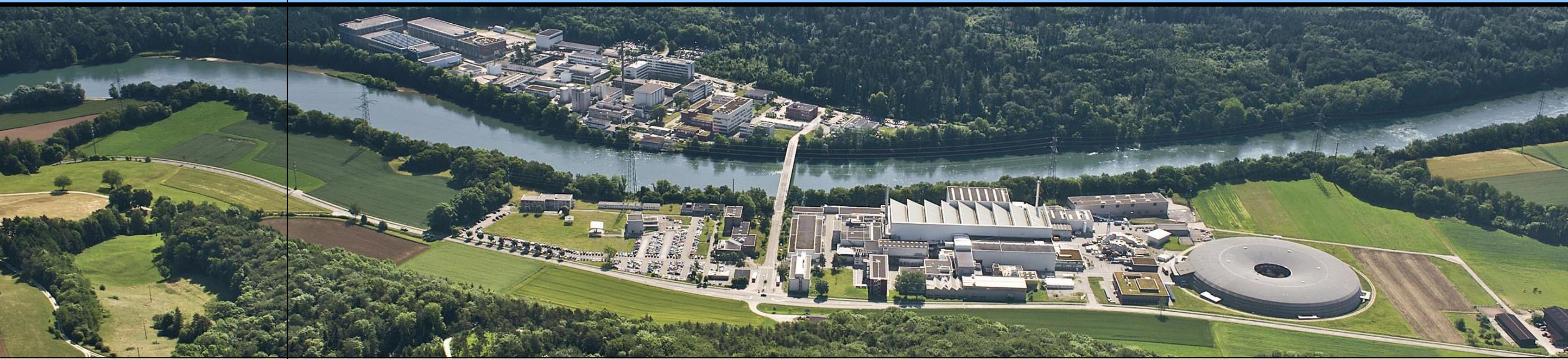


Wir schaffen Wissen – heute für morgen

Paul Scherrer Institut

I. Clifford, O. Zerkak, A. Pautz

OpenFOAM in Nuclear Applications

SERPENT and Multiphysics, LPSC, Grenoble, February 26-27, 2015

Remark

What this talk is:

- An introduction to OpenFOAM within the nuclear context
- A very brief summary of OpenFOAM development work over the years (work in which I have been involved)

What this talk is not:

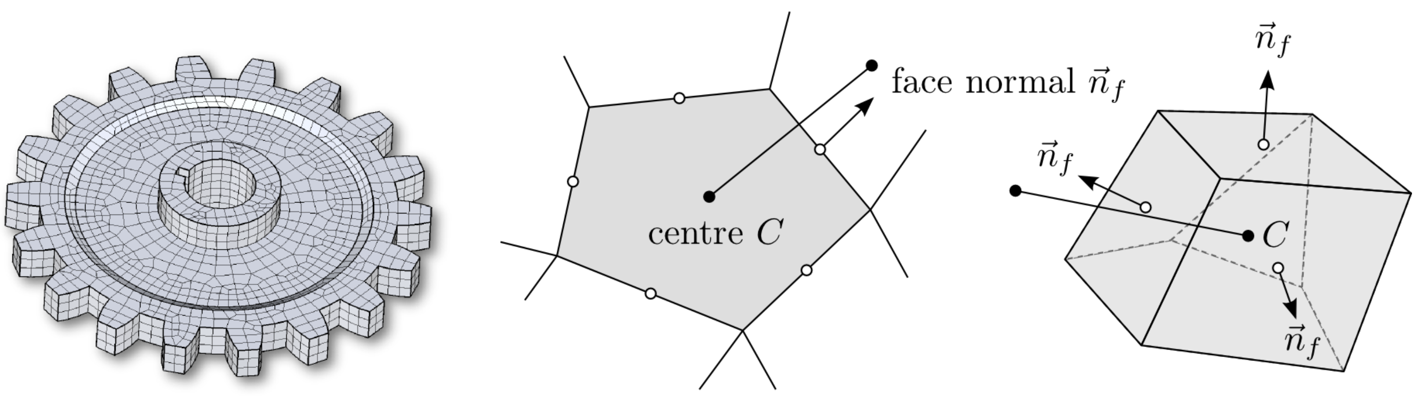
- A comprehensive overview of all nuclear-related work using OpenFOAM

Outline

- Introduction to OpenFOAM - a nuclear perspective
- OpenFOAM for nuclear applications
  - Pebble Bed Modular Reactor (PBMR)
  - Prismatic High Temperature Reactor (Pennstate University)
  - Light Water Reactors (STARS group at PSI)
- Summary and Outlook

What is OpenFOAM

- OpenFOAM stands for Open Field Operation and Manipulation
- Officially described as an open-source CFD toolbox
  - Capabilities mirror those of commercial CFD
  - Free-to-use software without paying for licensing and support
- Far more than simply a set of CFD solvers and tools
- Underlying design - a comprehensive multi-physics framework for solving sets of PDEs using cell-centred polyhedral finite-volume methods



Discretized Domain 2D 3D

Equation Mimicking

- Natural language of continuum mechanics: partial differential equations
- Example: turbulence kinetic energy equation

$$\frac{dk}{dt} + \nabla \cdot (\vec{u}k) - \nabla \cdot [(\nu + \nu_t)\nabla k] = \nu_t \left[\frac{1}{2}(\nabla\vec{u} + \nabla\vec{u}^T)\right]^2 - \frac{\epsilon_0}{k_0}k$$

- Objective: represent PDEs in their natural language

```
solve
(
      fvm::ddt(k)
    + fvm::div(phi, k)
    - fvm::laplacian(nu() + nut, k)
==
      nut*magSqr(symm(fvc::grad(U)))
    - fvm::Sp(epsilon/k, k)
);
```

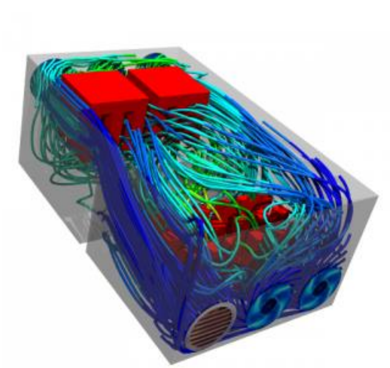
- Correspondence between implementation and equation is clear

