CHALMERS

Multiphysics simulations of nuclear reactors and more

Gothenburg Region OpenFOAM®User Group Meeting

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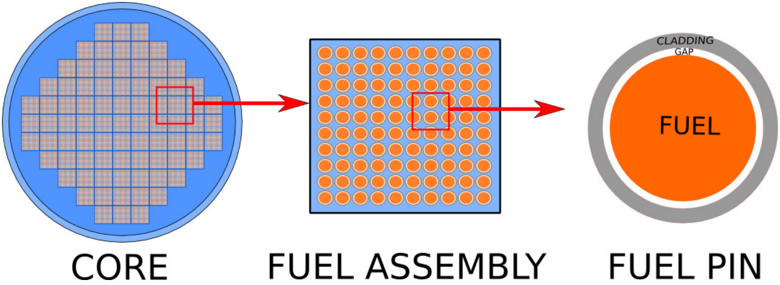
Outline

- Multiphysics and multiscale in Light Water Reactors (LWRs)
- Neutronics and thermal-hydraulics in OpenFOAM®:
- Multiple mesh methodology; mapping and parallelization
- Handling large sets of input parameters
- Example of a simplified Pressurized Water Reactor assembly

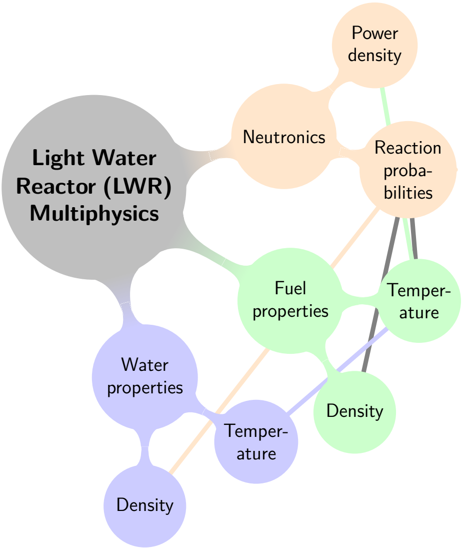
and more ...

- Coupled pressure and velocity solver in foam-extend-3.1

Multiscale systems



Multiphysics systems



Fuel reaction probabilities:
Temperature and density coupling

Power density:
Energy source in fuel temperature

Temperatures:
Dependence between water and fuel properties

Water cross-sections:
Water density coupling

FIRE - FIne mesh deterministic REactor modelling

Development of a fine mesh computational tool for nuclear fuel bundles:

- integrated approach for solving neutronics and thermal-hydraulics
- single and two-phase flow models based on first principles
- high-resolution coupling on fine meshes using HPC
- fuel bundle size calculations, ultimately coupled to coarse mesh solvers

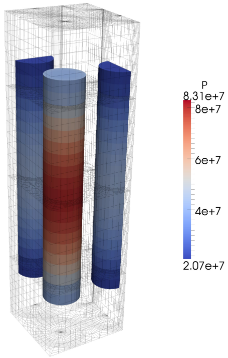


Figure: Power density distribution at fuel pins.

Financing:

- SKC - Swedish Center for Nuclear Technology

Supervisors:

- Christophe Demazière, Paolo Vinai, Srdjan Sasic

Neutronics solver

Steady-state eigenvalue problem

- Eigenvalue problem solved by power iteration method
- Diffusion solver based on multiple groups:

$$\nabla \cdot (D_g \nabla \Phi_g) + \Sigma_{T,g} \Phi_g = S_g + \frac{1}{k} F_g \qquad (1)$$

  - Fast but limited accuracy for fine-mesh with heterogeneous parameters
  - Implemented using a block matrix formulation
- Discrete ordinates method, multiple groups and multiple directions:

$$\Omega_m \cdot \nabla \Psi_{m,g} + \Sigma_{T,g} \Psi_{m,g} = S_{m,g} + \frac{\chi_g}{k} F_g \qquad (2)$$

  - More accurate, but computationally heavy
  - Transport method required for fine mesh problems

More information:

Block matrix systems in OFW9 training, Zagreb, 2014: "Block coupled matrix solvers in foam-extend-3", Klas Jareteg and Ivor Clifford

