Challenges and solution approaches for partitioned multiphysics simulations

Miriam Mehl,
Bernhard Gatzhammer, Janos Benk, Hans-Joachim Bungartz
Technische Universität München
Wolfgang Polifke: Thermoacoustic Instabilities

- fluid-structure-combustion-acoustics
- multiscale
- volume and surface coupling
- strong non-linear effects
- (physical) instabilities

Joris Degroote: HPC for Fluid-Structure Interaction

- surface coupling
- partitioned approach
- stable coupling strategies
- parallel simulations

http://www.fsi.ugent.be/gallery.htm
Frank Jenko: Plasmaphysics

- ITER (China, EU, India, Japan, Korea, Russia, USA) $\rightarrow$ 500 MW
- numerical ITER:
  - multi-scale in space and time
  - five- to seven-dimensional
  - gain by model improvements: $10^{16}$

Source: Jenko, EU-US Summer School on HPC Challenges, Catania, Italy, 4-7 October 2010
Sabine Roller: Fluid-Dynamics with Subscale Processes

- multiscale
- different types of models
- how to include all important scales with affordable costs?
Outline

- Fluid-Structure Interactions
- The Partitioned Approach
- Surface Coupling
  - Data Communication
  - Data Mapping for Non-Matching Grids
  - Coupling Strategies
- Lagrangian versus Eulerian Approaches
- Conclusion
Outline

- Fluid-Structure Interactions
- The Partitioned Approach
- Surface Coupling
  - Data Communication
  - Data Mapping for Non-Matching Grids
  - Coupling Strategies
- Lagrangian versus Eulerian Approaches
- Conclusion
Fluid-Structure Interactions

Vienna Online, 01/08/2009

TUM, 2009

Frederic Le Floch, 1999 ACO Le Mans Annual
Fluid-Structure Interactions

Characteristics:

- surface-coupled problem
- slightly different time scales
- same spatial scale (at least for laminar flows)
- non-linearities
- fluid computationally more expensive
Outline

- Fluid-Structure Interactions
- The Partitioned Approach
- Surface Coupling
  - Data Communication
  - Data Mapping for Non-Matching Grids
  - Coupling Strategies
- Lagrangian versus Eulerian Approaches
- Conclusion
The Partitioned Approach

Scenario 1: changing fields of application
Scenario 2: changing components (ideology-free coupling)
Outline

- Fluid-Structure Interactions
- The Partitioned Approach
- Surface Coupling
  - Data Communication
  - Data Mapping for Non-Matching Grids
  - Coupling Strategies
- Lagrangian versus Eulerian Approaches
- Conclusion
Surface Coupling – Data Communication

- coupling conditions
  - equality of forces $\sigma_f \cdot \vec{n} = \sigma_s \cdot \vec{n}$
  - equality of displacements/velocities $\vec{v}_f = \vec{v}_s$
Surface Coupling – Data Communication

preCICE – our inhouse coupling tool – direct communication, i.e.
local controllers
P2P solver communication
Surface Coupling – Data Mapping

octree-supported neighbourhood search

<table>
<thead>
<tr>
<th>octree depth</th>
<th>time (sec)</th>
<th>nodes</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>0.8</td>
<td>203,905</td>
</tr>
<tr>
<td>9</td>
<td>4.9</td>
<td>3,288,225</td>
</tr>
<tr>
<td>11</td>
<td>48.2</td>
<td>52,662,337</td>
</tr>
<tr>
<td>13</td>
<td>662.8</td>
<td>842,687,105</td>
</tr>
</tbody>
</table>
Surface Coupling – Data Mapping

- Conservation of energy at discrete interface
  \[ u_f^T f_f = u_s^T f_s \]

- Linear mapping of displacements from structure to fluid
  \[ u_f = H u_s \]

- Transposed mapping of forces enforced by conservation of energy
  \[ f_s = H^T f_f \]

- So far: explicit interface mesh

- Alternative: do without that – mesh-free interpolation
Surface Coupling – Coupling Strategies

unidirectional coupling

- small range of applicability
- fixed and almost rigid structures
Surface Coupling – Coupling Strategies

staggered coupling

- large range of applicability
- stability problems
- standard approach
Surface Coupling – Coupling Strategies

standard coupling: staggered iteration

interface equation: \( x = s(f(x)) \)
fixpoint iteration: \( x^{i+1} = s(f(x^i)) \)
(Aitken-)underrelaxation: \( x^{i+1} = (1 - \omega) \cdot x^i + \omega \cdot s(f(x^i)) \)
interface (quasi-)Newton: \( x^{i+1} = x^i + (I - J_{sf})^{-1}(s(f(x^i)) - x^i) \)
Surface Coupling – Coupling Strategies

