Improving Time Stepping in Partitioned Multi-Physics

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20. March 2018
**Fluid-Structure-Acoustics**

![Fluid-Structure-Acoustics simulation and partitioned setup](image)

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>

preCICE\textsuperscript{1}

\textbf{solver} \quad \textbf{adapter} \quad \textbf{libprecice}

\begin{itemize}
  \item \textbf{fluid solver}
    \begin{itemize}
      \item OpenFOAM
      \item SU2
      \item foam-extend
    \end{itemize}
  \item \textbf{in-house solver}
    \begin{itemize}
      \item Ateles (APES)
      \item Alya System
      \item Carat++
      \item FASTEST
    \end{itemize}
  \item API in:
    \begin{itemize}
      \item C / C++
      \item Fortran
      \item Python
    \end{itemize}
\end{itemize}

\textbf{structure solver}

\begin{itemize}
  \item \textbf{commercial solver}
    \begin{itemize}
      \item CalciX
      \item Code_Aster
    \end{itemize}
  \item \textbf{commercial solver}
    \begin{itemize}
      \item ANSYS Fluent
      \item COMSOL
      \item FEAP
    \end{itemize}
\end{itemize}

\begin{itemize}
  \item \textbf{coupling schemes}
  \item \textbf{communication}
  \item \textbf{data mapping}
  \item \textbf{time interpolation}
\end{itemize}

preCICE at GAMM

preCICE Coupling Library for Multi-Physics Simulation
Amin Totounferoush, University of Stuttgart S07.01 Coupled Problems
(today in the morning)

Quasi-Newton – A Universal Approach for Coupled Problems and Optimization
Miriam Mehl, University of Stuttgart S07.01 Coupled Problems
(just now)

Multi-physics simulations with OpenFOAM through preCICE
Gerasimos Chourdakis, Technical University of Munich S22.01 Scientific Computing
(Thursday morning)
Improving Time Stepping in Partitioned Multi-Physics

Requirements

Engineering:
- use different solvers
- use different discretization
- no degradation of solver performance

Informatics:
- black-box approach
- parallel

Multi-Scale Multi-Physics
Outline

Partitioned Heat Transport Equation

- introduce the partitioned heat transport equation example
- introduce classical and advanced coupling schemes
- show deficits of classical explicit and implicit coupling schemes
- show advantages of waveform relaxation coupling scheme

Simple setup

\[ \begin{align*}
    v^{n+1} & \quad \text{Solver A} \\
    t^{n+1} & \quad \tau \\
    w^{n+1} & \quad \text{Solver B} \\
    v^n & \quad \text{IE} \\
    t^n & \\
    w^n & \quad \text{IE}
\end{align*} \]
Reference Solution: The Monolithic Setup

Heat Transport equation

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

Dirichlet boundary conditions

\[ u(x = x_L, t) = u_L^D, \quad u(x = x_R, t) = u_R^D \]

Initial condition

\[ u(x, t = 0) = u_0(x) \]
The Partitioned Setup

**Dirichlet-Neumann coupling**

Get Ω\(_L\): \(v(x_C)\)

Set Ω\(_R\): \(w(x_C)\)

Heat Transport on Ω\(_L\):
\[
\frac{\partial v}{\partial t} = \frac{\partial^2 v}{\partial x^2}
\]

Heat Transport on Ω\(_R\):
\[
\frac{\partial w}{\partial t} = \frac{\partial^2 w}{\partial x^2}
\]

**Partitioning**

\(\tau = 0.2\)

\(\Omega_1: v(x, t)\)

\(\Omega_2: w(x, t)\)

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Classical Coupling Schemes

**Dirichlet-Neumann coupling**

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

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

Dirichlet BC

Heat Transport on $\Omega_L$

$$\frac{\partial v}{\partial t} = \frac{\partial^2 v}{\partial x^2}$$

Neumann BC

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

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

Heat Transport on $\Omega_R$

$$\frac{\partial w}{\partial t} = \frac{\partial^2 w}{\partial x^2}$$

**Explicit coupling**

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

$\mathbf{v}^n \rightarrow \mathbf{w}^n$

**Implicit coupling**

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

$\mathbf{v}^n \leftarrow \mathbf{w}^n$
Convergence order in time

- use constant spatial meshwidth $h$
- refine temporal meshwidth $\tau$
- compare to monolithic reference solution $u^n$ with fine $\tau$
Order Degradation: Trapezoidal rule

- order reduced to $\mathcal{O}(\tau)$
- $h = 0.2$
- stability problems for Fully implicit coupling

![Graph showing error in left domain $\Omega_l$ vs. time step $\tau$.]
Order Degradation: Trapezoidal rule

- order reduced to $O(\tau)$

- $h = 0.01$

- stability problems for Fully implicit coupling

- stability problems for Fully explicit coupling
Semi Implicit-Explicit Coupling

<table>
<thead>
<tr>
<th></th>
<th>update scheme</th>
<th>stability</th>
<th>order</th>
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<tbody>
<tr>
<td>fully explicit</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>
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## Semi Implicit-Explicit Coupling

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<tr>
<td>Coupling Type</td>
<td>Update Scheme</td>
<td>Stability</td>
<td>Order</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>semi explicit-implicit</td>
<td>$\mathbf{v}^{n+1} = \mathbf{v}^n + \frac{\tau}{2} \left[ f_v(\mathbf{v}^n, t_n, c_n) + f_v(\mathbf{v}^{n+1}, t_{n+1}, c_{n+1}) \right]$</td>
<td>???</td>
<td>???</td>
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<tr>
<td></td>
<td>$\mathbf{w}^{n+1} = \mathbf{w}^n + \frac{\tau}{2} \left[ f_w(\mathbf{w}^n, t_n, c_n) + f_w(\mathbf{w}^{n+1}, t_{n+1}, c_{n+1}) \right]$</td>
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Higher Order: Semi Implicit-Explicit Coupling

