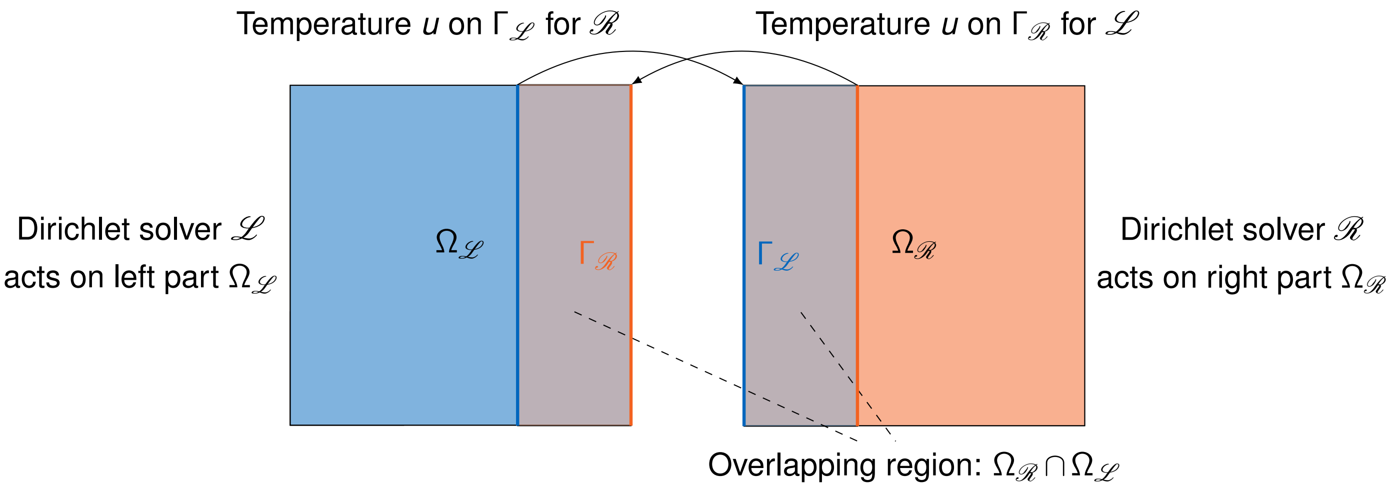


preCICE v3: waveform iteration (= PinT)

```
<data:vector name="Force" waveform-degree="2" />
<data:vector name="Displ" waveform-degree="3" />
...
<coupling-scheme:serial-implicit>
  <participants first="Fluid" second="Solid" />
  <exchange
    data="Force"
    from="Fluid"
    to="Solid"
    substeps="true" />
  <exchange
    data="Displ"
    from="Solid"
    to="Fluid"
    substeps="true" />
  ...
</coupling-scheme:serial-implicit>
```



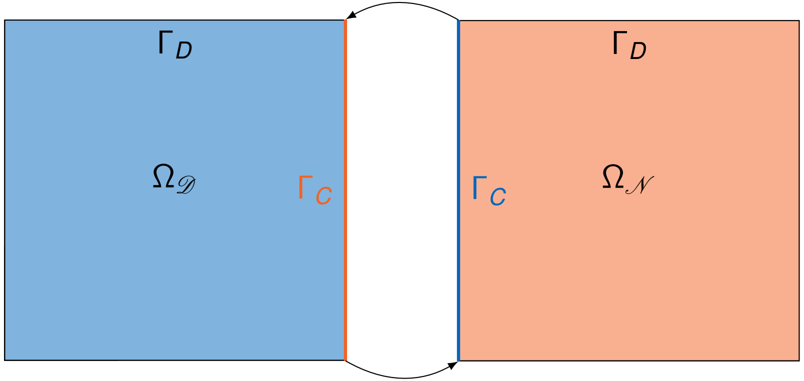
Partitioned heat equation



Partitioned heat equation

Dirichlet boundary condition on Γ_C for $\mathscr{D}$

temperature u_C



Dirichlet solver $\mathscr{D}$

(FEniCS, OpenFOAM, or Nutils)