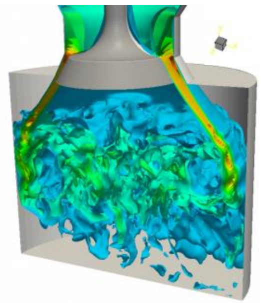
Open∇FOAM — What is OpenFOAM

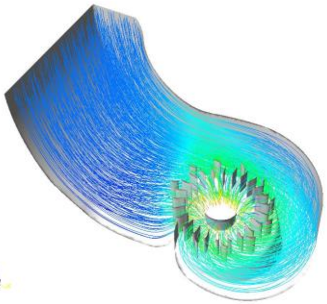
- Structure of OpenFOAM
  - Libraries
    - Foundation libraries: underlying mesh, field, matrix, etc. functionality
    - Physical modelling libraries: physics-specific functionality, eg. Material properties, specialized boundary conditions, turbulence models (largely focused on CFD)
    - Written in a reusable form
  - Executables
    - Solver applications (mostly focused on CFD)
    - Tools and utilities for creating, manipulating and post-processing meshes and field data
- Executables rely heavily on functionality provided by the underlying libraries
  - Typically only a few 100s of lines of code
  - Top level executables are easy to read, understand and modify
  - Low-level functions, eg. mesh handling, parallelisation, data I/O handled transparently: no need for special coding at top level
- Written from the base up in object-oriented C++
- Special Note: OpenFOAM is not a high-level language for scientific research like Matlab. This is production level optimized code suitable for large-scale computing
  - Fully parallelized: has been run successfully using thousands of cores

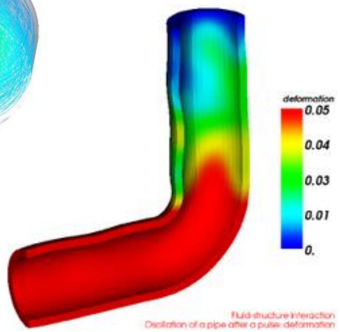
Open∇FOAM Physical Modelling Capability Highlights

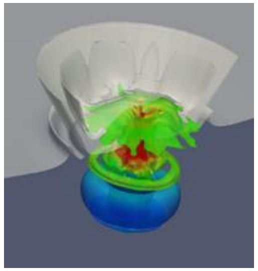
- Incompressible & compressible flow: segregated pressure-based algorithms
- Heat transfer: Buoyancy driven flow, conjugate heat transfer, thermal radiation
- Multiphase flows: Euler-Euler, VOF free surface capturing and surface tracking
- Turbulent flows: RANS, DES, LES
- Combustion and chemical reactions: Engine simulations
- Turbomachinery, Stress analysis, fluid-structure interaction, electromagnetics, MHD, particle tracking, etc.

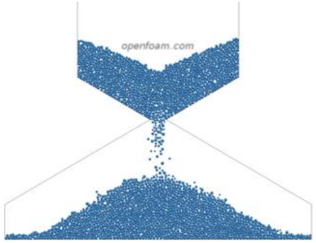












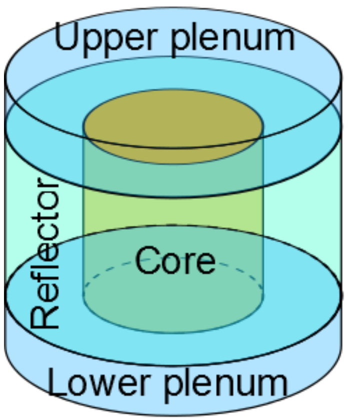
Open∇FOAM — In the Nuclear / Multiphysics Context

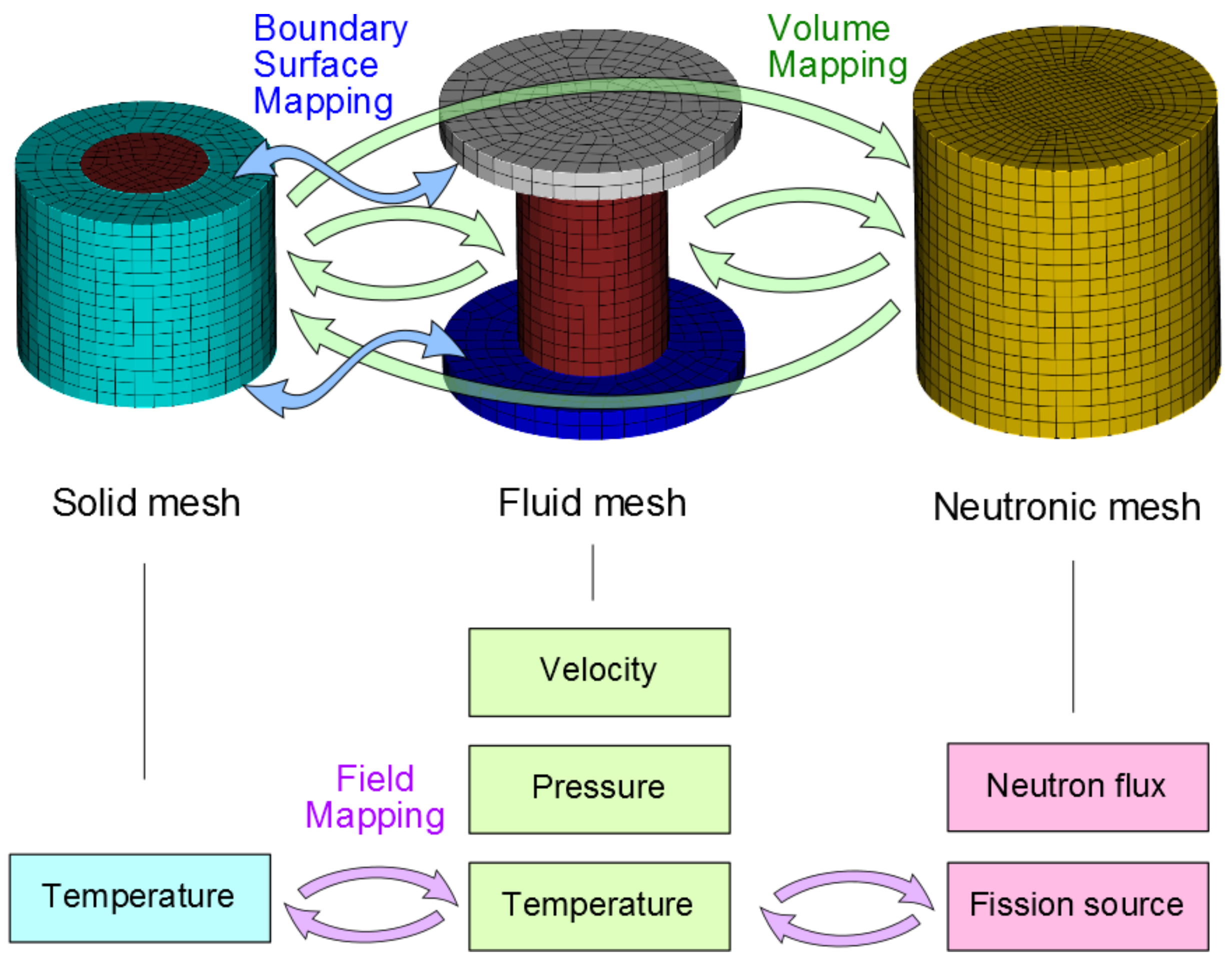
- Signification CFD jargon is used when talking about OpenFOAM
  - This can be confusing
  - Not immediately obvious how OpenFOAM may be applicable in the nuclear and reactor analysis context

I will try to give some basic insight!

