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

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

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

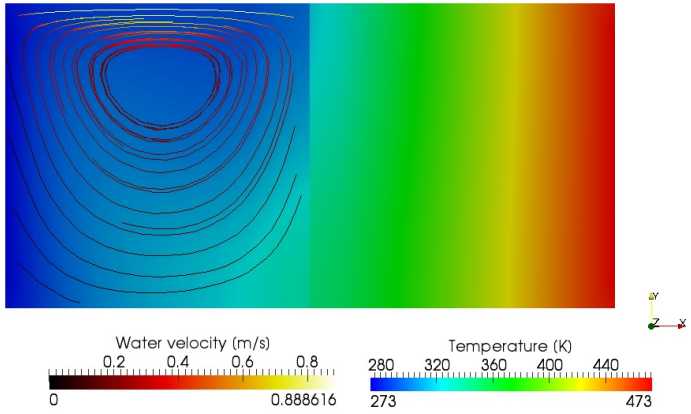
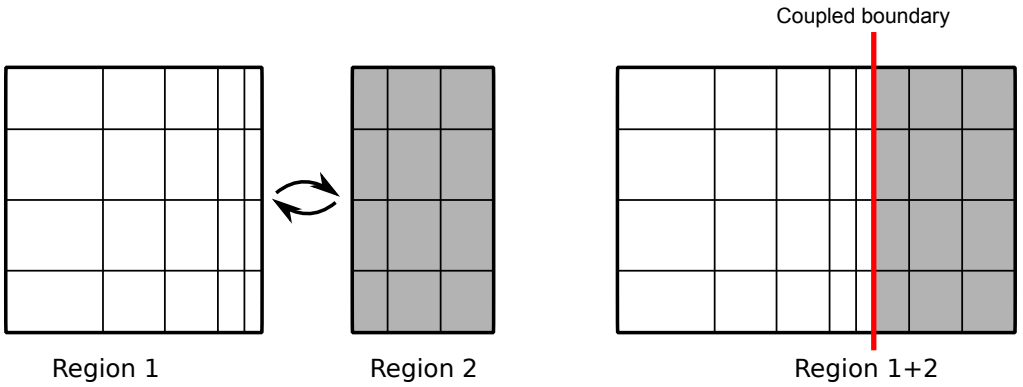