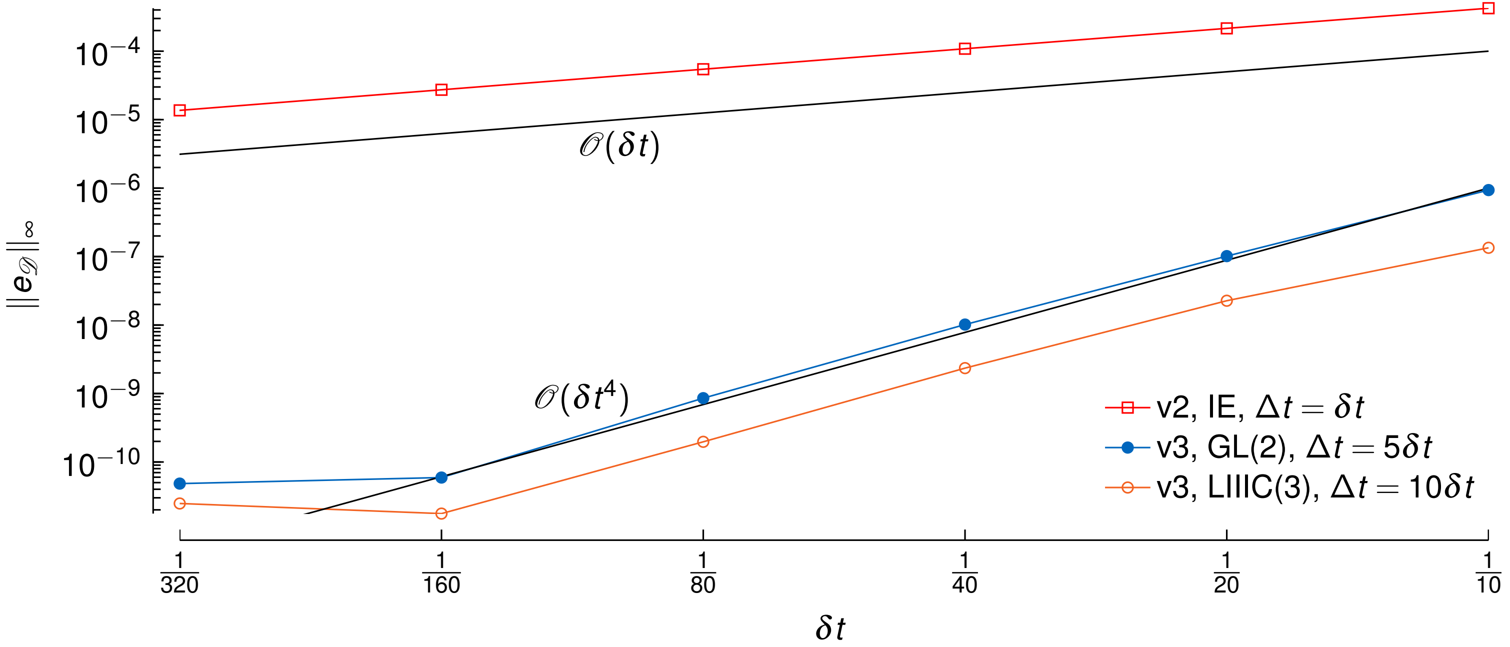
Neumann solver $\mathscr{N}$

(FEniCS, OpenFOAM, or Nutils)

