Coupled calculations in OpenFOAM -
Multiphysics handling, structures and solvers,
Gothenburg Region OpenFOAM User Group Meeting

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Outline

- Region coupling and block coupling
- Overview of coupled formats in OpenFOAM
- Application 1: Multiphysics simulations for nuclear reactors
- Application 2: Block coupled solver for incompressible flow
- Summary and future outlook
On coupled problems

Region coupling
  Background
  OpenFOAM
  Application: multiphysics in nuclear reactors

Field coupling
  Background
  Application: block coupled incompressible flow solver

Summary and future outlook
Coupled problems

- Multiple field problems and/or equations problems, e.g.:
  - Navier-Stokes
  - Conjugate heat-transfer
  - Nuclear reactor modeling
  - Multi-group radiation
  - Multiphase modeling
- Not enough to solve one problem.

How to solve the coupling of the fields/equations/regions?
Region coupling

On coupled problems
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Summary and future outlook
Background

- **Characteristic:**
  - Multiple materials (solid/fluid)
  - Similar physics in many regions ($T$)
  - Coupled boundaries

- **Solution methods:**
  - Segregated solver - Iterative solution of region by region
  - Coupled solver - Solve multiple regions at once

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**Figure:** conjugateCavity, dual region simulation
Regional coupling available through `coupleFvMatrix`.

```cpp
 coupledFvScalarMatrix TEqns(2);

 // Add fluid equation
 TEqns.set
 (0,
  new fvScalarMatrix
  (
    fvm::ddt(T)
   + fvm::div(phi, T)
   - fvm::laplacian(DT, T)
  )
 );

 // Add solid equation
 TEqns.set
 (1,
  new fvScalarMatrix
  (fvm::ddt(Tsolid) - fvm::laplacian(DTsolid, Tsolid)
  )
 );

 TEqns.solve();
```

*Energy equation in `conjugateHeatFoam`*
Regional coupling in OpenFOAM II

- regionCouple boundary condition at coupled patches
- Existing solvers CG, BiCGStab, BiCG, smoothSolver
- Parallelizable
- Utilities (mostly) compatible with multiple regions (splitMesh, foamToVTK, sample, decomposePar, reconstructPar)

Additional sources:
- H. Jasak. “Coupled Multiphysics with OpenFOAM Inter-Region and Inter-Equation Coupling”
Application: multiphysics in nuclear reactors

Nuclear reactor cores: multiphysics environment

Neutron density field

Flow properties

Fuel properties

Water density

Fuel temperature

Power

Flow properties

Region coupling — Application: multiphysics in nuclear reactors
- **Multi-region environment**: Both solid and fluid, different types of materials

- **Fields in all regions**:
  - Temperature (solid: conduction, fluid: convection)
  - Multi-group neutron density field (same model equation all regions)

![Figure: Slice of nuclear fuel pin](image)
OpenFOAM implementation

- Implemented using OpenFOAM 1.6-ext.
- Region coupling for an arbitrary number of pins
- Segregated solver considering field dependencies

Details:
- K. Jareteg. Klas Jareteg, PhD Student, Personal web page. 2012. URL: klas.nephy.chalmers.se
Example results

(a) All regions

(b) Moderator only

Figure: Radial temperature profiles.
Field coupling

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Coupling 2: Field coupling

- **Characteristic:**
  - Multiple fields ($\alpha$, $U_g$, $U_l$, $p$)
  - Couplings between fields
  - Same mesh (typically)
  - Field dependent parameters

- **Solution methods:**
  - Segregated solver - Iterative solution. Solve one field at a time. Explicit coupling.
  - Coupled solver - Solve all/multiple fields at once. Implicit coupling.