Figure: `conjugateCavity`, dual region simulation



Regional coupling in OpenFOAM I

- Regional coupling availble through `coupleFvMatrix`.

```
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

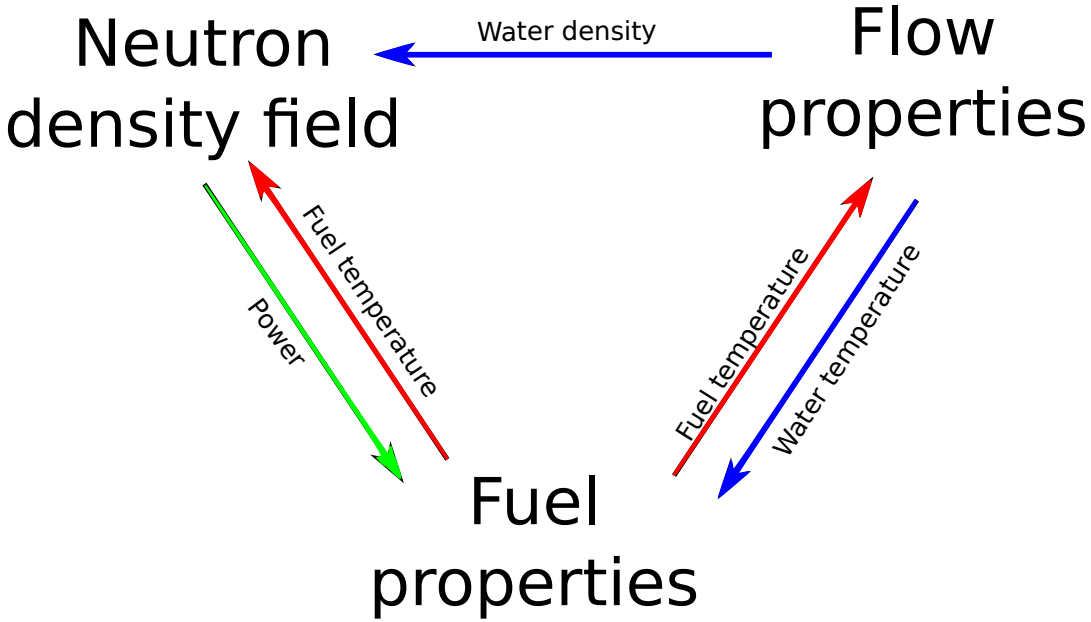
- `regionCouple` boundary condition at coupled patches
- Existing solvers `CG`, `BiCGStab`, `BiCG`, `smoothSolver`
- Parallelizable
- Utilities (mostly) compatible with multiple regions (`splitMesh`, `foamToVTK`, `sample`, `decomposePar`, `reconstructPar`)

Additional sources:

- H. Jasak. "Coupled Multiphysics with OpenFOAM Inter-Region and Inter-Equation Coupling"
- K. Jareteg. "Development of an integrated deterministic neutronic/thermalhydraulic model using a CFD solver". MA thesis. Chalmers University of Technology, 2012

Application: multiphysics in nuclear reactors

Nuclear reactor cores: multiphysics environment



- **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)

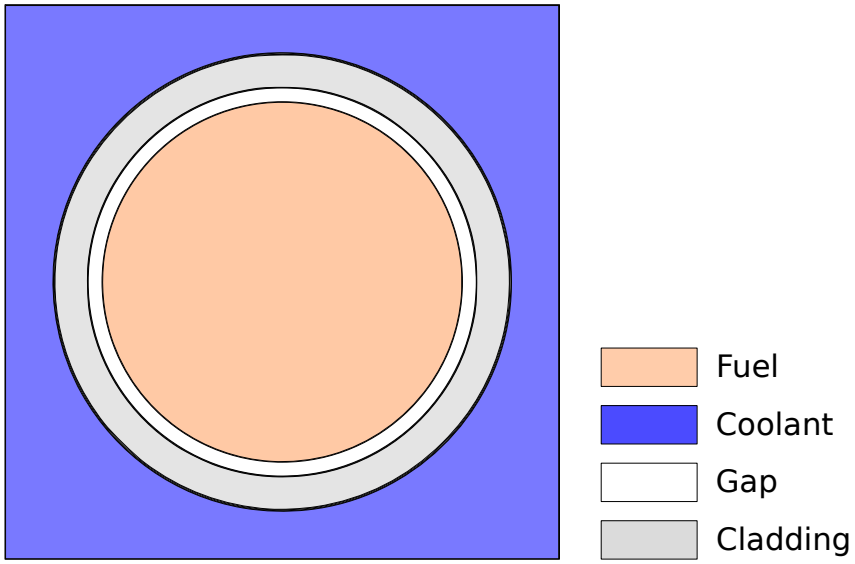


Figure: Slice of nuclear fuel pin