heat flux $q_C = \vec{\nabla} u \,|_{\Gamma_C}$

Neumann boundary condition on Γ_C for $\mathscr{N}$

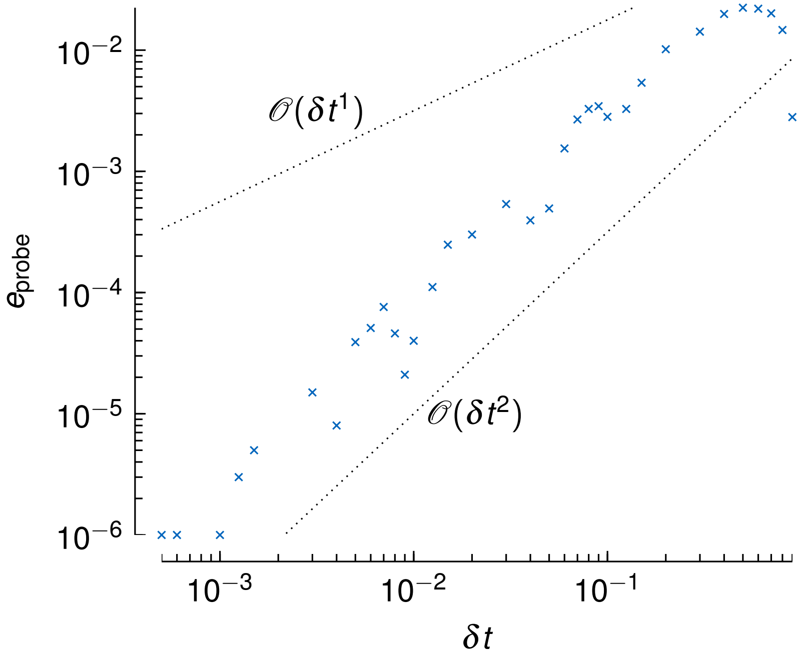
Partitioned heat equation



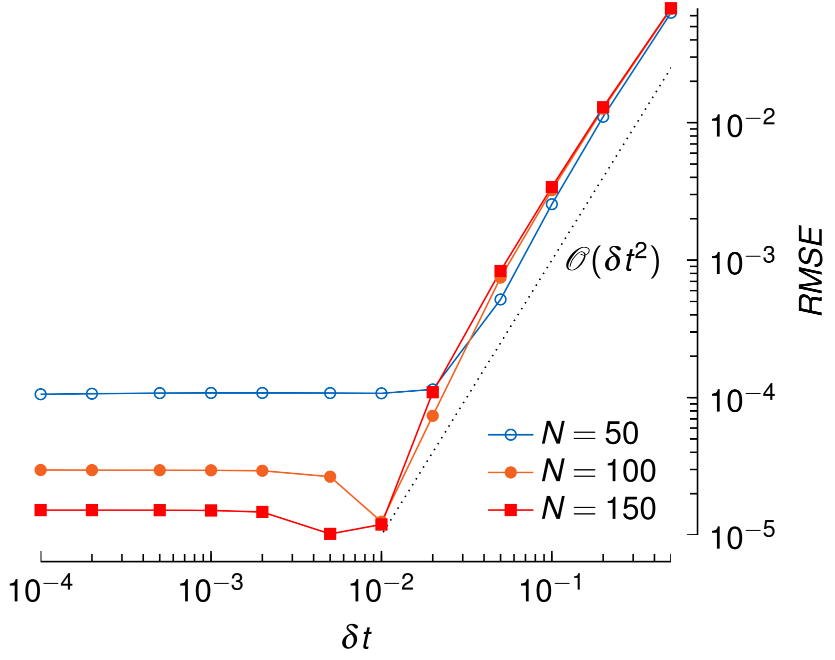
Bachelor's thesis by Niklas Vinnitchenko *Evaluation of Higher-Order Coupling Schemes with FEniCS-preCICE*[1]

[1] https://github.com/precice/tutorials/pull/415

Outlook: FS (atm) without I



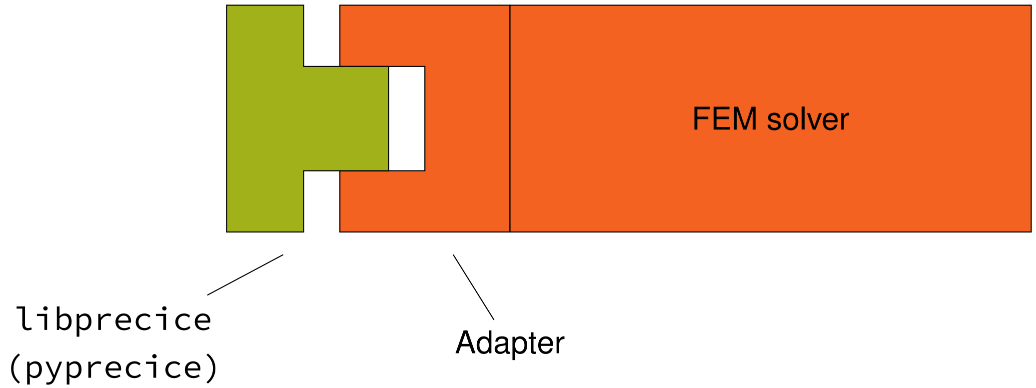
CalculiX beam (Probe at beam tip, compare to $\delta t = 10^{-5}$)



OpenFOAM Taylor-Green vortex

Guided research project by Marc Amorós Trepat *Review of higher-order time stepping schemes in open-source solvers*

preCICE user interface + waveform iteration



Goal: Black-box + higher-order interpolation + waveform iteration

- Numerics: Accuracy, convergence order, energy conservation
- API Design: Simple user interface!
- Move as much waveform iteration logic *inside* preCICE as possible
- preCICE v2.5 is the current version, preCICE v3 + new API is almost released

$\mathscr{F}(d) = u$ in python: API example

```python
# example: FSI coupling, perspective of fluid solver $\mathscr{F}$:
participant = precice.Participant("Fluid", "precice-config.xml")

# leaving out coupling mesh and data initialization

participant.initialize()

while participant.is_coupling_ongoing():
  # store checkpoint, if needed
  dt = participant.get_max_time_step_size()
  displacement = participant.read_data(dt)  # Read displacement at $t_n+\Delta t$: $d_{n+1}$
  forces = forces + dt * dfdt(displacements)  # Implicit Euler
  participant.write_data(forces)
  participant.advance(dt)
  # read checkpoint, if needed

participant.finalize()
```

API with RK4, with subcycling

```python
# example: FSI coupling, perspective of fluid solver $\mathcal{F}$:
# ...
participant.initialize()

while participant.is_coupling_ongoing():
  # store checkpoint, if needed
  precice_dt = participant.get_max_time_step_size()  # until end of window
  solver_dt = time_stepper.get_max_dt()  # stability, adaptivity
  dt = np.min([precice_dt, solver_dt])  # actual time step size $\delta t$
  # time_stepper represents s-stage RK scheme
  ts = time_stepper.rhs_eval_points(dt)  # $t_n+c_1, t_n+c_2 \ldots, t_n+c_s$
  displacements = [participant.read_data(t) for t in ts]  # $d(t_n+c_1), d(t_n+c_2) \ldots, d(t_n+c_s)$
  forces = time_stepper.do_step(displacements, dt)  # $f_{n+1} = f_n + \delta t \sum_{i=1}^{s} b_i k_i$
  participant.write_data(forces)
  participant.advance(dt)
  # read checkpoint, if needed

participant.finalize()
```