Neutronics solver - Discrete ordinates method

Implementation of discrete ordinates:

- Standard matrix solvers potentially inefficient
- Following ordinate Ω_m, a direct sweep through the domain allows $\Psi_{m,g}$ to be computed in one sweep
- Sweeping order of the cells calculated at initialization
- Parallelization handled as in `GaussSeidel` solvers (corresponding to full boundary exchange after finisihed sweep)

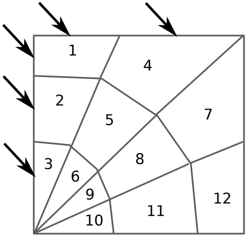


Figure: Example of a sweep ordering for an unstructured mesh

Code: steadyDOMSweeNeutronics.C

```
for (register label cellI=0; cellI<nCells; cellI++)
{
    // Modification for ordered sweep
    register label cellJ = sweepOrder[cellI];
```

Thermal-hydraulics single-phase solver

Steady state single phase solver:

- Approach equivalent to `simpleFoam`
- Buoyancy taken into account for density variation from heating
- Generally slow convergence for pressure and velocity

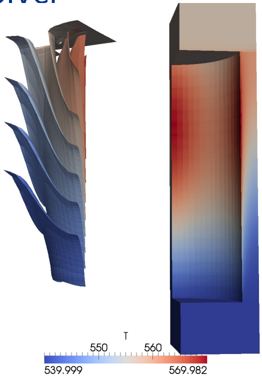


Figure: Temperature distribution in coolant around a single fuel pin.

More information:

Presentation on coupled pressure and velocity solver from OFW9, Zagreb, 2014: "`puCoupledFoam` - an open source coupled incompressible pressure-velocity solver based on foam-extend" Klas Jareteg, Vuko Vukcevic, Hrvoje Jasak

Thermal-hydraulics: conjugate heat transfer

- Multiregion approach, separate meshes for all solid and liquid regions
- Implicit heat transfer by using `regionCouple`
  - Explicit iteration over all regions not an alternative, too many regions
- Temperature dependent thermophysical properties
  - Based on table interpolation, inheriting `basicThermo`

Thermal-hydraulics two-phase solver

- Two-phase flow model under development to extend solver to Boiling Water Reactors (BWRs)
- Large variety of complex behavior to be covered
- Solver based on a population balance methods

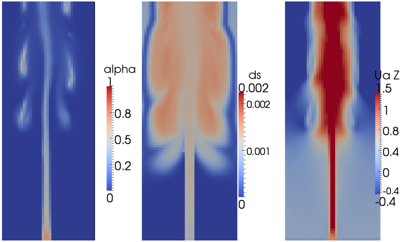


Figure: Void fraction, bubble mean diameter and axial velocity

Steady state coupling algorithm

- Explicit scheme, coupled convergence iteration
- Neutronics and thermal-hydraulic modules implemented as classes. Easy testing of different implementations using inheritance and run-time choosable mechanism

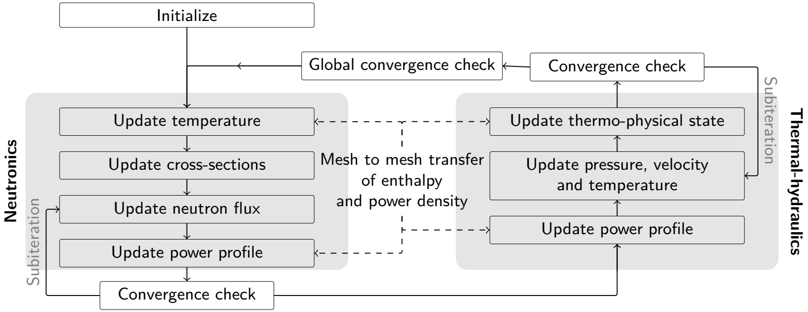


Figure: Iterative coupled scheme. [1]

Class structure

- Solvers for each field written as objects
- Direct inheritance allows for different models to be tested in the coupled scheme