- A typical OpenFOAM case
  - Time control
  - One or more meshes: Spatial description of the domain with boundaries defined
  - One or more fields: Unknown variables associated with a mesh with boundary conditions defined
    - Fields on the same mesh can be manipulated and combined directly
    - Fields on different meshes can be mapped between meshes and thereafter manipulated and combined directly
  - One or more equations: Partial differential equations in terms of the unknown variables with source terms
    - Coupling between equations typically uses segregated algorithms
    - Newton-based nonlinear solvers are not currently available (eg. MOOSE platform)

Conceptual demonstration: A simple nuclear reactor

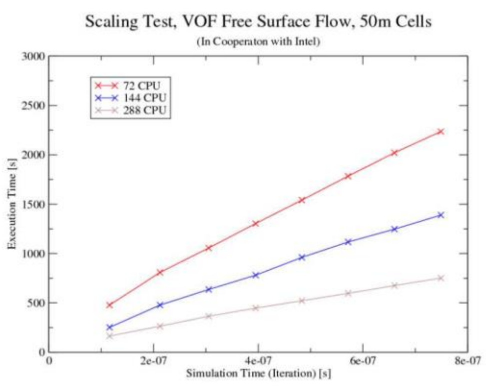


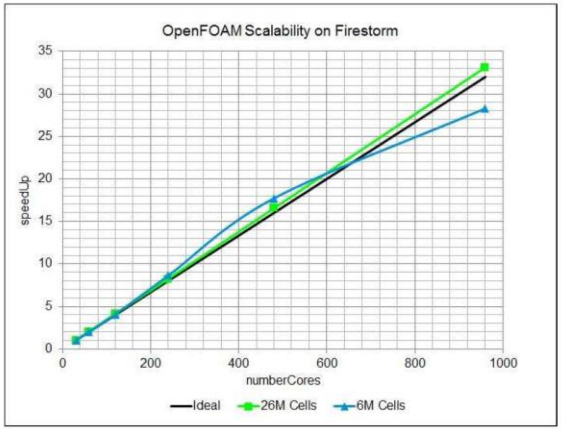


Open∇FOAM Massively Parallel Scaling

Massively Parallel Scaling

- Mesh size and resolution environment in 21st century are revolutionary different from (the comfortable) 1990s: thousands of processors, a billion cell mesh
- Complex hardware architecture without proper programming support complicates the programming and roll-out into real-world applications
- Still learning GPU lessons: potentially changing the way we write CFD codes back towards structured mesh codes and fixed internal infrastructure
- What about parallel CFD clouds: do we need custom infrastructure?





Cyprus Advanced HPC Workshop Winter 2012. Tracking: FH6190763 Feb/2012

OpenFOAM: Introduction, Capabilities and HPC Needs – p. 8

Open∇FOAM — Advantages

- Open architecture
  - Access to complete source: no secret tricks or cutting corners
  - Readily extendable – Custom boundary conditions, physical models, etc.
  - Significant community-based support available
- Open-source
  - No license costs
- Problem-independent numerics and discretization
  - Tackle non-standard continuum mechanics problems
  - Tackling complex multi-physics problems is made easier through equation mimicking
  - Runtime selection of discretization schemes and physical models
    - Case setup is highly flexible
  - Good track record in non-linear and strongly coupled problems
- Excellent piece of C++ code and software engineering

Open∇FOAM — Disadvantages

- Library is LARGE: 1000s of classes
  - Steep learning curve for non-standard physics
  - Good knowledge of C++ programming is essential
- Finite-volume methods have relatively low order accuracy (2nd order)
  - Significant mesh refinement may be needed to achieve the desired accuracy
  - This disadvantage is partly offset by the simplicity of the method
- Limited number of users in the nuclear community
  - Less community support for your particular project
  - Less existing code from which to borrow ideas
- In-house verification and validation is typically needed: community-based efforts may not consider your particular problem
- Recently: The OpenFOAM project has branched into two separate groups and development tracks (OpenFOAM Foundation and OpenFOAM Extend Project)
  - The developments are no longer closely compatible
  - The choice of which project to follow can have unexpected consequences down the line

Code Verification

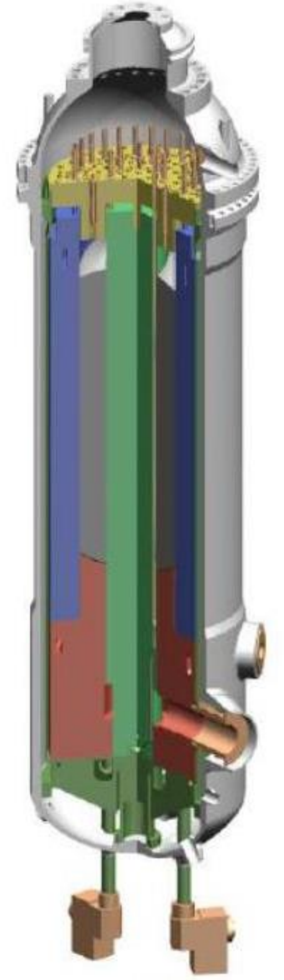
- Primary responsibility of code developer
- In many respects, code verification also carried out by user community: with so many users, errors inevitably get identified quickly
  - In a sense: Direct Peer Review by the community
- Layered development assists verification efforts
  - Underlying libraries don't change
  - If you have not recompiled or re-linked the code, you have not broken it!
  - Object-oriented code design
    - Component-wise V&V (unit tests) can easily be carried out
    - Data protection prevents unexpected data corruption from higher levels

Validation

- At basic level, validation of open-source code is identical to other efforts
  - Choose well established validation examples (experiments)
  - Perform detailed studies, varying model parameters and studying mesh dependence effects
  - Compare results with reference values
- Huge amount of effort: cannot be avoided
- Code validation done in a traditional way… helped by the fact that top-level solvers are very simple
  - single-physics solvers can be used to validate individual physical models
  - All critical functionality is shared and reused from library components

PBMR — Pebble Bed Modular Reactor

- Legacy pebble bed reactor analysis codes originally developed at Forschungszentrum Jülich (FZJ) in 1980s
  - Fast and effective but severely limited
    - Inherently 2D (axisymmetric)
    - Rectangular r-z discretization
    - Difficult to implement new methods
    - Difficult to couple with other codes
- PBMR design
  - New reactor → New codes and methods
- Modern simulation platform was conceived
- OpenFOAM chosen as basis for reactor dynamics solver (Vulashaka)
  - Steady-state (eigenvalue) and transient solver
  - Coupled multigroup neutron diffusion and coarse mesh thermal-fluids



Multigroup Neutron Diffusion

- OpenFOAM is proven and tested for CFD, i.e. thermal-fluids
- Neutronics was never considered by the developers or community

Can it be done?