Conclusion

State of development

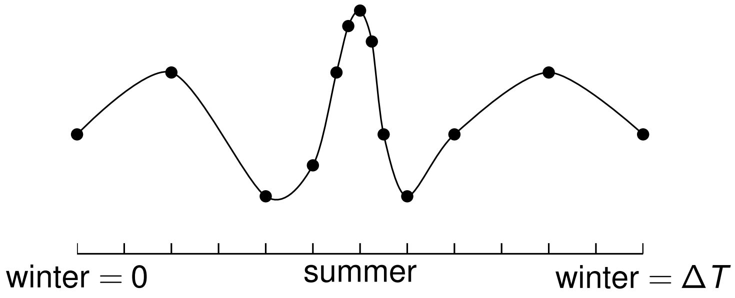
- Achievements: Black-box waveform iteration + usable API (+ multirate)
- Goal: Release preCICE v3. (we are very very close)
- If you want to try experimental version now: `https://github.com/precice/precice/pull/1914`

Where to be careful:

- Requirement: High order interpolation needs subcycling
- Restriction: Only simple acceleration with substeps, `https://github.com/precice/precice/pull/1834`

Many questions:

- Synchronization, subcycling, and performance?
- Fluid-structure interaction case?
- Adaptivity (inside window / across windows)



Community

preCICE Workshop 2023@Munich

Stay in touch?

- `precice.org/community`
- `precice.discourse.group`

Conferences

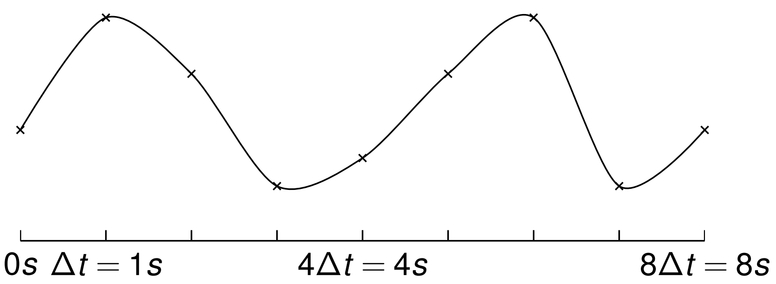
- WCCM + preCICE course
  July 2024@Vancouver
  Deadline: this Friday
  preCICE MS[1]
- preCICE Workshop
  Sept 2024@Stuttgart
- COUPLED
  2025@Sicily

[1] Multi-Physics and Multi-Scale Simulations with the Coupling Library preCICE (0415)

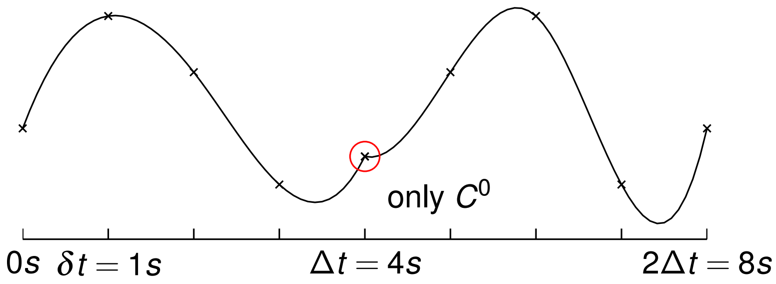
Subcycling

- Time window size $\Delta t \geq$ time step size δt_1 and δt_2.
- Do n time steps in window: $\Delta t = n_1 \delta t_1 = n_2 \delta t_2$
- Allows to create BSpline of degree $n - 1$. (Goal reached: Something better than linear interpolation)
- Restriction: Only use data of current window!
- Larger window + subcycling has impact on number of QN iterations[1]

Without subcycling



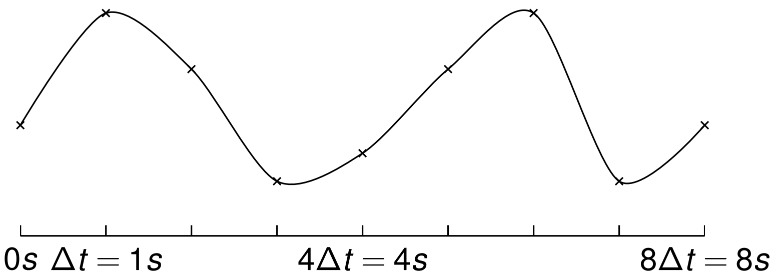
With subcycling (third order BSpline)



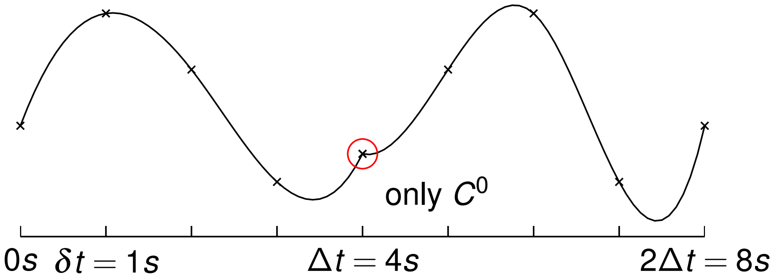
[1] Rüth, B, Uekermann, B, Mehl, M, Birken, P, Monge, A, Bungartz, H-J. Quasi-Newton waveform iteration for partitioned surface-coupled multiphysics applications. Int J Numer Methods Eng. 2021; 122: 5236– 5257. `https://doi.org/10.1002/nme.6443`