equation application:
rigid-body motion

\[ \nu(t) = \frac{A}{A - A_b} u(t) - \frac{A_b}{A - A_b} \ddot{x}(t) \quad \text{(mass conservation)} \]

\[ \dot{\nu}(t) + \frac{1}{\rho_f} \frac{\rho_r - \rho_i}{L} = 0 \quad \text{(conservation of momentum)} \]

\[ m\ddot{x}(t) = \frac{F}{A_b} = A_b (\rho_l - \rho_r) \quad \text{(Newton's law of motion)} \]
Surface Coupling – Coupling Strategies

dir example application: rigid-body motion

Dirichlet-Neumann coupling

\[
\text{fluid: } F^{n+1,k+1} = \frac{m_f}{dt} \frac{1}{A - A_b} \left[ A(u^{n+1} - u^n) - A_b(\dot{x}^{n+1,k} - \dot{x}^n) \right]
\]

\[
\text{structure: } \dot{x}^{n+1,k+1} = \dot{x}^n + dt \frac{F^{n+1,k+1}}{m}
\]
Surface Coupling – Coupling Strategies

example application: rigid-body motion

Dirichlet-Neumann coupling

\[
\text{fluid: } F^{n+1,k+1} = m_f \frac{1}{dt} \left[ A(u^{n+1} - u^n) - A_b(\dot{x}^{n+1,k} - \dot{x}^n) \right]
\]

\[
\text{structure: } \dot{x}^{n+1,k+1} = \dot{x}^n + dt \frac{F^{n+1,k+1}}{m}
\]

\[
\Rightarrow e^{n+1,k+1} = -m_f \frac{A_b}{m \left( A - A_b \right)} e^{n+1,k} \]

✓ for small or heavy structures

✗ for large or light structures
Surface Coupling – Coupling Strategies

example application: 
rigid-body motion

Neumann-Dirichlet coupling

\[
\text{fluid} : \dot{x}^{n+1,k+1} = \dot{x}^n + dt \frac{A - A_b}{A_b m_f} F^{n+1,k} + \frac{A}{A_b} (u^{n+1} - u^n)
\]

\[
\text{structure} : F^{n+1,k+1} = \frac{m}{dt} (\dot{x}^{n+1,k+1} - \dot{x}^n)
\]
Surface Coupling – Coupling Strategies

example application:
rigid-body motion

Neumann-Dirichlet coupling

\[ \dot{x}^{n+1,k+1} = \dot{x}^n + dt \frac{A - A_b}{A_b m_f} F^{n+1,k} + \frac{A}{A_b} (u^{n+1} - u^n) \]

\[ F^{n+1,k+1} = \frac{m}{dt} (\ddot{x}^{n+1,k+1} - \dot{x}^n) \]

\[ e^{n+1,k+1} = \frac{m}{m_f} \frac{A - A_b}{A_b} e^{n+1,k} \]

- for large or light structures
- for small or heavy structures
Surface Coupling – Coupling Strategies

example application:
rigid-body motion

Dirichlet-Neumann coupling or
Neumann-Dirichlet coupling
Newton

convergence in one step (linear problem)
Surface Coupling – Coupling Strategies

example involving frequency modes:
flexible tube

Dirichlet-Neumann coupling

results with preCICE

<table>
<thead>
<tr>
<th>algorithm</th>
<th>runtime</th>
<th>#iterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>constant underrelaxation</td>
<td>136.5</td>
<td>852.38</td>
</tr>
<tr>
<td>Aitken underrelaxation</td>
<td>8.3</td>
<td>50.94</td>
</tr>
<tr>
<td>IQN-ILS</td>
<td>3.0</td>
<td>16.21</td>
</tr>
<tr>
<td>IQN-ILS(2)</td>
<td>1.3</td>
<td>6.20</td>
</tr>
<tr>
<td>IQN-ILS(4)</td>
<td>1.0</td>
<td>4.60</td>
</tr>
</tbody>
</table>

Compare:
Degroote, Bruggemann, Haeltermann, Vierendeels, Computation & Structure 86, 2008
Surface Coupling – Coupling Strategies

example involving frequency modes:
flow over a membrane

Dirichlet-Neumann coupling

\[ e^{n+1,i} = c \cdot \exp(i\kappa x + i\mu t) \]
\[ e^{n+1,i+1} = \frac{\rho_f}{m} |\kappa|^{-1} \]


Aitken:

- stabilizing low frequencies
- slowing down high frequencies

interface quasi-Newton:

- capturing several frequencies
Surface Coupling – Coupling Strategies

example involving frequency modes: flow over a membrane

Dirichlet-Neumann coupling

\[
\begin{align*}
\mathbf{u}_s^{i+1} &= A_{ss}^{-1}(\mathbf{b}_s - A_{sf} \mathbf{u}_f^{i+1}) \\
\mathbf{u}_s^{i+1,g,new}|_{\Gamma_{fs}} &= (1 - \omega_{i,g}) \cdot \mathbf{u}_s^{i,g}|_{\Gamma_{fs}} + \omega_{i,g} \cdot \mathbf{u}_s^{i+1,g}|_{\Gamma_{fs}} \text{ for all levels } \varrho
\end{align*}
\]
Surface Coupling – Coupling Strategies

example involving frequency modes:
flow over a membrane

Dirichlet-Neumann coupling

\[ e^{n+1,i} = c \cdot \exp(i\kappa x + i\mu t) \]

\[ e^{n+1,i+1} = \frac{\rho_f}{m} |\kappa|^{-1} \]

unstable modes

more expensive coupling???
Surface Coupling – Coupling Strategies

non-staggered coupling

- parallel!!!
- stability?
- efficiency?
Surface Coupling – Coupling Strategies

non-staggered coupling

interface equation: \( s(x) = f(x) \)

Richardson iteration: \( x^{i+1} = x^i \pm (f(x^i) - s(x^i)) \)

underrelaxation: \( x^{i+1} = x^i + \omega \cdot (f(x^i) - s(x^i)) \)

interface (quasi-)Newton: \( x^{i+1} = x^i - (J_f - J_s)^{-1}(f(x^i) - s(x^i)) \)
Surface Coupling – Coupling Strategies

example application:
rigid-body motion

\[ \nu(t) = \frac{A}{A - A_b} u(t) - \frac{A_b}{A - A_b} \dot{x}(t) \quad \text{(mass conservation)} \]

\[ \dot{\nu}(t) + \frac{1}{\rho_f} \frac{p_r - p_l}{L} = 0 \quad \text{(conservation of momentum)} \]

\[ m\ddot{x}(t) = \frac{F}{A_b} = A_b(p_l - p_r) \quad \text{(Newton's law of motion)} \]
Surface Coupling – Coupling Strategies

example application: rigid-body motion

equality of velocities

\[ \text{fluid: } \dot{x}_{f}^{n+1,k+1} = \dot{x}^{n} + \frac{A}{A_{b}} (u_{n+1}^{n} - u^{n}) - \frac{A - A_{b}}{A_{b}} \frac{dt}{m_f} F_{n+1,k}^{n+1} \]

\[ \text{structure: } \dot{x}_{s}^{n+1,k+1} = \dot{x}^{n} + \frac{dt}{m} F_{n+1,k}^{n+1} \]

\[ \text{interface equation: } \dot{x}_{f}^{n+1,k+1} = \dot{x}_{s}^{n+1,k+1} \]
Surface Coupling – Coupling Strategies

example application:
rigid-body motion

equality of velocities

\[
\text{fluid: } \dot{x}_{f}^{n+1,k+1} = \dot{x}^n + \frac{A}{A_b} (u_{n+1}^n - u^n) - \frac{A - A_b}{A_b} \frac{dt}{m_f} F_{n+1,k}^{n+1,k}
\]

\[
\text{structure: } \dot{x}_{s}^{n+1,k+1} = \dot{x}^n + \frac{dt}{m} F_{n+1,k}^{n+1,k}
\]

Richardson: \[\dot{F}^{n+1,k+1}_{n+1,k} = F^{n+1,k} + \left( \dot{x}_{f}^{n+1,k+1} - \dot{x}_{s}^{n+1,k+1} \right) \]
Surface Coupling – Coupling Strategies

example application:
rigid-body motion

equality of velocities

fluid: $\dot{x}_{f}^{n+1,k+1} = \dot{x}^{n} + \frac{A}{A_{b}}(u_{n+1}^{n} - u^{n}) - \frac{A - A_{b}}{A_{b}} \frac{dt}{m_{f}} F^{n+1,k}$

structure: $\dot{x}_{s}^{n+1,k+1} = \dot{x}^{n} + \frac{dt}{m} F^{n+1,k}$

Richardson: $F^{n+1,k+1} = \left(1 - dt \frac{m_{f} A_{b} + (A - A_{b})m}{m_{f} \cdot m \cdot A_{b}}\right) F^{n+1,k} + \frac{A}{A_{b}} (u_{n+1}^{n} - u^{n})$
Surface Coupling – Coupling Strategies

example application:
rigid-body motion

equality of velocities

\[
\text{fluid: } \dot{x}_f^{n+1,k+1} = \dot{x}^n + \frac{A}{A_b} (u^{n+1} - u^n) - \frac{A - A_b}{A_b} \frac{dt}{m_f} F^{n+1,k}
\]

\[
\text{structure: } \dot{x}_s^{n+1,k+1} = \dot{x}^n + \frac{dt}{m} F^{n+1,k}
\]