- Multigroup neutron diffusion equation

$$\frac{1}{v_g}\frac{\mathrm{d}\phi_g}{dt} - \nabla \cdot D_g \nabla \phi_g + \left(\Sigma_a^g + \Sigma_s^g\right)\phi_g = S_S^g + \frac{1}{k}\mathrm{X}_P^g S_P + \mathrm{X}_D^g S_D$$

- In OpenFOAM this is easily implemented for each equation

```
solve
(
      fvm::ddt(invV[g], phi[g])
    - fvm::laplacian(D[g], phi[g])
    + fvm::Sp(sigma_a[g]+sigma_s[g], phi[g])
==
      S_s[g]
    + (1/k)*chi_p[g]*S_p
    + chi_d[g]*S_d
);
```

PBMR

Multigroup Neutron Diffusion

- Simple segregated approach
  - Works for steady-state problems (simple power iteration)
  - Fails miserably in many cases for time-dependent problems (stiff equations)

Back to the drawing board?

Not quite!

- Block-coupled solver recently developed for OpenFOAM
  - Solves systems of linearly coupled PDEs implicitly

$$\boldsymbol{v}^{-1}\frac{\mathrm{d}\Phi}{dt} - \nabla \cdot \boldsymbol{D}\nabla\Phi + (\boldsymbol{\Sigma}_a + \boldsymbol{\Sigma}_s)\Phi = \cdots$$

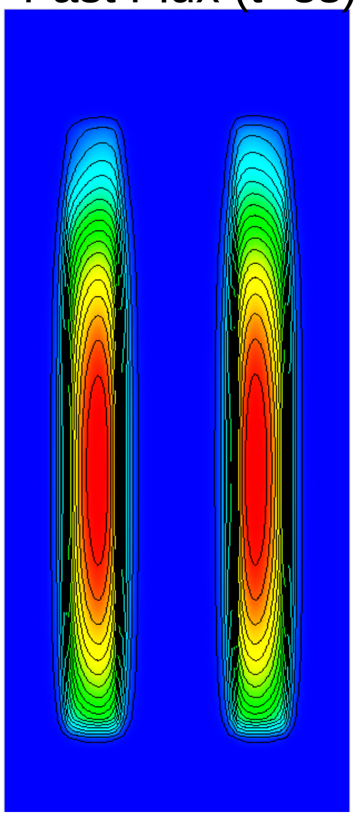
  - Solution variables and coefficients become vectors and tensors, eg.

$$\boldsymbol{\Phi} = \begin{bmatrix} \phi_1 \\ \vdots \\ \phi_G \end{bmatrix}, \boldsymbol{\Sigma}_a = \begin{bmatrix} \Sigma_a^1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \Sigma_a^G \end{bmatrix}$$

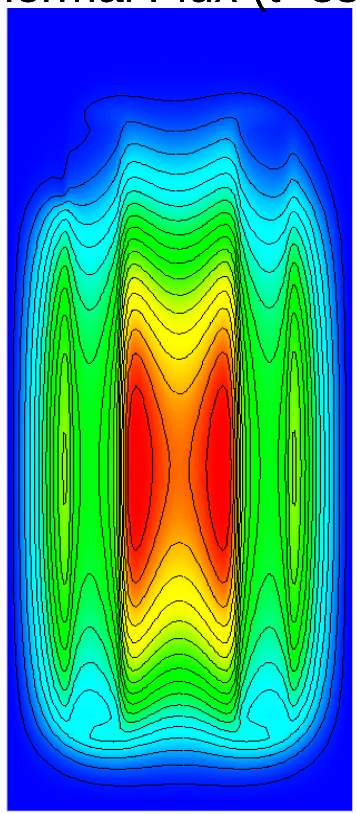
  - Additional work needed since the equation mimicking cannot be readily applied to general coupled sets of equations
- Block-coupled approach works for both steady-state and transient simulations

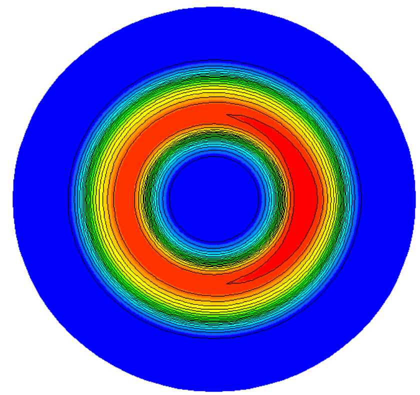
PBMR400 Benchmark: Single Control Rod Ejection Transient

Fast Flux (t=3s)

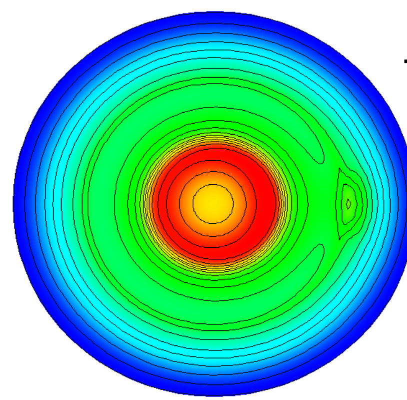


Thermal Flux (t=3s)