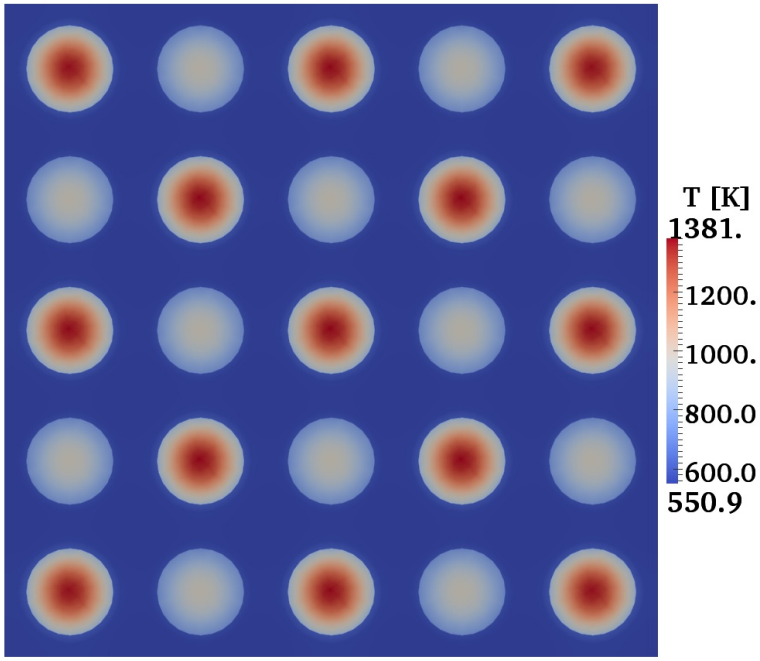
OpenFOAM implementation

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

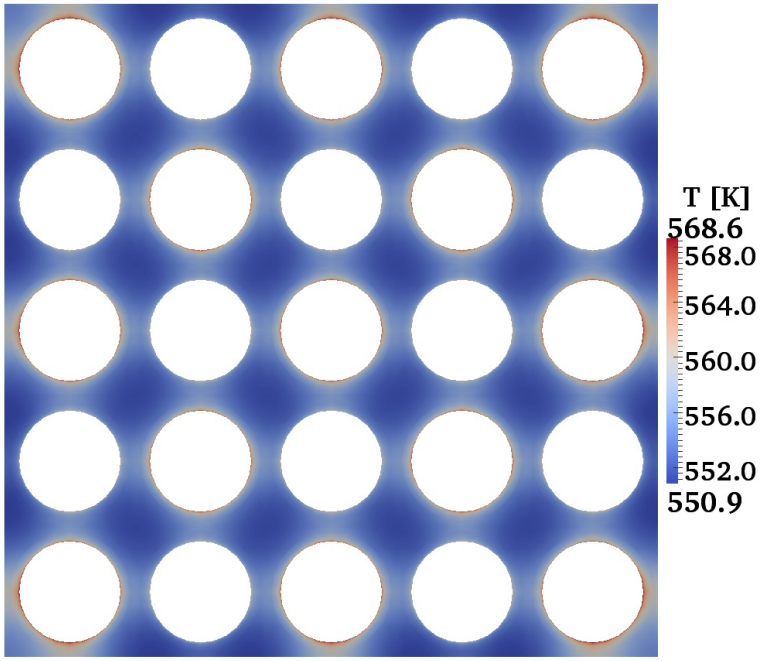
Details:

- K. Jareteg. "Development of an integrated deterministic neutronic/thermalhydraulic model using a CFD solver". MA thesis. Chalmers University of Technology, 2012
- 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

Coupling 2: Field coupling

- **Characteristic:**
  - Multiple fields (α, 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.

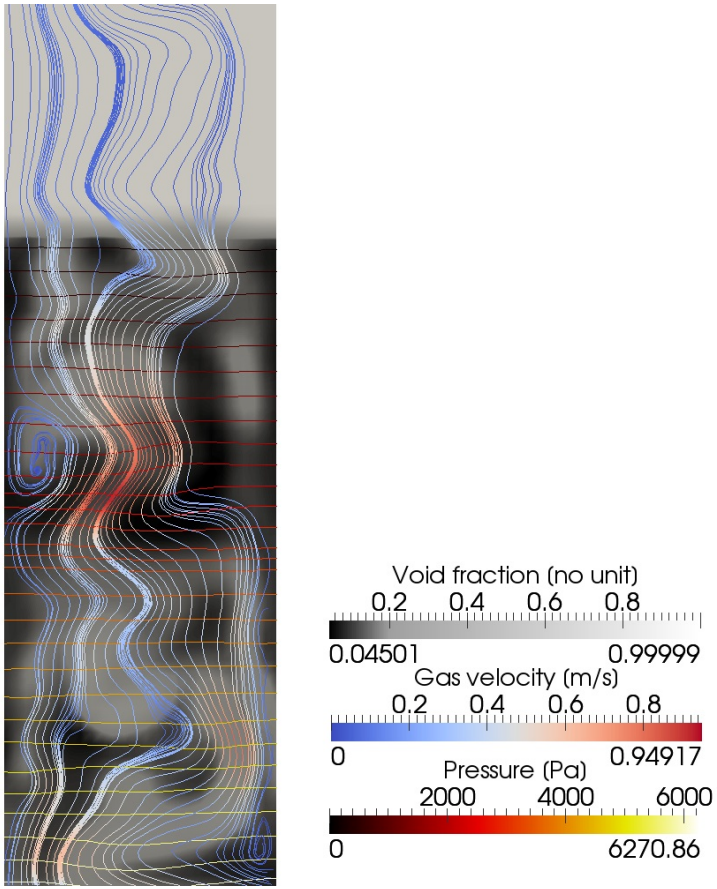


Figure: `bubbleColumn`

Application block coupled incompressible flow solver

- Incompressible steady-state Navier-Stokes:

$$\nabla \cdot (\mathbf{U}) = 0 \tag{1}$$

$$\nabla \cdot (\mathbf{U}\mathbf{U}) - \nabla(\nu \nabla \mathbf{U}) = -\frac{1}{\rho}\nabla p \tag{2}$$

- Traditionally segragated 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

Theory

- SIMPLE algorithm: pressure equation from the continuity equation, explicit use of velocity (from momentum predictor step)
- Alternative approach: Rhie-Chow interpolation:

$$\sum_{\text{faces}} \left[\overline{\mathbf{U}_\mathrm{f}} - \overline{\mathbf{D}_\mathrm{f}} \left(\nabla P_\mathrm{f} - \overline{\nabla P_\mathrm{f}}\right)\right] \cdot \mathbf{S}_\mathrm{f} = 0 \tag{3}$$

$$\sum_{\text{faces}} \left[\mathbf{U}\mathbf{U} - \nu \nabla \mathbf{U}\right]_\mathrm{f} \cdot \mathbf{S}_\mathrm{f} = -\sum_{\text{faces}} P_\mathrm{f} \mathbf{S}_\mathrm{f} \tag{4}$$

Additional sources:

- M. Darwish, I. Sraj, and F. Moukalled. "A coupled finite volume solver for the solution of incompressible flows on unstructured grids". In: *Journal of Computational Physics* 228 (2009), pp. 180–201
- L. Mangani and C. Bianchini. *A coupled finite volume solver for the solution of laminar/turbulent incompressible and compressible flows*. June 2010
- F. Peng Kärrholm. "Rhie-Chow interpolation in OpenFOAM". 2006

OpenFOAM implementation I

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