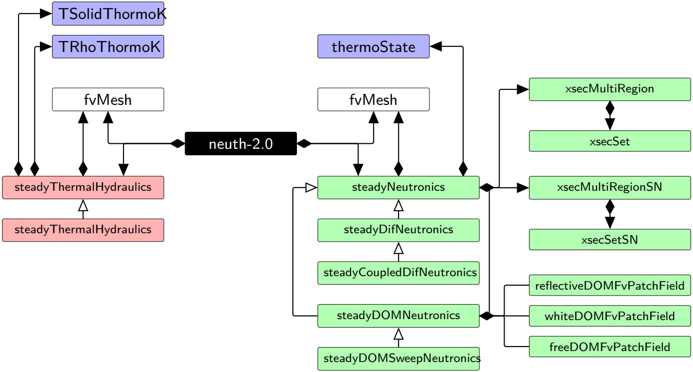
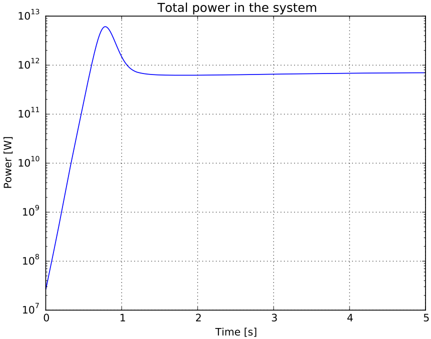


Figure: Simplified class structure of coupled solver

Transient multiphysics calculations

Master thesis project by Rasmus Andersson

- Currently developing a transient multiphysics solver
- Thermal-hydraulic solvers based on PISO algorithm, with variable density
- Neutronics solver based on diffusion solver



Multiple meshes - Generation and setup

- Repeating structure of fuel pins allows for repeated mesh
- Automatic setup of region coupled interfaces for the thermal-hydraulics

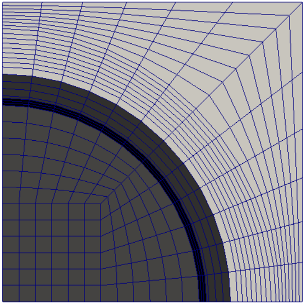


Figure: Mesh example for a quarter of a fuel pin

Multiple meshes - Mapping I

Different meshes in different regions:

- Finer mesh in the liquid coolant than in neutronics in general
- Mapping algorithm needed for data exchange:

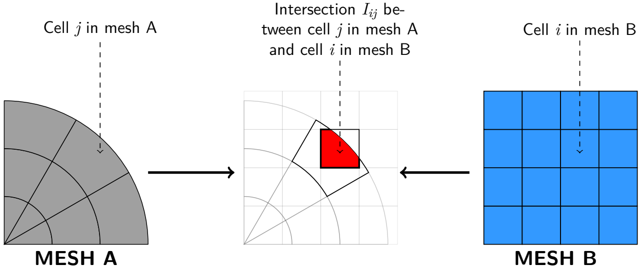


Figure: Example of mapping of two overlapping meshes. [1]

- Fully conservative transfer of extensive quantities
- Geometric overlaps computed equivalent to GGI face overlaps, extended to 3D

Multiple meshes - Mapping II

- Mapping handled locally on each CPU

Code: neuthFoam-2.0.C

```
// Compute cell intersection between all fuel meshes and neutronics
PtrList<intersectionChecker> iSolid(I);

forAll(iSolid,i)
{
    iSolid.set(i, new intersectionChecker(solidMeshes[i], neutronicsMesh));
}
```

Code: neuthFoam-2.0.C

```
// Transper power distribution from neutronics to fuel meshes
const volScalarField& Pnk = neutronics->P();
PtrList<volScalarField>& PS = thermalhydraulics->P();

forAll(solidMeshes,i)
{
    // Transfer the power field and immediately normalize
    solidMeshes[i].backwardFieldVolumetric(PS[i],Pnk);
}
```

Multiple meshes - Mapping III

- Parallelization: all meshes are split in same planes
- `meshPartitionerRegion` (not yet released) used to generate cell sets.