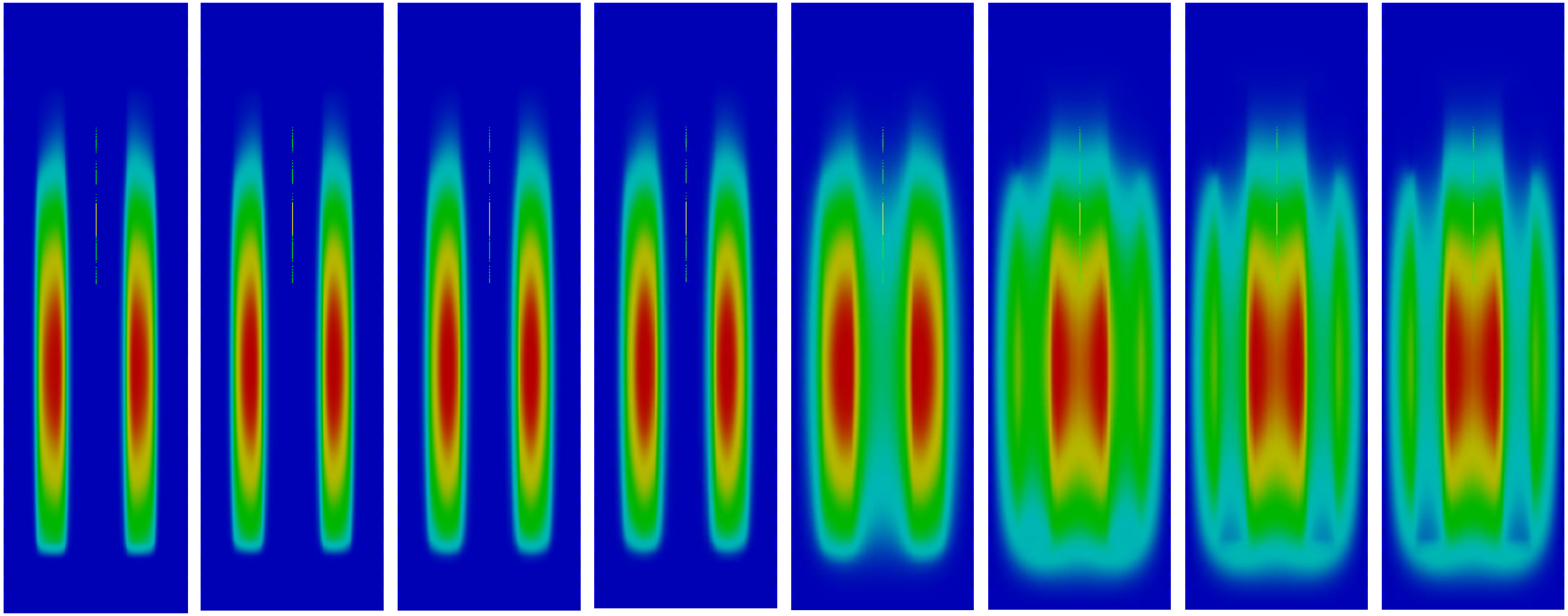


Fast Flux (t=3s)



Thermal Flux (t=3s)

PBMR400 Benchmark: Neutron flux profiles for steady-state operation



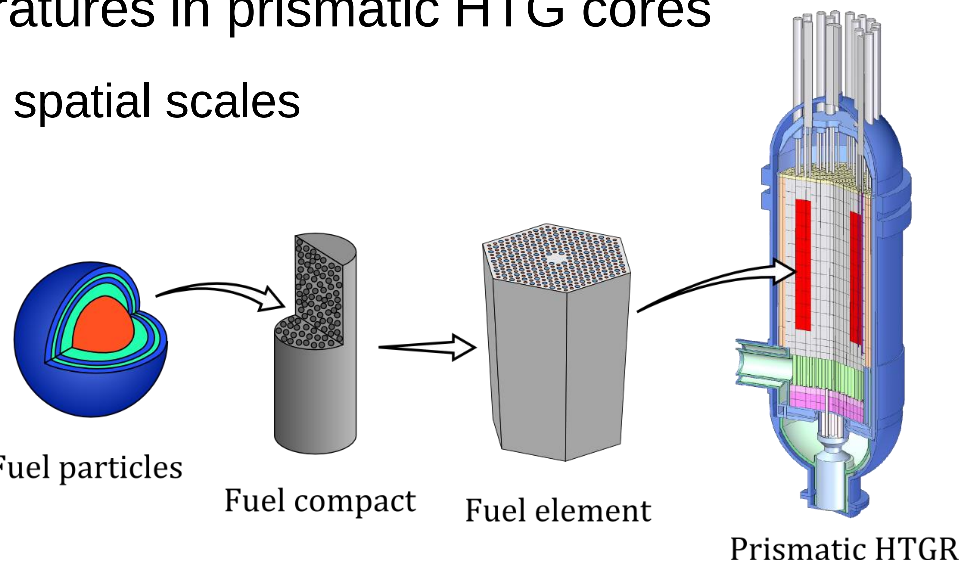
Fast Thermal

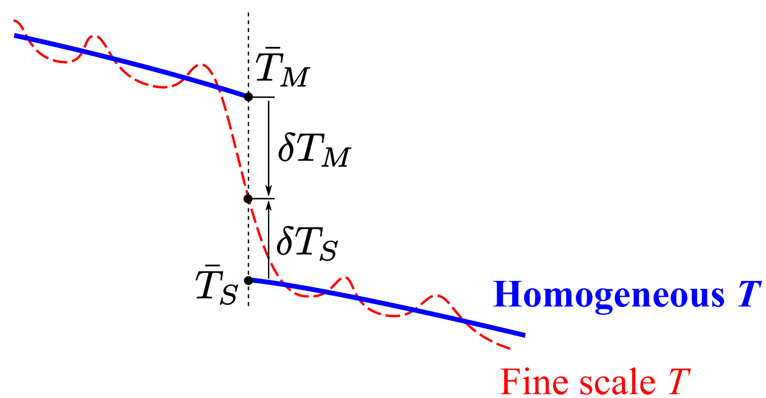
Pennstate — Prismatic High Temperature Reactor