QN iterations

Without subcycling



With subcycling (third order BSpline)

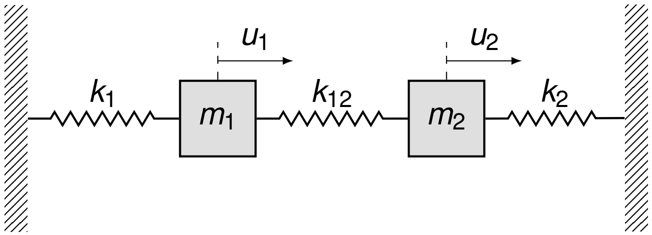


rQN-WI | Δt	0.5	0.1
WI$(1,1;1)$	7.85	5.45
WI$(5,5;1)$	10.95	7.48

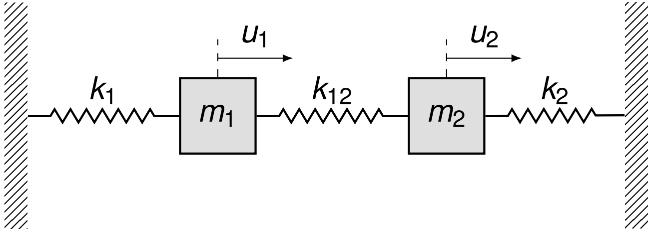
rQN-WI means we only use the data at the end of the window for Quasi-Newton. Different example case, but similar implementation. More possibilities shown in[1].

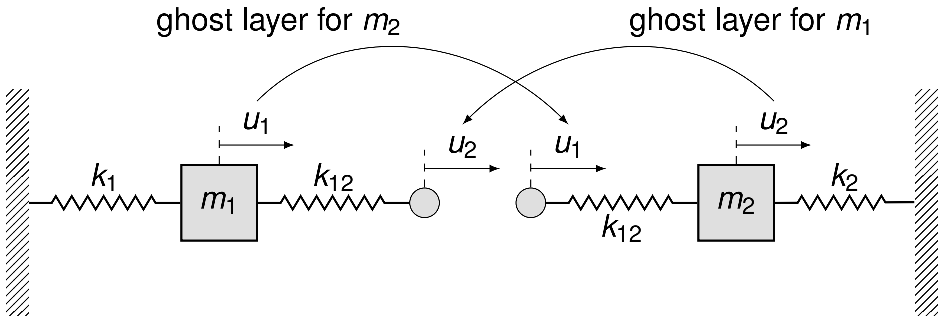
[1] Rüth, B, Uekermann, B, Mehl, M, Birken, P, Monge, A, Bungartz, H-J. Quasi-Newton waveform iteration for partitioned surface-coupled multiphysics applications. Int J Numer Methods Eng. 2021; 122: 5236– 5257. `https://doi.org/10.1002/nme.6443`