Code: meshPartitionerDict

```
Directions (1 1 4);
Mode "manual";
X (0.0 1.0);
Y (0.0 1.0);
Z (-100.0 0.4 0.7 1.1 100.0);
```

Neutronics mesh - cross-section handling

- Different cross-sections in different materials
- Handled using cell sets

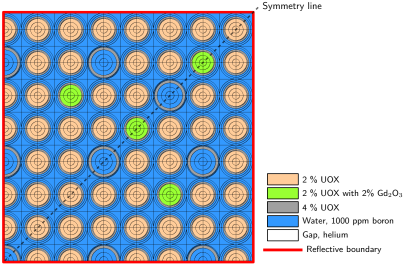


Figure: Horizontal view of test system. [1]

Code: Cell sets for cross-sections

```
// Automatically generated cell set for fuel region, input to setSet
cellSet fue\_I0\_J0\_U100\_out new cylinderToCell
    (0.0e+00 0.0e+00 0.0e+00) (0.0e+00 0.0e+00 1.0e-02) 1.340407e-03
 ...
cellSet fue_I0_J0_U100 new rotatedBoxToCell
    (0.0e+00 0.0e+00 0.0e+00) (1.366667e-03 0.0e+00 0.0e+00)
    (8.368420e-20 1.366667e-03 0.0e+00) (0.0e+00 0.0e+00 1.0e-02)
cellSet fue_I0_J0_U100 delete cellToCell fue_I0_J0_U100_box
```

Example case

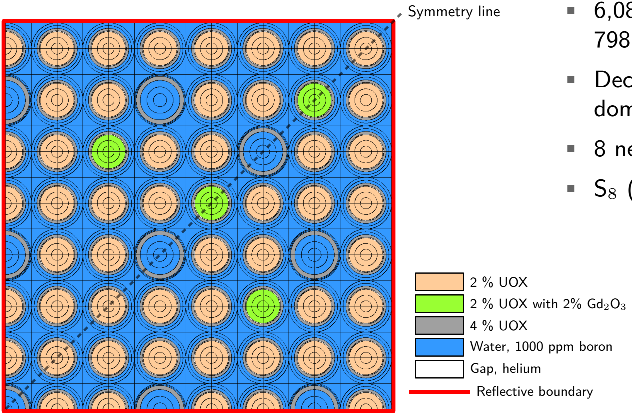


Figure: Horizontal view of test system. [1]

- Quarter of 15×15 system
- PWR conditions
- System height 100 cm ($+2 \times 20$ cm reflector)
- 6,088,000 cells in coolant, 798,000 in neutronics
- Decomposed in 64 domains
- 8 neutron energy groups
- S_8 (80 directions)

Example case - Results I I

- Problem converged in 14 hours using 64 CPUs (Nehalem Intel® Xeon® E5520, 2.27GHz)
- Multiphysics coupling converged in 8 iterations

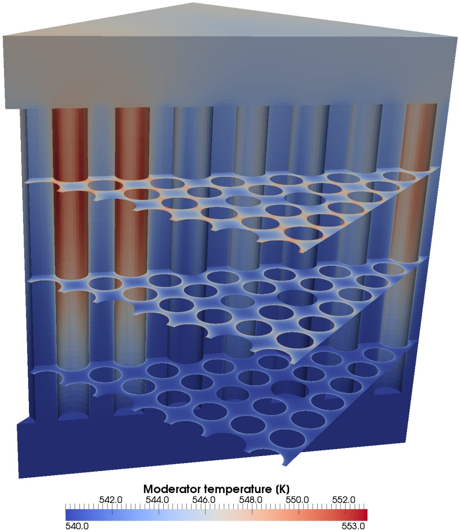


Figure: Moderator temperature. [1]

Example case - Results I I

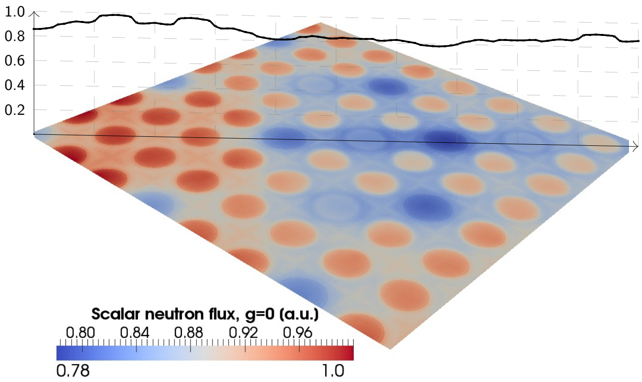


Figure: Scalar flux at mid-elevation for the fast group. [1]