Multi-scale solution of solid temperatures in prismatic HTG cores

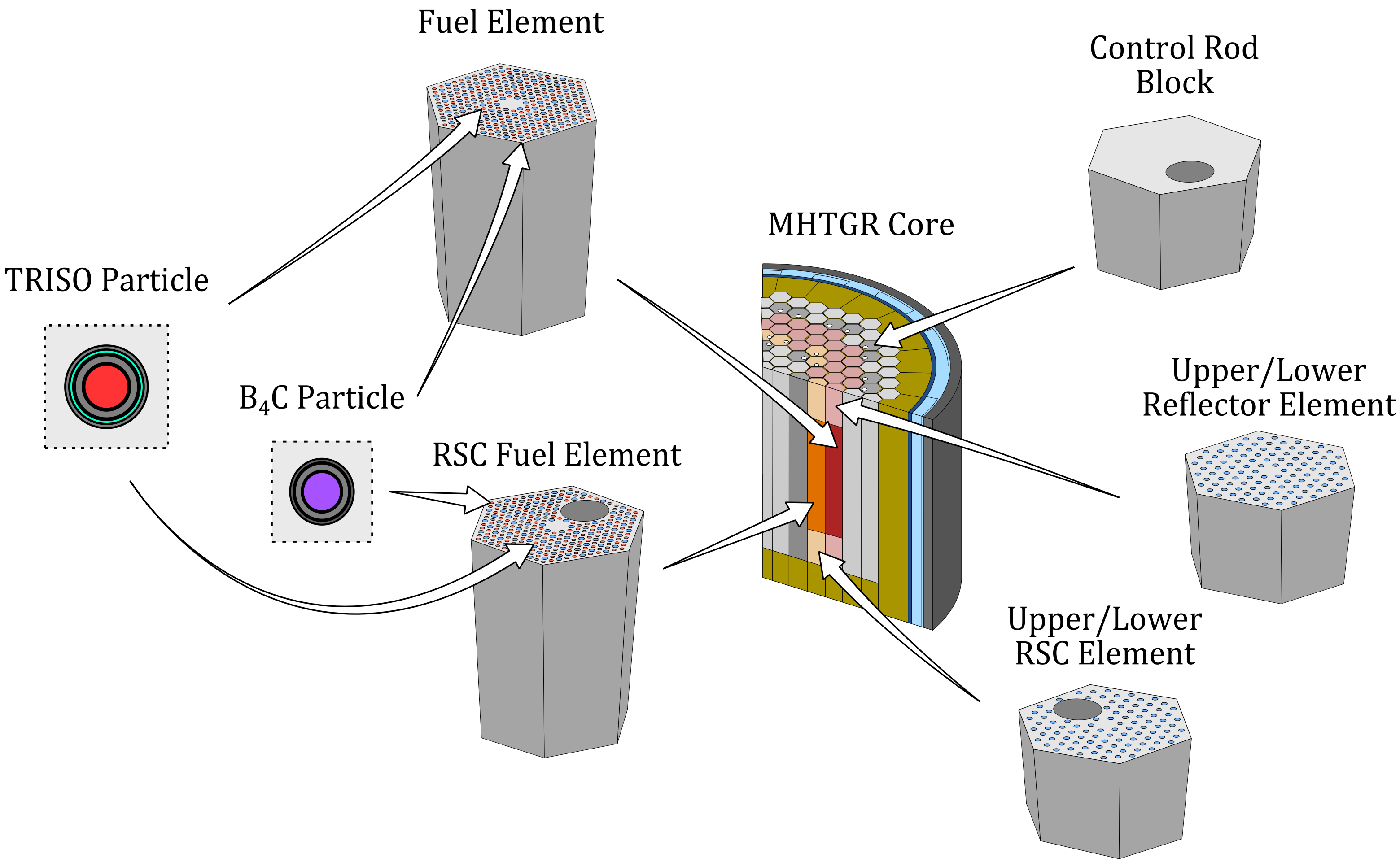
- Reactor design has multiple distinct spatial scales

- Basic concept: Hierarchical multi-scale solution for temperature in solid materials
  - Borrows concepts from homogenization theory (unit cell calculations, discontinuity factors, etc.)
  - Subscale temperatures modelled using reduced order models



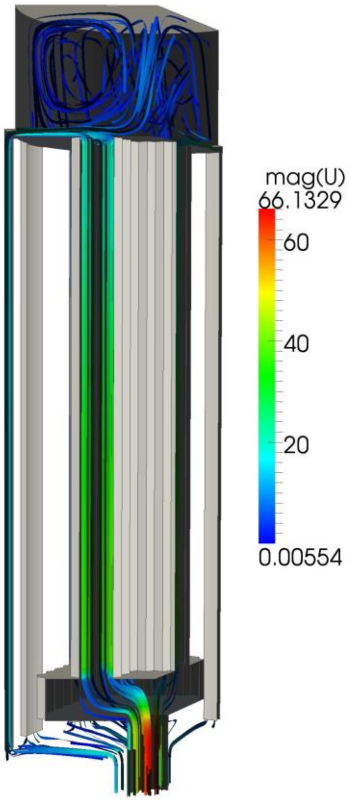


MHTGR-350MW Benchmark: Hierarchical Model Development

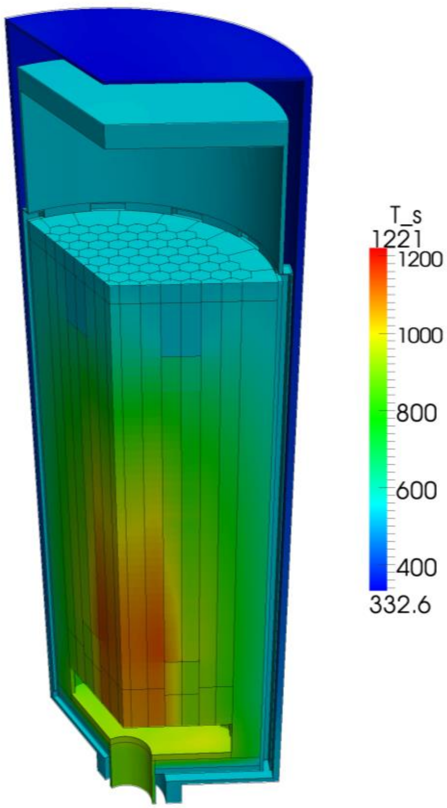


Pennstate Benchmark Results

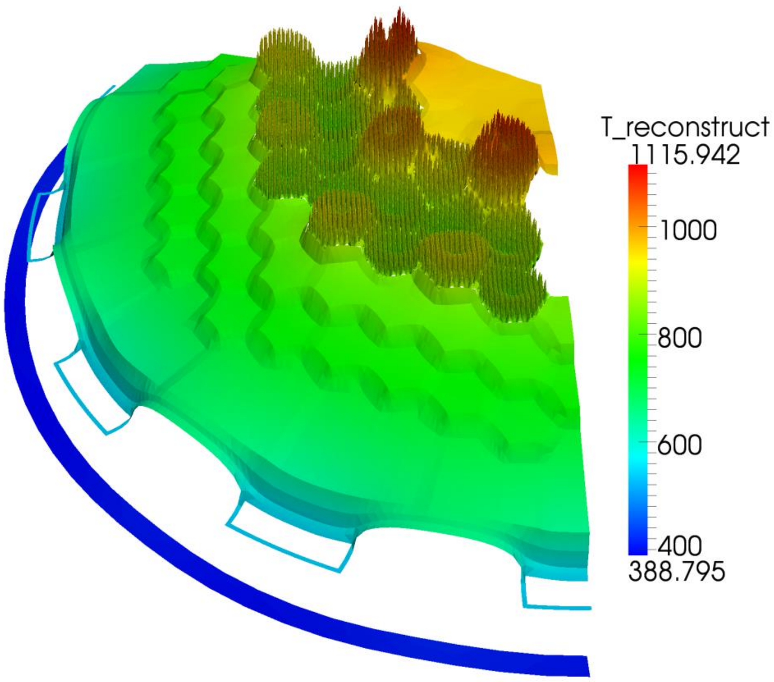
MHTGR-350MW Benchmark: Multi-scale solid temperature solution