```
//- 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))

$$\sum_{\text{faces}} \left[\overline{\mathbf{U}_\mathrm{f}} - \overline{\mathbf{D}_\mathrm{f}}\left(\nabla P_\mathrm{f} - \overline{\nabla P_\mathrm{f}}\right)\right] \cdot \mathbf{S}_\mathrm{f} = 0$$

$$\sum_{\text{faces}} \left[\mathbf{U}\mathbf{U} - \nu \nabla \mathbf{U}\right]_\mathrm{f} \cdot \mathbf{S}_\mathrm{f} = -\sum_{\text{faces}} P_\mathrm{f} \mathbf{S}_\mathrm{f}$$

OpenFOAM implementation II

- For 3D solver: $\mathbf{A}x = f$
  - Matrix element:

$$a_{i,j} = \begin{bmatrix} a_{u,u} & 0 & 0 & a_{p,u} \\ 0 & a_{v,v} & 0 & a_{p,v} \\ 0 & 0 & a_{w,w} & a_{p,w} \\ a_{u,p} & a_{v,p} & a_{w,p} & a_{p,p} \end{bmatrix}_{i,j} \tag{5}$$

  - Solution vector:

$$x_i = \begin{bmatrix} u \\ v \\ w \\ p \end{bmatrix}_i \tag{6}$$

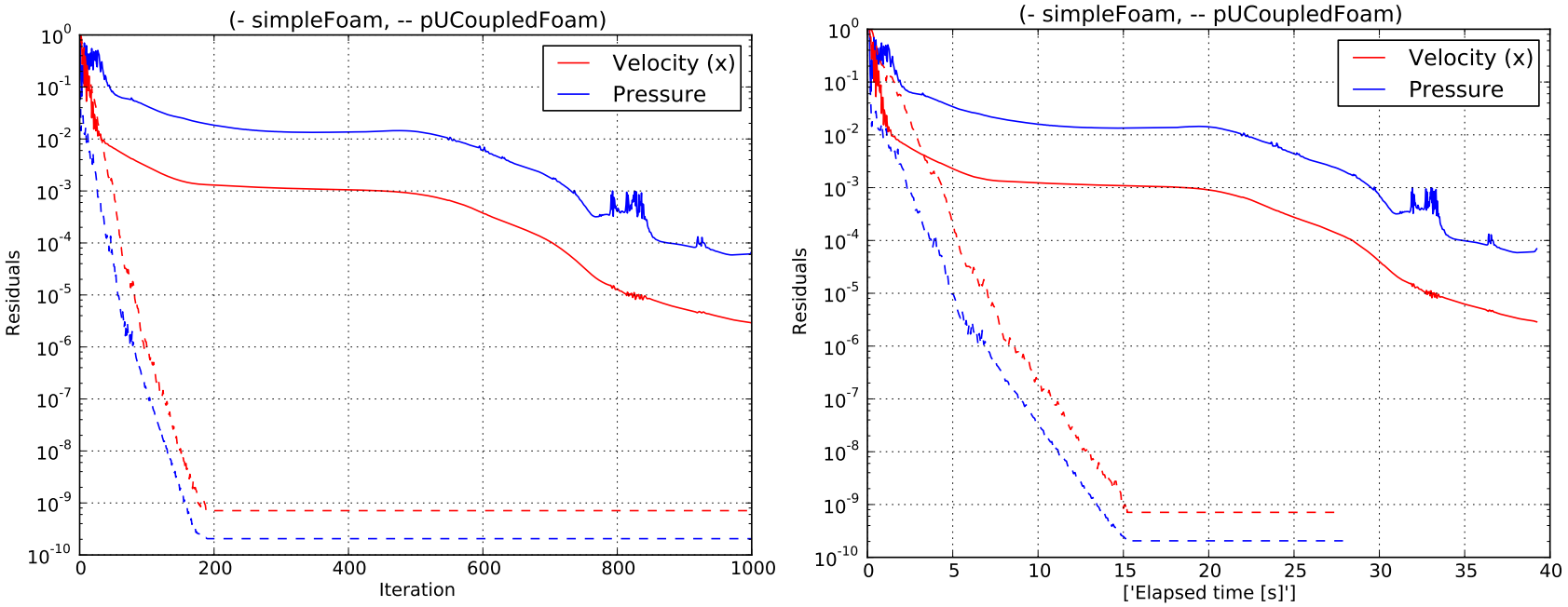
- Off-diagonal coefficients giving the implicit coupling between pressure and velocity
- New solvers implemented (`GMRES`, `BiCGStab`, `CG`)

Description of work:

- K. Jareteg. "Block coupled calculations in OpenFOAM: A coupled incompressible flow solver". Project work within: CFD with OpenSource software, 2012, Chalmers. Oct. 2012