Slow convergence in incompressible flow solvers

Background

- Generally slow convergence of segregated steady-state incompressible solvers
- A large number of iterations needed to resolve coupling between pressure and velocity
- Coupled solvers potentially give an increased convergence rate

Applications

- Single-phase flow around PWR between fuel pins
- Low mach simulations around external surfaces
- ...

Implicit formulation

- Navier-Stokes, incompressible, steady-state equations:

$$\nabla \cdot (\mathbf{U}) = 0 \tag{3}$$

$$\nabla \cdot (\mathbf{U}\mathbf{U}) - \nabla(\nu \nabla \mathbf{U}) = -\frac{1}{\rho}\nabla p \tag{4}$$

- with the semi-discretized form:

$$\sum_{\text{faces}} \mathbf{U}_\text{f} \cdot \mathbf{S}_\text{f} = 0 \tag{5}$$

$$\sum_{\text{faces}} [\mathbf{U}\mathbf{U} - \nu \nabla \mathbf{U}]_\text{f} \cdot \mathbf{S}_\text{f} = -\sum_{\text{faces}} P_\text{f} \mathbf{S}_\text{f} \tag{6}$$

- Rhie-Chow interpolation in the continuity equation:

$$\sum_{\text{faces}} \left[\overline{\mathbf{U}_\text{f}} - \overline{\mathbf{D}_\text{f}} \left(\nabla P_\text{f} - \overline{\nabla P_\text{f}}\right)\right] \cdot \mathbf{S}_\text{f} = 0 \tag{7}$$

a coupled system of four equations is formulated.

pUCoupledFoam - Coupled incompressible solver I

Coupled solver

- Coupled solver implemented in foam-extend-3

Example case

- Structured mesh, 4800 cells, laminar case
- Comparison of SIMPLE algorithm and coupled algorithm

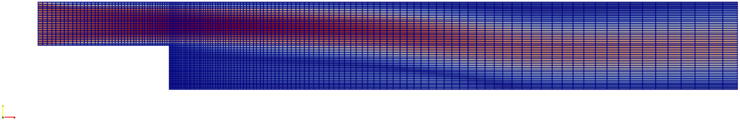


Figure: Geometry and velocity solution for back facing step case

`pUCoupledFoam` - Coupled incompressible solver II

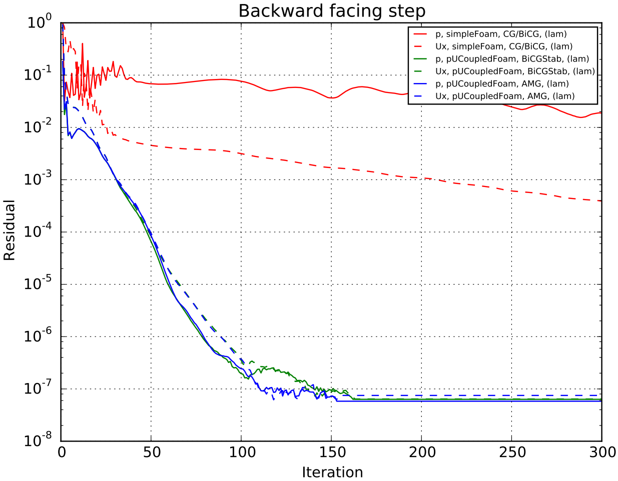


Figure: Performance of `simpleFoam` compared to `pUCoupledFoam`.

Questions?

More information:

[1] K. Jareteg et al. "Coupled fine-mesh neutronics and thermal-hydraulics - modeling and implementation for PWR fuel assemblies". In: *Submitted to Annals of Nuclear Energy, Special Issue: "Multi-Physics Modeling of LWR Static and Transient Behavior"* (2014).