Oscillator example: Setup



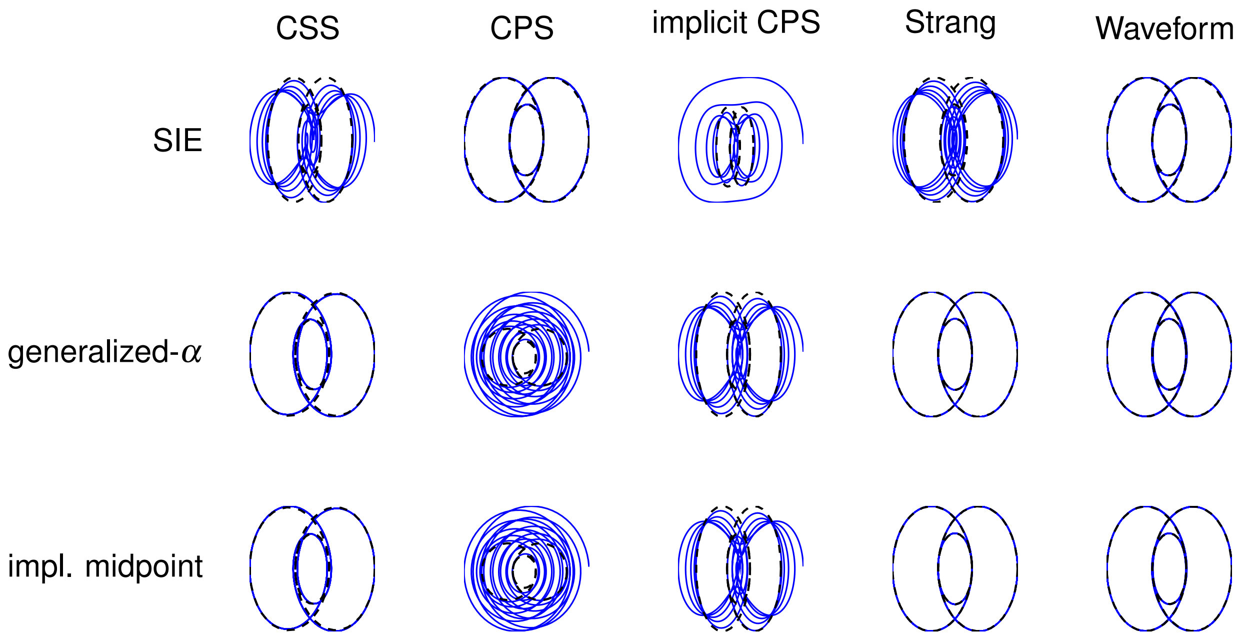
Oscillator example: Setup





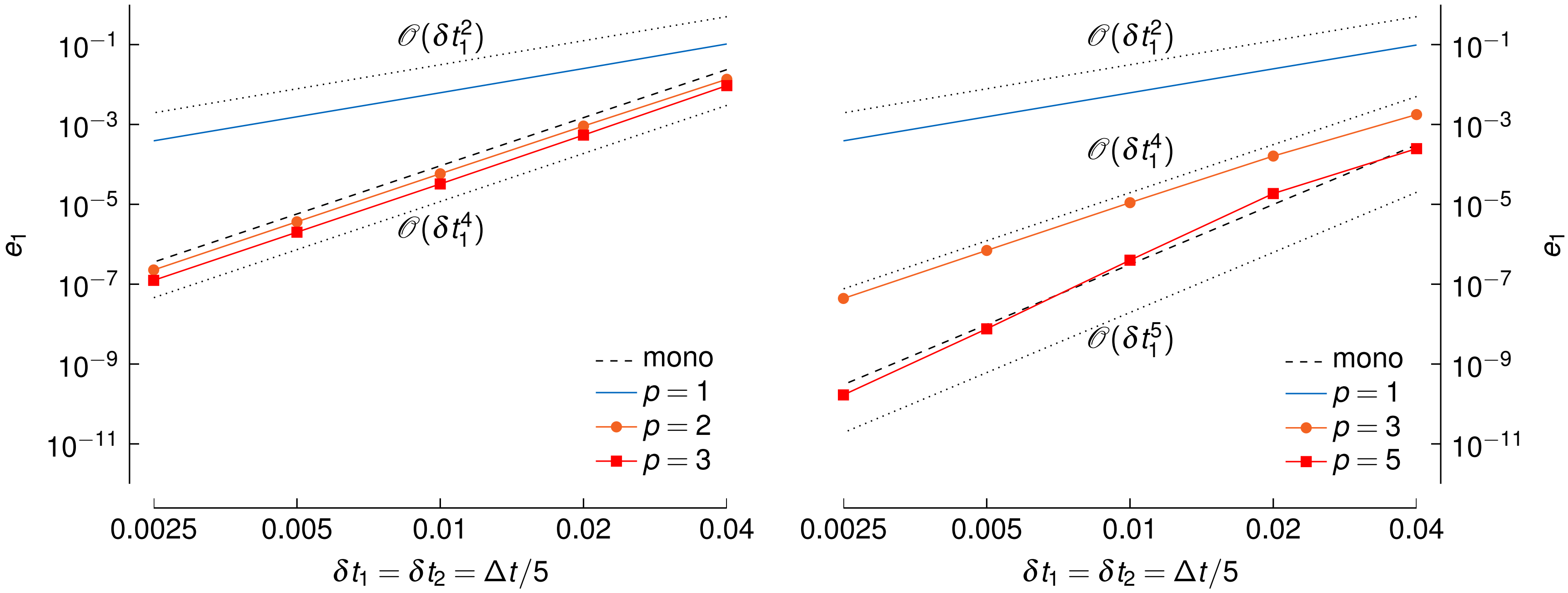
Not Dirichlet-Neumann coupling, but overlapping Schwarz for this setup. Still: Same idea.

Oscillator example: Energy conservation



A Simple Test Case for Convergence Order in Time and Energy Conservation of Black-Box Coupling Schemes. 2022.