Case study pitzDailyFoam

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

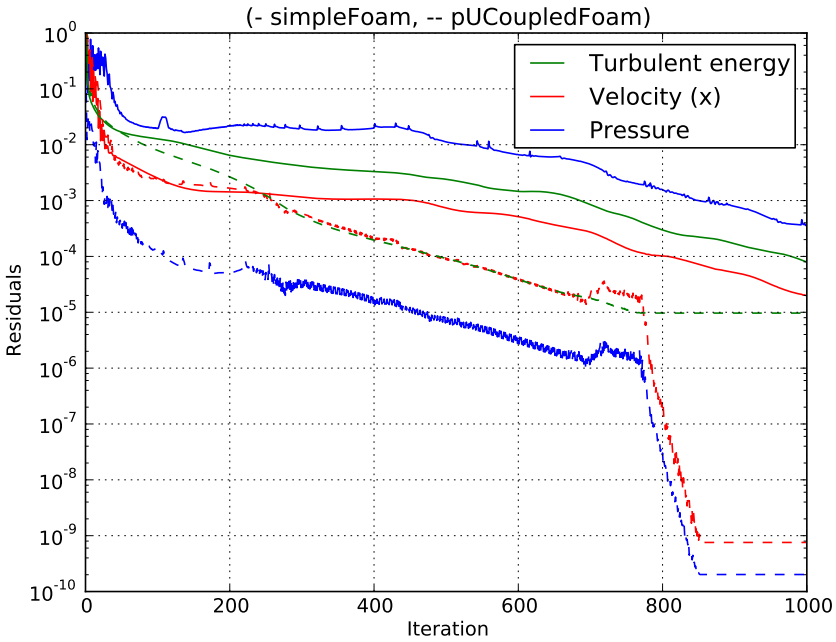


(a) Iterations

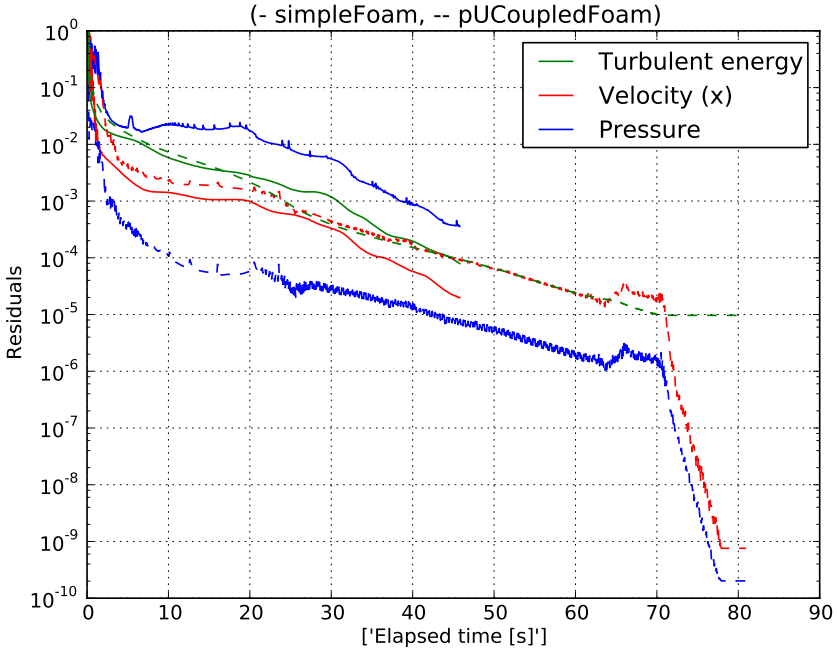
(b) Elapsed time

Figure: Comparison of convergence for `simpleFoam` and `pUCoupledFoam`. Laminar case.

- Convergence profile (turbulent case):



(a) Iterations



(b) Elapsed time

Figure: Comparison of convergence for `simpleFoam` and `pUCoupledFoam`. Turbulent case.

Summary and future outlook

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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