Richardson: \[e^{n+1,k+1} = \left( 1 - dt \frac{m_f A_b + (A - A_b) m}{m_f \cdot m \cdot A_b} \right) \cdot e^{n+1,k}\]

☑ for \(dt\) small enough
Surface Coupling – Coupling Strategies

example application:
rigid-body motion

equality of forces

\[
\text{fluid: } F_{f}^{n+1,k+1} = \frac{m_f}{dt} \left[ \frac{A}{A - A_b} (u_n^{n+1} - u_n^n) - \frac{A_b}{A - A_b} (\dot{x}_n^{n+1,k} - \dot{x}_n^n) \right]
\]

\[
\text{structure: } F_{s}^{n+1,k+1} = \frac{m}{dt} (\dot{x}_n^{n+1,k} - \dot{x}_n^n)
\]

interface equation: \( F_{f}^{n+1,k+1} = F_{s}^{n+1,k+1} \)
Surface Coupling – Coupling Strategies

different example application:
rigid-body motion

equality of forces

fluid: \( F_{f}^{n+1,k+1} = \frac{m_f}{d} \left[ \frac{A}{A - A_b} (u^{n+1} - u^n) - \frac{A_b}{A - A_b} (\dot{x}^{n+1,k} - \dot{x}^n) \right] \)

structure: \( F_{s}^{n+1,k+1} = \frac{m}{d} (\dot{x}^{n+1,k} - \dot{x}^n) \)

Richardson: \( \dot{x}^{n+1,k+1} = \dot{x}^{n+1,k} + \left( F_{f}^{n+1,k+1} - F_{s}^{n+1,k+1} \right) \)
Surface Coupling – Coupling Strategies

example application:
rigid-body motion

equality of forces

\[ \text{fluid: } F_{f}^{n+1,k+1} = \frac{m_f}{dt} \left[ \frac{A}{A - A_b} (u^{n+1} - u^n) - \frac{A_b}{A - A_b} (\dot{x}^{n+1,k} - \dot{x}^n) \right] \]

\[ \text{structure: } F_s^{n+1,k+1} = \frac{m}{dt} (\ddot{x}^{n+1,k} - \ddot{x}^n) \]

Richardson: \[ e^{n+1,k+1} = \left( 1 - \frac{m_f A_b + m_s (A - A_b)}{dt (A - A_b)} \right) e^{n+1,k} \]

\[ \times \text{ for } dt \text{ small!!} \]
Surface Coupling – Coupling Strategies

example application:
rigid-body motion

Equality of velocities or equality of forces
Newton

convergence in one step (linear problem)
Surface Coupling – Coupling Strategies

non-staggered coupling

equality of displacements for non-matching grids

explicit time-step
solve interface equation exactly

- **LLM** (compressible fluids, Ross, Park, Felippa)

Mike Ross, Phd thesis, 2006
Surface Coupling – Coupling Strategies

non-staggered coupling

general convergence?
frequency dependency?
Surface Coupling – Coupling Strategies

fully parallel coupling

\[
\begin{pmatrix}
M_{ff} & M_{fl} \\
M_{lf} & M_{ll} & M_{ls} \\
M_{sl} & M_{ss}
\end{pmatrix}
\begin{pmatrix}
u_f \\
u_l \\
u_s
\end{pmatrix}
= \begin{pmatrix}
f_f \\
f_l \\
f_s
\end{pmatrix}
\]