Velocity



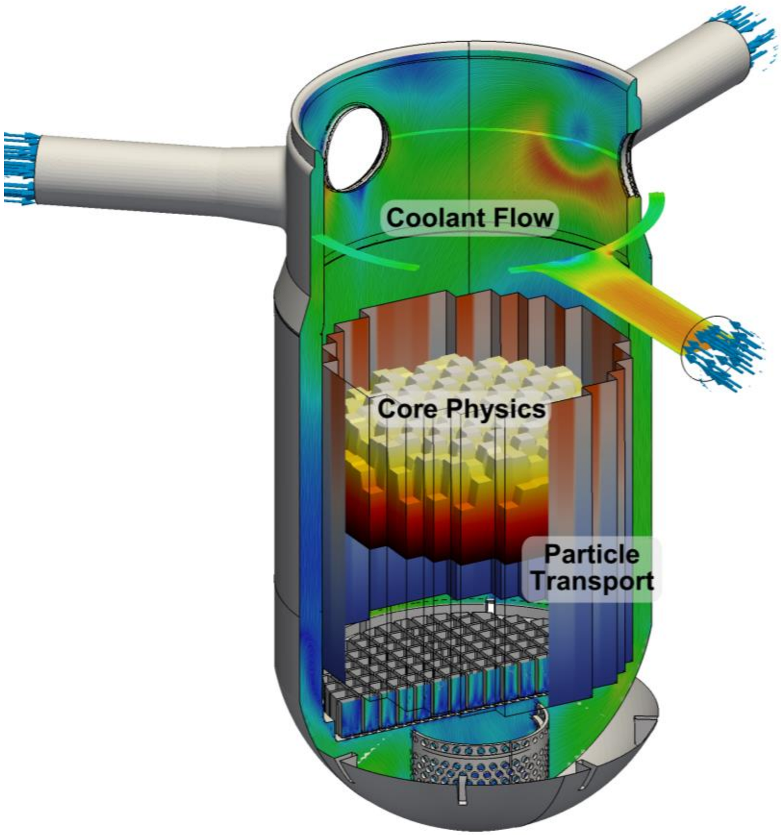
Homogeneous temperature



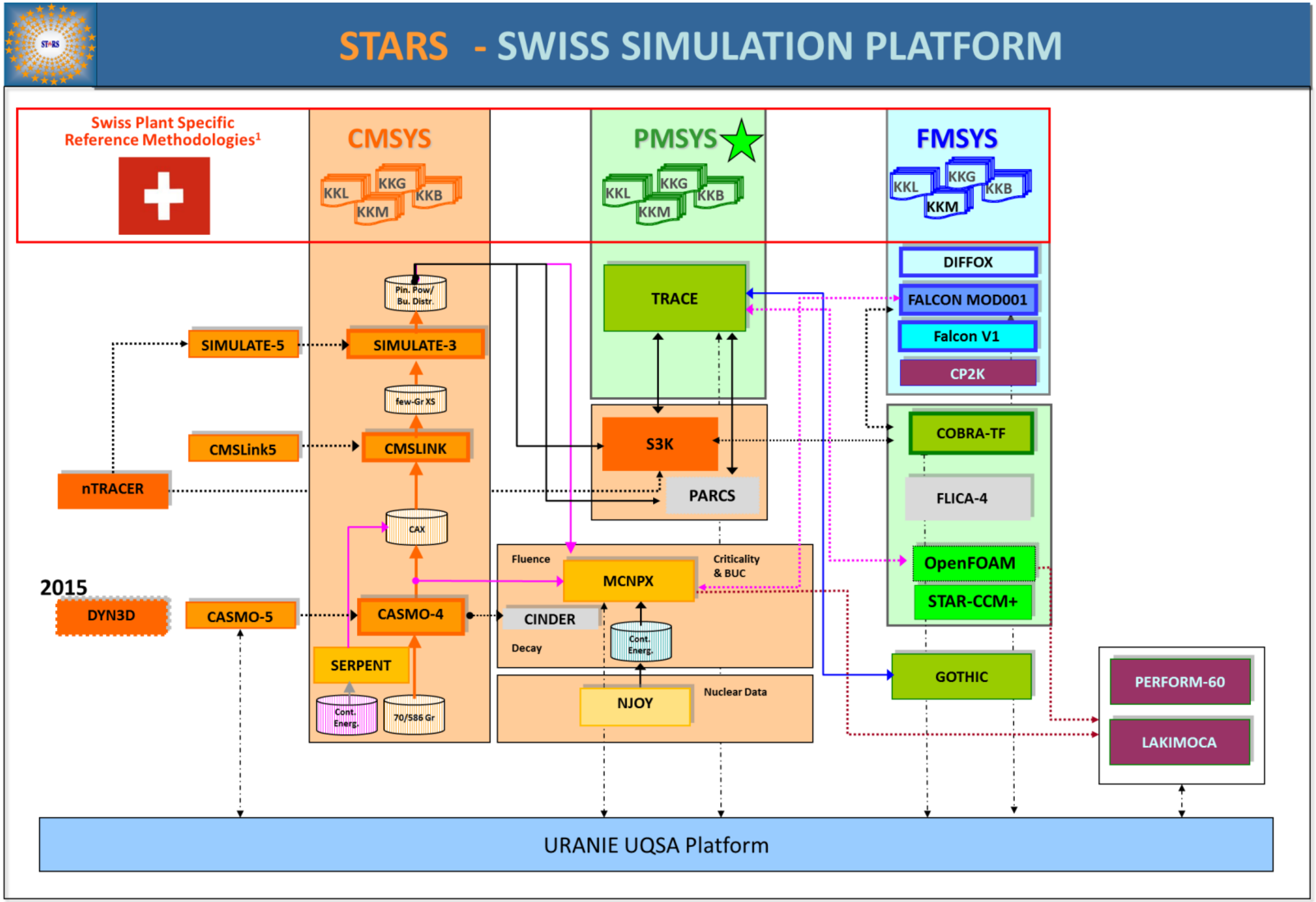
Reconstructed temperature (z=8.2m)

STARS — Light Water Reactors

- STARS project at PSI
  - Development of analysis models for the Swiss reactors
  - Continually strive to improve modeling techniques
  - Continually expanding our validation database
  - Participate in several OECD international programs
- Hi fidelity multi-physics simulations are key to better understanding many phenomena
  - Fluence, activation and ageing
  - Recriticality following LOCA
- OpenFOAM use within STARS is focused on CFD analysis
- OpenFOAM is the current preferred CFD software for coupled simulations
  - Flexibility and availability of source code
  - More implicit coupling strategies can be investigated



STARS Multi-physics and Multi-scale Analysis Framework

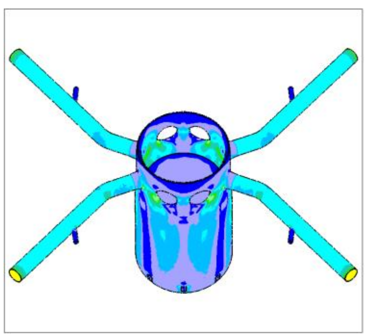


TRACE/ANSYS-CFX

CFX: "Master" Program
- ❑ Data Exchange
- ❑ Data Manipulation
- ❑ Data Conversion