- order $\mathcal{O}(\tau^2)$ maintained for semi explicit-implicit coupling
- no stability problems for semi explicit-implicit coupling

![Graph showing error in left domain $\Omega_L$](image)

- Trapezoidal Rule - Monolithic Approach
- Trapezoidal Rule - Semi Implicit Explicit Coupling
Higher Order: Semi Implicit-Explicit Coupling

- order $\mathcal{O}(\tau^2)$ maintained for semi explicit-implicit coupling
- no stability problems for semi explicit-implicit coupling

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<tr>
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<th>order</th>
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<tr>
<td>fully explicit</td>
<td>depends on $\tau$</td>
<td>$\mathcal{O}(\tau)$</td>
</tr>
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<td>fully implicit</td>
<td>depends on $\tau$</td>
<td>$\mathcal{O}(\tau)$</td>
</tr>
<tr>
<td>semi explicit-implicit</td>
<td>unconditionally</td>
<td>$\mathcal{O}(\tau^2)$</td>
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Intermediate Summary

<table>
<thead>
<tr>
<th>Semi-Explicit-Implicit</th>
<th>Goal</th>
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<tr>
<td>identical timesteps</td>
<td>subcycling</td>
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<tr>
<td>simple schemes</td>
<td>substepping</td>
</tr>
<tr>
<td>identical solvers</td>
<td>inhomogeneous setup</td>
</tr>
<tr>
<td>$\mathcal{O}(\tau^2)$</td>
<td>Higher order</td>
</tr>
<tr>
<td>tailored schemes</td>
<td>general solution strategy</td>
</tr>
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Multi-Scale Multi-Physics
What is Waveform Relaxation?

Background Information

Algorithm

We want to solve the coupled problem

$$F_v(v, c) = 0, \ F_w(w, c) = 0.$$ 

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 $T_{n+1}$

---

Waveform Relaxation (WR) Coupling Scheme

WR with our example

- Semi-Explicit-Implicit coupling equals WR with linear interpolation of
  \[ c^k(t) = \frac{c_n(t_{n+1} - t)}{\tau} + \frac{c_{n+1}(t - t_n)}{\tau}. \]

- Semi-Explicit-Implicit coupling:
  \[ v^{n+1} = v^n + \frac{\tau}{2} \left[ f_v(c^k(t_n)) + f_v(c^k(t_{n+1})) \right] \]
  \[ w^{n+1} = w^n + \frac{\tau}{2} \left[ f_w(c^k(t_n)) + f_w(c^k(t_{n+1})) \right] \]

- Other interpolation methods are spline or dense output interpolation

Multi-Scale Setup

\[ \tau_1 = 0.5 \]
\[ \tau_2 = 0.2 \]
High Order and Subcycling

<table>
<thead>
<tr>
<th>scheme-solvers</th>
<th>time step</th>
<th>order</th>
<th>stable</th>
</tr>
</thead>
<tbody>
<tr>
<td>M-RK4</td>
<td>$\tau_1 = \tau_2$</td>
<td>$O(\tau^4)$</td>
<td>small $\tau_2$</td>
</tr>
<tr>
<td>Im-TR/TR</td>
<td>$\tau_1 = \tau_2$</td>
<td>$O(\tau)$</td>
<td>small $\tau_2$</td>
</tr>
<tr>
<td>Im-RK4/RK4</td>
<td>$\tau_1 = \tau_2$</td>
<td>$O(\tau)$</td>
<td>small $\tau_2$</td>
</tr>
<tr>
<td>WR-RK4/RK4</td>
<td>$\tau_1 &gt; \tau_2$</td>
<td>$O(\tau^4)$</td>
<td>small $\tau_2$</td>
</tr>
<tr>
<td>WR-RK4/TR</td>
<td>$\tau_1 = \tau_2$</td>
<td>$O(\tau^2)$</td>
<td>$\forall \tau_2$</td>
</tr>
</tbody>
</table>

Diagram:
- Error in left domain $\Omega_L$
ylabel

$\tau$: $10^{-15}$ to $10^{-4}$

$\tau$: $10^{-12}$ to $10^{-9}$

$\tau$: $10^{-6}$ to $10^{-3}$

$\tau$: $10^{-3}$ to $10^0$

$\tau$: $\Delta x$
Conclusion

Partitioned Heat Transport

✓ introduce the partitioned heat transport equation example
✓ introduce classical and advanced coupling schemes
✓ deficits of classical explicit and implicit coupling schemes
  • order and stability degradation
✓ advantages of waveform relaxation coupling scheme
  • order and stability maintained
  • inhomogeneous setup
  • subcycling

Multi-Scale

\[
\begin{align*}
\tau_1 & \quad \text{EE} \\
\tau_2 & \quad \text{RK4}
\end{align*}
\]

\[
\begin{align*}
\tau_1 & \quad \text{EE} \\
\tau_2 & \quad \text{RK4}
\end{align*}
\]

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

\[
\begin{align*}
w^{n+1} & \quad \tau_2 \\
w^{n+0.9} & \quad \text{RK4} \\
w^{n+0.1} & \quad \tau_2 \\
w^n & \quad \text{RK4}
\end{align*}
\]

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Outlook

Implementation

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

Further Tests

1D Tube\(^1\):

preCICE examples\(^2\):


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