Time stepping algorithms for partitioned multi-scale multi-physics in preCICE

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Partitioned multi-physics

preCICE

A Coupling Library for Partitioned Multi-Physics Simulations

coupling schemes
communication
data mapping
time interpolation

solver
adapter
libprecice

in-house
fluid solver

OpenFOAM
SU2
foam-extend

in-house
solver

Ateles (APES)
Alya System
Carat++
FASTEST

API in:
C / C++
Fortran
Python

structure
solver

CalculiX
Code_Aster

commercial
solver

ANSYS Fluent
COMSOL
FEAP

API in:
C / C++
Fortran
Python

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Example application: fluid-structure-acoustics

Fluid-structure-acoustics simulation and partitioned setup\(^1\).

<table>
<thead>
<tr>
<th>physics</th>
<th>timescale</th>
<th>solver</th>
<th>scheme</th>
<th>order</th>
</tr>
</thead>
<tbody>
<tr>
<td>(A)</td>
<td>small</td>
<td>Ateles</td>
<td>RK</td>
<td>2 or 4</td>
</tr>
<tr>
<td>(A)</td>
<td>small</td>
<td>FASTEST</td>
<td>EE</td>
<td>1</td>
</tr>
<tr>
<td>(F)</td>
<td>medium</td>
<td>FASTEST</td>
<td>CN</td>
<td>2</td>
</tr>
<tr>
<td>(S)</td>
<td>large</td>
<td>FEAP</td>
<td>N-(\beta)</td>
<td>1 or 2</td>
</tr>
</tbody>
</table>


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Example application: acoustics-acoustics

Three-field flow coupling around a 2D subsonic free jet

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**Partitioned multi-physics**

**Time stepping requirements**

**Engineering:**
- Use different solvers (EE + RK4)
- Use different time discretization
- No degradation of solver performance

**Informatics:**
- Black-box approach (nodal data)
- Parallel (Exa-Scale)

---

![Diagram](image-url)
Partitioned heat transport equation

A simple model problem

- introduce a model problem
- review different coupling schemes
- evaluate performance of schemes

Simple setup

\[ \begin{align*}
&v^{n+1} \\
&\tau \\
&v^n
\end{align*} \quad \begin{align*}
&t^{n+1} \\
&\tau \\
&w^{n+1}
\end{align*} \]

\[ \begin{align*}
&w^n
\end{align*} \]

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Partitioned heat transport equation

Monolithic setup

Heat Transport equation

\[ \frac{\partial u(x, t)}{\partial t} = \alpha \frac{\partial^2 u(x, t)}{\partial x^2}, \quad x \in \Omega, \ t \in \mathbb{R}^+ \]

Dirichlet boundary conditions

\[ u(x = x_L, t) = u_D^L, \quad u(x = x_R, t) = u_D^R \]

Initial condition

\[ u(x, t = 0) = u_0(x) \]
Partitioned heat transport equation

Partitioned setup

Dirichlet-Neumann coupling

Get $\Omega_1$: $v(x_C)$

Set $\Omega_2$: $w(x_C)$

Dirichlet BC

Heat Transport on $\Omega_1$

$\frac{\partial v}{\partial t} = \frac{\partial^2 v}{\partial x^2} = f_v(\ldots)$

Neumann BC

Set $\Omega_1$: $v_x(x_C)$

Get $\Omega_2$: $w_x(x_C)$

Heat Transport on $\Omega_2$

$\frac{\partial w}{\partial t} = \frac{\partial^2 w}{\partial x^2} = f_w(\ldots)$

Partitioning

$\tau = 0.2$

$t$

$\Omega^L_h$

$\Omega^R_h$

$\Omega_h$

$\Sigma : x_C$

$X_L$

$X_R$
Review and experiments on coupling schemes

We are interested in higher order coupling

- different coupling schemes
- use constant spatial meshwidth $h$
- refine temporal meshwidth $\tau$
- compare partitioned result to monolithic solution $u^n$ with fine $\tau$