**Figure:** bubbleColumn
Application block coupled incompressible flow solver

- Incompressible steady-state Navier-Stokes:

$$ \nabla \cdot (U) = 0 $$  \hspace{1cm} (1)

$$ \nabla \cdot (UU) - \nabla (\nu \nabla U) = -\frac{1}{\rho} \nabla p $$  \hspace{1cm} (2)

- Traditionally segregated solvers (OpenFOAM simpleFoam)

- Often slow convergence, pressure equation elliptic behaviour

- Possible remedy: coupled calculation using OpenFOAM 1.6-ext: BlockLduMatrix

Additional sources:

- Henrik Rusche and Hrvoje Jasak. *Implicit solution techniques for coupled multi-field problems – Block Solution, Coupled Matrices*. June 2010

- Julia Springer et al. *A coupled pressure based solution algorithm based on the Volume-of-Fluid approach for two or more immiscible fluids*. June 2010

- Ivor Clifford. *Block-Coupled Simulations Using OpenFOAM*. June 2011
• SIMPLE algorithm: pressure equation from the continuity equation, explicit use of velocity (from momentum predictor step)

• Alternative approach: Rhie-Chow interpolation:

\[
\sum_{\text{faces}} \left[ \overline{U_f} - \overline{D_f} \left( \nabla P_f - \overline{\nabla P_f} \right) \right] \cdot S_f = 0 \tag{3}
\]

\[
\sum_{\text{faces}} \left[ \overline{UU} - \nu \nabla \overline{U} \right]_f \cdot S_f = - \sum_{\text{faces}} P_f S_f \tag{4}
\]

Additional sources:


- L. Mangani and C. Bianchini. *A coupled finite volume solver for the solution of laminar/turbulent incompressible and compressible flows*. June 2010

OpenFOAM implementation I

- Implemented using OpenFOAM-1.6-ext
- Block matrix class: BlockLduMatrix
  - Templated matrix class. Elements of arbitrary size:

```cpp
//— Diagonal coefficients
CoeffField<Type>* diagPtr_;

//— Upper triangle coefficients. Also used for symmetric matrix
CoeffField<Type>* upperPtr_;

//— Lower triangle coefficients
CoeffField<Type> *lowerPtr_;
```

BlockLduMatrix.H

- In this case: manual assembling of matrix coefficients and source for each term in the continuity and momentum equations (Eqs. (3) and (3))

\[
\sum_{faces} \left[ \mathbf{U}_f - \mathbf{D}_f (\nabla P_f - \nabla \mathbf{P}_f) \right] \cdot \mathbf{S}_f = 0
\]

\[
\sum_{faces} \left[ \mathbf{U} \mathbf{U} - \nu \nabla \mathbf{U} \right]_f \cdot \mathbf{S}_f = - \sum_{faces} \mathbf{P}_f \mathbf{S}_f
\]
OpenFOAM implementation II

- For 3D solver: \( \mathbf{A} \mathbf{x} = \mathbf{f} \)
  - Matrix element:
    \[
    a_{i,j} = \begin{bmatrix}
      a_{u,u} & 0 & 0 & a_{p,u} \\
      0 & a_{v,v} & 0 & a_{p,v} \\
      0 & 0 & a_{w,w} & a_{p,w} \\
      a_{u,p} & a_{v,p} & a_{w,p} & a_{p,p}
    \end{bmatrix}_{i,j}
    \]
    \( (5) \)
  - Solution vector:
    \[
    \mathbf{x}_i = \begin{bmatrix}
      u \\
      v \\
      w \\
      p
    \end{bmatrix}_{i}
    \]
    \( (6) \)
  - Off-diagonal coefficients giving the implicit coupling between pressure and velocity
  - New solvers implemented (GMRES, BiCGStab, CG)

Description of work:

Case study pitzDailyFoam

- New solver benchmarked against simpleFoam using the standard pitzDailyFoam.
- Convergence profile (non-turbulent case):

**Figure:** Comparison of convergence for simpleFoam and pUCoupledFoam. Laminar case.
Convergence profile (turbulent case):

- Iterations
- Elapsed time

**Figure:** Comparison of convergence for simpleFoam and pUCoupledFoam. Turbulent case.
Summary and future outlook

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Summary and future outlook
Summary:

- Great possibilities
- Successful parallelized multiphysics simulations of nuclear reactor cores
- Faster convergence for incompressible flow simulations

Future developments:

- Multi-grid methods for region and block coupling?
- Combining region and block coupling?
- ...

Community needs:

- Documentation
- Examples (e.g. parallelization of region coupling)
- Tutorials
Thank you! Questions?

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