Block - Jacobi:

fluid: \( u_f^{i+1} = M_{ff}^{-1}(f_f - M_{fl}u_l^i) \)

interface: \( u_l^{i+1} = M_{ll}^{-1}(f_l - M_{lf}u_f^i - M_{ls}u_s^i) \)

structure: \( u_s^{i+1} = M_{ss}^{-1}(f_s - M_{sl}u_l^i) \)
Surface Coupling – Coupling Strategies

eexample application: rigid-body motion

\[ v(t) = \frac{A}{A - A_b} u(t) - \frac{A_b}{A - A_b} \dot{x}(t) \quad \text{(mass conservation)} \]
\[ \dot{v}(t) + \frac{1}{\rho_f} \frac{p_r - p_l}{L} = 0 \quad \text{(conservation of momentum)} \]
\[ m \ddot{x}(t) = \frac{F}{A_b (\rho_l - \rho_r)} \quad \text{(Newton's law of motion)} \]
Surface Coupling – Coupling Strategies

example application: rigid-body motion

block-Jacobi

\[
\begin{pmatrix}
1 & \frac{A_b}{A - A_b} & \frac{m_f A}{A - A_b} & \frac{m_s (A - A_b)}{A - A_b} \\
- & - & - & - \\
M_{II} & - & - & - \\
\end{pmatrix}
\begin{pmatrix}
\nu^{n+1} \\
\dot{\nu}^{n+1} \\
\dot{x}^{n+1} \\
- \\
\end{pmatrix}
= 
\begin{pmatrix}
\frac{A}{A - A_b} u^{n+1} \\
\frac{m_f A}{A - A_b} (u^{n+1} - u^n) + M_{II} \dot{x}^n \\
- \\
- \\
\end{pmatrix}
\]

\[M_{II} = \frac{m_f A_b + m_s (A - A_b)}{A - A_b} \]

✔ solution in one step (empty fluid and structure)
Surface Coupling – Coupling Strategies

fully parallel coupling

general convergence?
frequency dependency?
non-matching grids?
black-box solvers?
Outline

- Fluid-Structure Interactions
- The Partitioned Approach
- Surface Coupling
  - Data Communication
  - Data Mapping for Non-Matching Grids
  - Coupling Strategies
- Lagrangian versus Eulerian Approaches
- Conclusion
Lagrangian versus Eulerian Approaches
Lagrangian versus Eulerian Approaches
Lagrangian versus Eulerian Approaches

monolithic FE: $\text{fluideq} \cdot \chi_f + \text{structureeq} \cdot \chi_s$

partitioned FE: weakly enforce boundary conditions at cell-cuts

Fluid with Dirichlet boundary (FE):

$$a(\bar{u}, p)(\bar{\phi}, \xi) + c(\bar{u}, p)(\bar{\phi}) + b(\bar{u})(\bar{\phi}, \xi)$$

standard FE boundary integrals from partial integration boundary condition enforcing

$= f(\bar{\phi}) + b(\bar{g})(\bar{\phi}, \xi)$

right hand side boundary condition enforcing
Lagrangian versus Eulerian Approaches

monolithic FE: \[ \text{fluideq} \cdot \chi_f + \text{structureeq} \cdot \chi_s \]

partitioned FE: weakly enforce boundary conditions at cell-cuts

Janos Benk, method implemented in Sundance
Lagrangian versus Eulerian Approaches

monolithic FE: \[ \text{fluid eq} \cdot \chi_f + \text{structure eq} \cdot \chi_s \]

partitioned FE: weakly enforce boundary conditions at cell-cuts


<table>
<thead>
<tr>
<th>( \gamma = 1,000 )</th>
<th>drag</th>
<th>lift</th>
</tr>
</thead>
<tbody>
<tr>
<td>111x21</td>
<td>5.57919</td>
<td>0.012239</td>
</tr>
<tr>
<td>221x41</td>
<td>5.57935</td>
<td>0.010597</td>
</tr>
<tr>
<td>441x81</td>
<td>5.57935</td>
<td>0.010622</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( \gamma = 10,000 )</th>
<th>drag</th>
<th>lift</th>
</tr>
</thead>
<tbody>
<tr>
<td>111x21</td>
<td>5.57936</td>
<td>0.0120811</td>
</tr>
<tr>
<td>221x41</td>
<td>5.57936</td>
<td>0.0105961</td>
</tr>
<tr>
<td>441x81</td>
<td>5.57936</td>
<td>0.0106214</td>
</tr>
</tbody>
</table>

reference 5.579535 0.0106189
Lagrangian versus Eulerian Approaches

monolithic FE: \( \text{fluideq} \cdot \chi_f + \text{structureeq} \cdot \chi_s \)

partitioned FE: weakly enforce boundary conditions at cell-cuts

Source: Janos Benk
Outline

- Fluid-Structure Interactions
- The Partitioned Approach
- Surface Coupling
  - Data Communication
  - Data Mapping for Non-Matching Grids
  - Coupling Strategies
- Lagrangian versus Eulerian Approaches
- Conclusion
Conclusion

- modular multiphysics simulations require partitioned approaches
- new partitioned coupling strategies required for massively parallel simulations
- numerical properties of such methods remain to be analysed
- generalisation to black-box solvers?