Monolithic setup

Partitioned setup
Review and experiments on coupling schemes

Classical coupling schemes

**Dirichlet-Neumann coupling**

1. **Get** $\Omega_1$: $v(x_C)$
2. **Set** $\Omega_2$: $w(x_C)$
3. **Heat Transport on** $\Omega_1$:
   \[
   \frac{\partial v}{\partial t} = \frac{\partial^2 v}{\partial x^2} = f_v(\ldots)
   \]
4. **Heat Transport on** $\Omega_2$:
   \[
   \frac{\partial w}{\partial t} = \frac{\partial^2 w}{\partial x^2} = f_w(\ldots)
   \]
5. **Dirichlet BC**
6. **Neumann BC**

**Explicit/loose coupling**

**Implicit/strong coupling**
Review and experiments on coupling schemes

Classical coupling schemes

\[ L_2 \text{ error on } \Omega_h^L \]

![Graph comparing \( L_2 \) error for different coupling schemes, including Heun(\( \tau \)), TR(\( \tau \)) - Mono, and RK4(\( \tau \)) - Mono.

1. Heun(\( \tau \)), TR(\( \tau \)) - Mono
2. RK4(\( \tau \)) - Mono
Review and experiments on coupling schemes

Classical coupling schemes

- RK4(τ), Heun(τ), TR(τ) - IC
- Heun(τ), TR(τ) - Mono
- RK4(τ) - Mono

$L_2$ error on $\Omega_h^i$
Review and experiments on coupling schemes

Customized 2nd order schemes

Heun(τ) - EC
TR(τ) - IC

Heun(τ) - Monolithic
TR(τ) - Monolithic

$L_2$ error on $\Omega_h$
Review and experiments on coupling schemes

Customized 2nd order schemes

$10^{-3}$ $10^{-2}$ $10^{-1}$

$10^{-4}$ $10^{-5}$ $10^{-6}$

$10^{-7}$ $10^{-8}$

$L_2$ error on $\Omega_h$

TR($\tau$) - IC

Heun($\tau$) - EC

Heun($\tau$) - Monolithic

TR($\tau$) - Monolithic

Semi E-I

$\mathbf{v}^{n+1}$ $\mathbf{v}^n$ $\mathbf{w}^{n+1}$

$\mathbf{w}^n$ $\mathbf{v}^n$ $\mathbf{w}^{n+1}$

$\mathbf{v}^n$ $\mathbf{w}^n$ $\mathbf{v}^{n+1}$

$\mathbf{w}^n$ $\mathbf{v}^{n+1}$

$\mathbf{v}^n$ $\mathbf{w}^n$
Review and experiments on coupling schemes

Customized 2nd order schemes

Heun(\(\tau\)) - EC
TR(\(\tau\)) - IC

Heun(\(\tau\)) - Monolithic
TR(\(\tau\)) - Monolithic
Semi E-I

\[ L_2 \text{ error on } \Omega_h \]

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Review and experiments on coupling schemes

Splitting methods

Godunov splitting (= explicit coupling)

\[ v^{n+1} \rightarrow \frac{1}{2} (v^n + v^{n+1}) \]

\[ w^{n+1} \rightarrow \frac{1}{2} (w^n + w^{n+1}) \]

Strang splitting

\[ v^{n+1} = v^n + \frac{1}{2} f_v \]

\[ w^{n+1} = w^n + \frac{1}{2} f_w \]
Review and experiments on coupling schemes

Splitting methods

\begin{figure}
\begin{center}
\includegraphics[width=\textwidth]{plot.png}
\end{center}
\end{figure}

\textbf{Heun(\(\tau\)) - Strang}

\textbf{TR(\(\tau\)) - Mono}

\textbf{TR(\(\tau\)) - Strang}

\(L_2\) error on \(\Omega_h\)

\(10^{-3}\) \quad \(10^{-4}\) \quad \(10^{-5}\) \quad \(10^{-6}\)

\(\tau_i\)

\(10^{-3}\) \quad \(10^{-2}\) \quad \(10^{-1}\)
Review and experiments on coupling schemes

Splitting methods

\begin{align*}
\text{Heun}(\tau) - \text{Strang} \\
\text{RK4}(\tau) - \text{Strang} \\
\text{TR}(\tau) - \text{Mono} \\
\text{TR}(\tau) - \text{Strang}
\end{align*}

\[ L_2 \text{ error on } \Omega^L_h \]
Review and experiments on coupling schemes