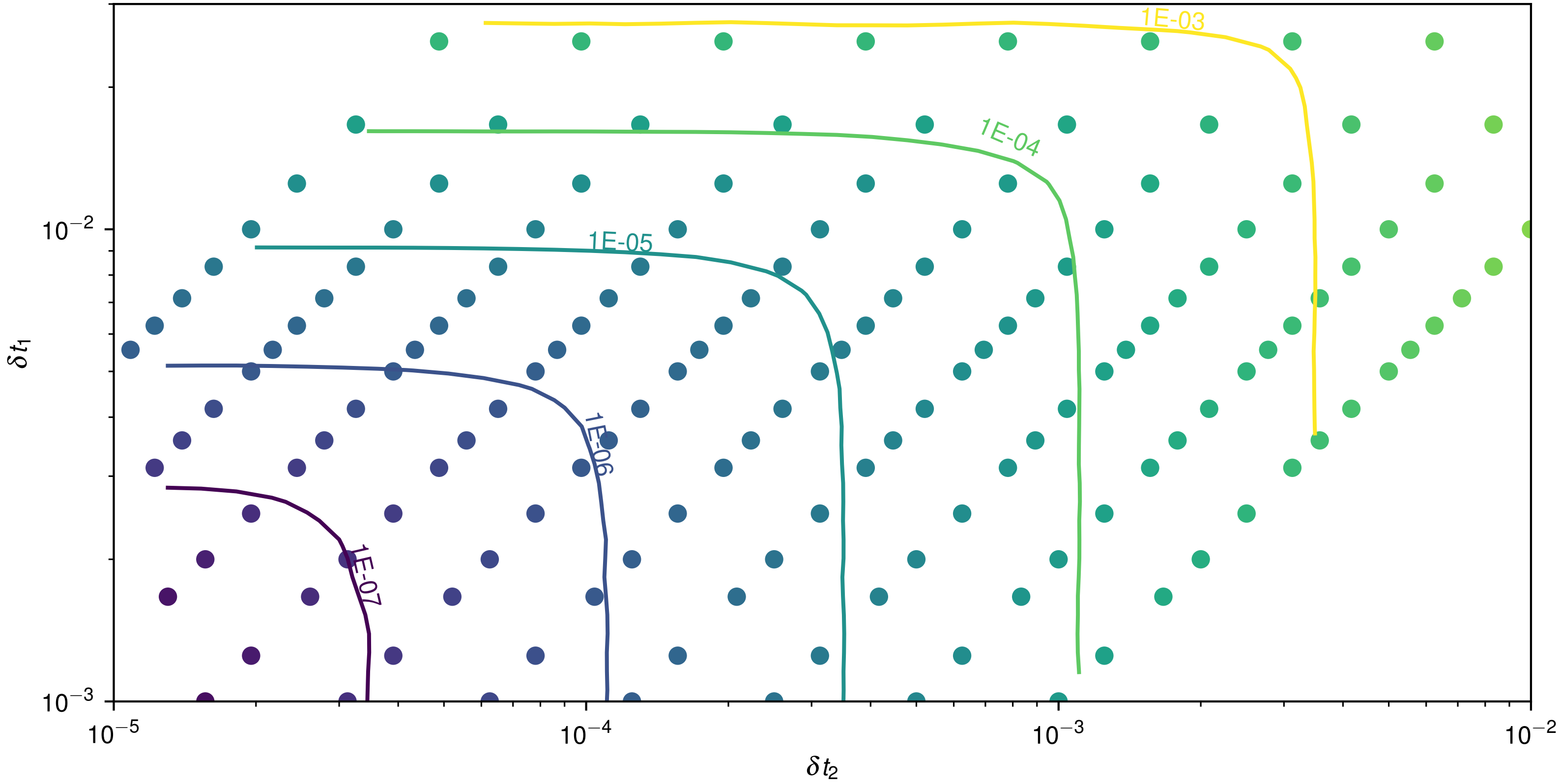
Oscillator example: Higher-order TS



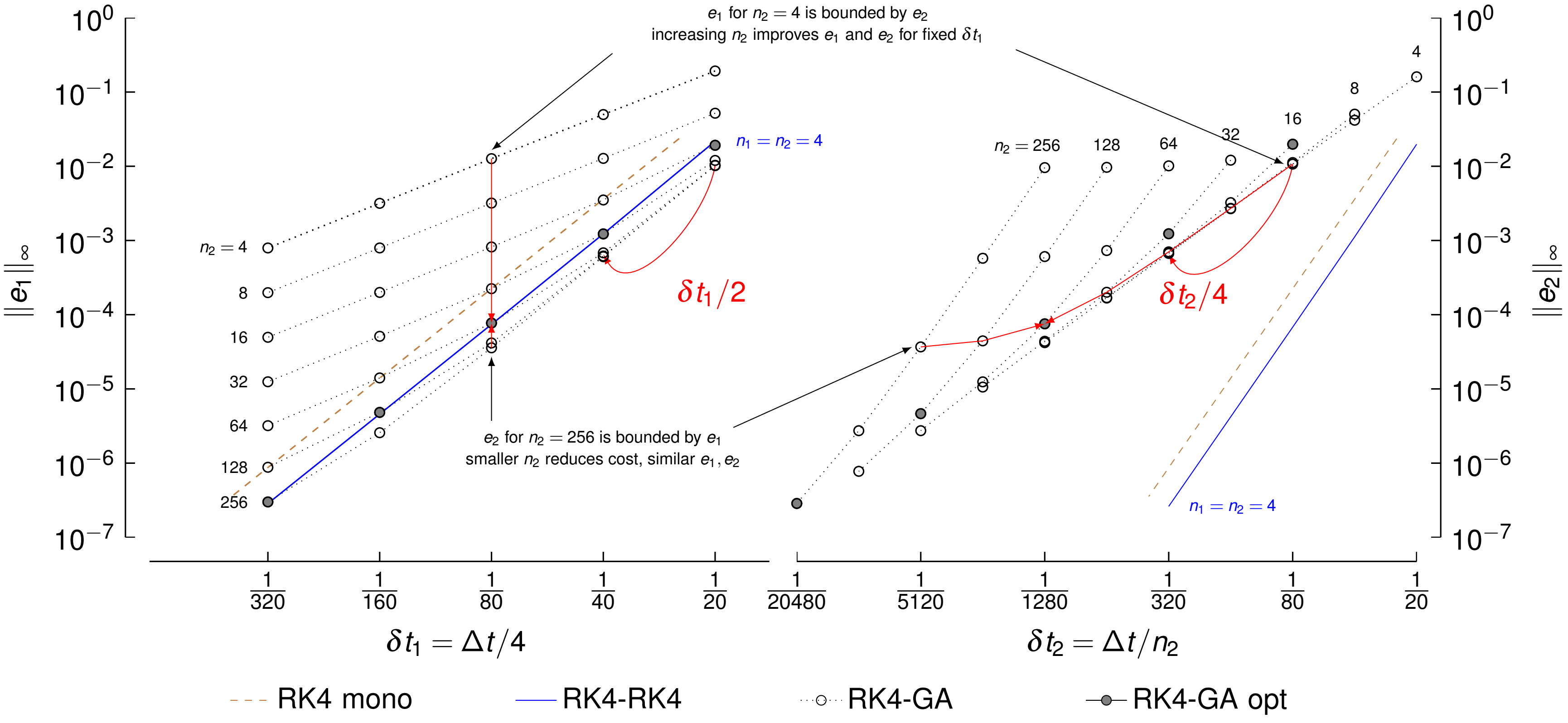
classic Runge-Kutta method

Radau IIA

Oscillator example: Different schemes, different δt



Oscillator example: Different schemes, different δt



RK4 in code

```
# determine time step size δt for this time step
dt = participant.get_max_time_step_size()

# compute stages k_i and evaluate waveform at times c_iδt
k1 = A.dot(x) + participant.read_data("Displ", 0.0 * dt)
k2 = A.dot(x + k1 * 0.5 * dt) + participant.read_data("Displ", 0.5 * dt)
k3 = A.dot(x + k2 * 0.5 * dt) + participant.read_data("Displ", 0.5 * dt)
k4 = A.dot(x + k3 * 1.0 * dt) + participant.read_data("Displ", 1.0 * dt)
# assemble new solution
x_new = x + dt / 6 * (k1 + 2 * k2 + 2 * k3 + k4)