Splitting methods

- Heun($\tau$) - Strang
- RK4($\tau$) - Strang
- TR($\tau$) - Strang
- RK4($\tau$)/TR($\tau$) - Strang

$L_2$ error on $\Omega_h$

$t$

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Review and experiments on coupling schemes

Waveform relaxation

Implicit/strong coupling

Waveform relaxation

\[ \tilde{v}(t) \]

\[ \tau_L, \text{BDF2} \]

\[ \tau_R, \text{RK4} \]
Review and experiments on coupling schemes

Waveform relaxation

\[ \tau_i \]

\[ L_2 \text{ error on } \Omega_h \]

\[ \text{TR}(\tau) - \text{Monolithic Waveform Relaxation} \]
Review and experiments on coupling schemes

Waveform relaxation

![Graph showing L2 error on $\Omega_t^j$ as a function of $\tau_i$. The graph compares different coupling schemes: TR($\tau$) - Monolithic Waveform Relaxation, RK4($\tau$)/RK4($\tau$) - WR, and RK4($\tau$) - Monolithic. The x-axis represents $\tau_i$ ranging from $10^{-3}$ to $10^{-1}$, while the y-axis represents the L2 error ranging from $10^{-15}$ to $10^{-2}$. The graph includes data points for each scheme, showing the error level for different $\tau_i$ values.]

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Review and experiments on coupling schemes

Waveform relaxation

\[ L_2 \text{ error on } \Omega_h \]

\[ 10^{-15} \quad 10^{-14} \quad 10^{-13} \quad 10^{-12} \quad 10^{-11} \quad 10^{-10} \quad 10^{-9} \quad 10^{-8} \quad 10^{-7} \quad 10^{-6} \quad 10^{-5} \quad 10^{-4} \quad 10^{-3} \quad 10^{-2} \quad 10^{-1} \]

\[ \tau_i \]

RK4(\tau) - Monolithic

RK4(\tau)/RK4(0.1\tau) - WR

TR(\tau) - Monolithic Waveform Relaxation

RK4(\tau)/RK4(\tau) - WR

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Review and experiments on coupling schemes

Waveform relaxation

\[ L_2 \text{ error on } \Omega^L_i \]

- RK4(\(\tau\))/TR(\(\tau\)) - WR
- TR(\(\tau\)) - Monolithic Waveform Relaxation
- RK4(\(\tau\))/RK4(0.1\(\tau\)) - WR
- RK4(\(\tau\))/RK4(\(\tau\)) - WR

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Conclusion

Algorithmic requirements

- inhomogeneous setup
- subcycling
- black-box
- parallel

Partitioned Heat Transport

- model problem
- experimental study

Short discussion

- implicit/explicit
- semi explicit-implicit
- predictor
- √ Strang
- √ Waveform Relaxation

Multi-Scale

\[ t^n \]

\[ t^{n+0.1} \]

\[ t^{n+0.9} \]

\[ v^n \]

\[ v^{n+1} \]

\[ w^n \]

\[ w^{n+0.1} \]

\[ w^{n+0.9} \]

FACTEST

Ateles

\[ k_1 \]

\[ k_2, k_3 \]

\[ k_4 \]

\[ \tau_L \]

\[ \tau_R \]

\[ \text{EE} \]

RK4

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Further steps

Implementation

- Interpolation methods?
- Convergence of acceleration schemes
- Parallel performance

Tests

1D Tube\(^1\):

preCICE examples\(^2\):

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\(^1\)figure from Degroote, J., et al. (2008). Stability of a coupling technique for partitioned solvers in FSI applications. [https://doi.org/10.1016/j.compstruc.2008.05.005](https://doi.org/10.1016/j.compstruc.2008.05.005)

\(^2\)figure from Cheung Yau, L. (2016). Conjugate Heat Transfer with the Multiphysics Coupling Library preCICE. TUM.
Thank you!¹

**Website:** precice.org  
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- Join our mailing list
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- Ask me for stickers

¹The financial support of the managing board of ECCOMAS and of SPPEXA, the German Science Foundation Priority Programme 1648 – Software for Exascale Computing is thankfully acknowledged.

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### Appendix

#### Semi Implicit-Explicit Coupling

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<tr>
<th></th>
<th>Update Scheme</th>
<th>Stability</th>
<th>Order</th>
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<tbody>
<tr>
<td><strong>Fully Explicit</strong></td>
<td>$\mathbf{v}^{n+1} = \mathbf{v}^n + \frac{\tau}{2} \left[ f_v (\mathbf{v}^n, t_n) + f_v (\mathbf{v}^{n+1}, t_{n+1}) \right]$</td>
<td>depends on $\tau$</td>
<td>$O(\tau)$</td>
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<td></td>
<td>$\mathbf{w}^{n+1} = \mathbf{w}^n + \frac{\tau}{2} \left[ f_w (\mathbf{w}^n, t_n) + f_w (\mathbf{w}^{n+1}, t_{n+1}) \right]$</td>
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**Diagram:**

- **Fully Explicit** coupling:
  - $\mathbf{v}^n$ to $\mathbf{v}^{n+1}$ via $f_v$
  - $\mathbf{w}^n$ to $\mathbf{w}^{n+1}$ via $f_w$

- **Fully Implicit** coupling:
  - $\mathbf{v}^n$ to $\mathbf{v}^{n+1}$ via $f_v$
  - $\mathbf{w}^n$ to $\mathbf{w}^{n+1}$ via $f_w$

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<tr>
<td><strong>semi explicit-implicit</strong></td>
<td>( v^{n+1} = v^n + \frac{\tau}{2} \left[ f_v(v^n, w^n, t_n) + f_v(v^{n+1}, w^{n+1}, t_{n+1}) \right] )</td>
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Appendix

Predictor Coupling

Heun’s method

\[
\begin{pmatrix}
    v^{n+1} \\
    w^{n+1}
\end{pmatrix}
= \begin{pmatrix}
    v^n \\
    w^n
\end{pmatrix}
+ \frac{dt}{2} \left( \begin{pmatrix}
    f_v(v^n, w^n, t_n) + f_v(\tilde{v}^{n+1}, \tilde{w}^n, t_{n+1}) \\
    f_w(v^n, w^n, t_n) + f_w(v^n, \tilde{w}^{n+1}, t_{n+1})
\end{pmatrix} \right),
\]

- \tilde{v}^{n+1}, \tilde{w}^{n+1} from explicit Euler
- only coupling at the beginning of timestep happening

With predictor

\[
\begin{pmatrix}
    v^{n+1} \\
    w^{n+1}
\end{pmatrix}
= \begin{pmatrix}
    v^n \\
    w^n
\end{pmatrix}
+ \frac{dt}{2} \left( \begin{pmatrix}
    f_v(v^n, w^n, t_n) + f_v(\hat{v}^{n+1}, \hat{w}^{n+1}, t_{n+1}) \\
    f_w(v^n, w^n, t_n) + f_w(\hat{v}^n, \hat{w}^{n+1}, t_{n+1})
\end{pmatrix} \right)
\]

- \hat{v}^{n+1}, \hat{v}^{n+1}, \hat{w}^{n+1} and \hat{w}^{n+1} from explicit Euler
- coupling also for stages of scheme
Appendix

What is Waveform Relaxation?

Algorithm

We want to solve the coupled problem

\[ F_v(v, c) = 0, \quad F_w(w, c) = 0. \]

with \( v, w, c \) known for \( t < t_n \) on the window \( T_n = [t_n, t_{n+1}] \).

1. set \( k = 0 \) and extrapolate \( c^0(t) = c_n \) for \( t \in T \)
2. solve decoupled \( F_v, F_w \) using \( c^k \) to obtain \( v^{k+1}, w^{k+1} \) for \( t \in T \)
3. use \( v^{k+1}, w^{k+1} \) to obtain \( c^{k+1} \)
4. if not converged:
   a. set \( k = k + 1 \) and go to step 2,
   b. otherwise proceed to next window \( T_{n+1} \)

---

\(^1\)Adapted from Schöps, S., et al. (2017). Application of the Waveform Relaxation Technique to the Co-Simulation of Power Converter Controller and Electrical Circuit Models. https://doi.org/10.1109/MMAR.2017.8046937

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