# do writing
displ = extract_force(x_new)
participant.write_data("Force", cpl_write)
# end time step of size δt
precice_dt = participant.advance(dt)
```

API for subcycling

Read interpolated data from current time t_n:

```
displacement = precice.read_data(dt)
```

No more substeps:

```
precice.advance(precice_dt)
```

t_n

```
dt = 0
```

$t_{n+1} = t_n + \Delta t$

```
dt = precice_dt
```

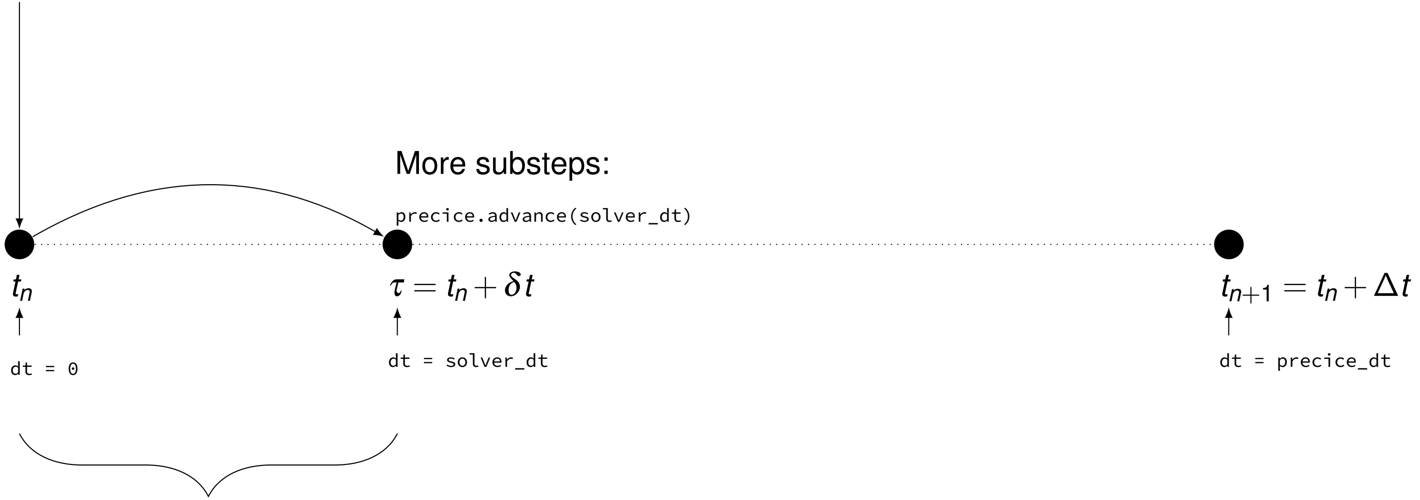
Complete time window size Δt

```
precice_dt = precice.get_max_time_step_size()
```

API for subcycling

Read interpolated data from current time t_n:

```
displacement = precice.read_data(dt)
```



Solver time step size δt

```
solver_dt < precice_dt
```

API for subcycling

Read interpolated data from current time t_n:

```
displacement = precice.read_data(dt)
```