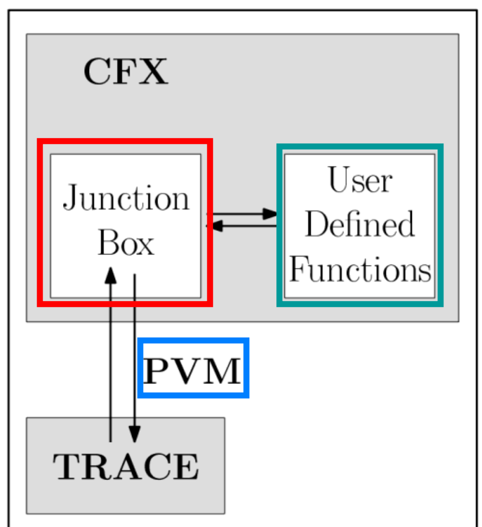
+

TRACE: "Slave" Program
- ❑ Data Exchange

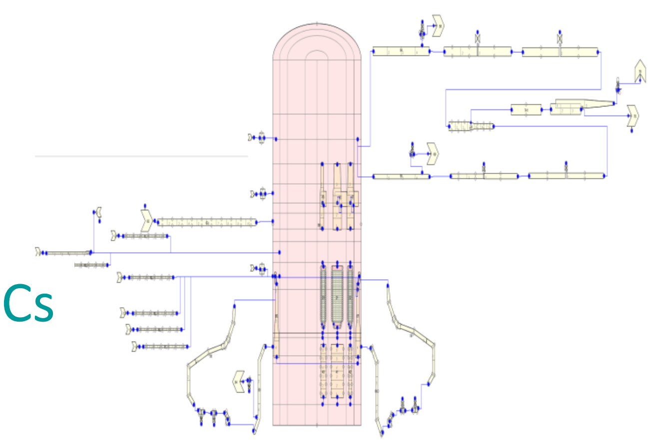


Master

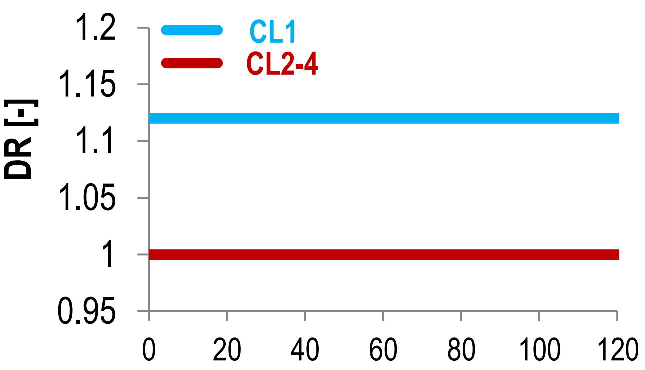
Data exchange

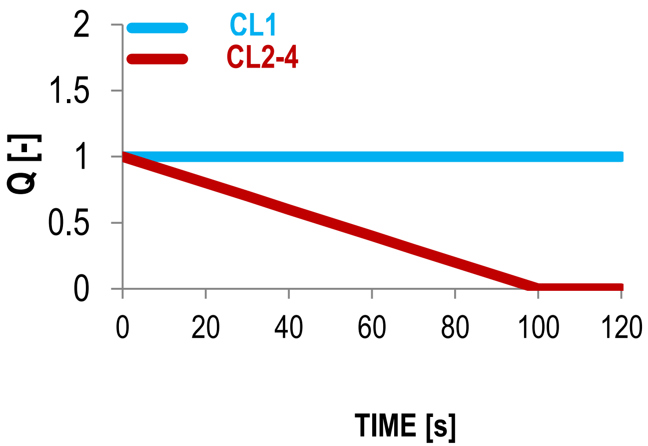


BCs



STARS CFD: Downcomer Mixing in LWRs

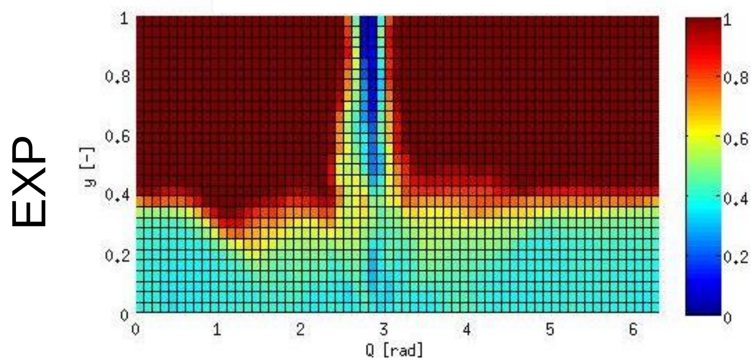


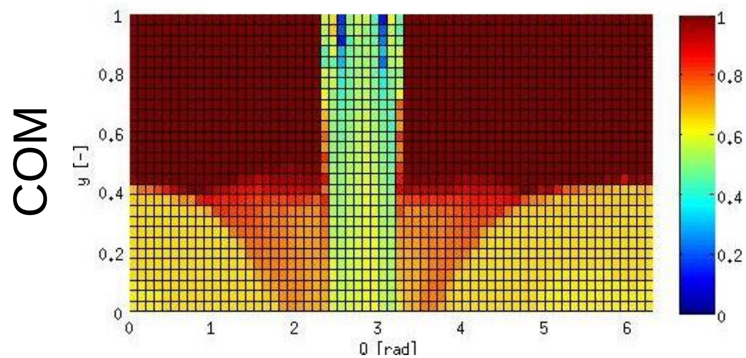


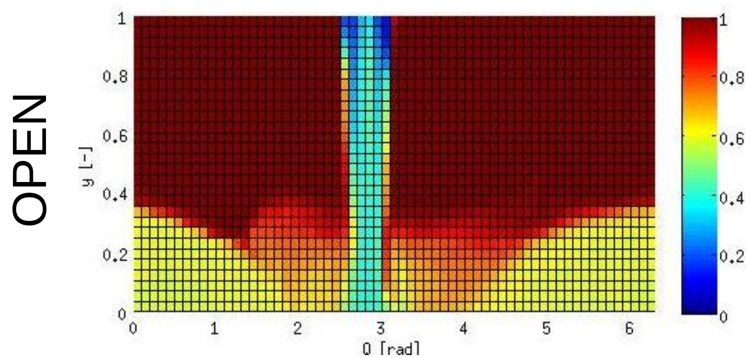
Comparison of commercial vs. open-source CFD and experimental data

- Snapshots of dimensionless temperature maps @ Downcomer sensors, t = 0.875 [-]. Width of the plume is largely over-estimated by the commercial code when standard water properties are used.

- OpenFOAM solution obtained with physical property correction and variable turbulent Prandtl model shows flow patterns and features that are more similar to the experiment.



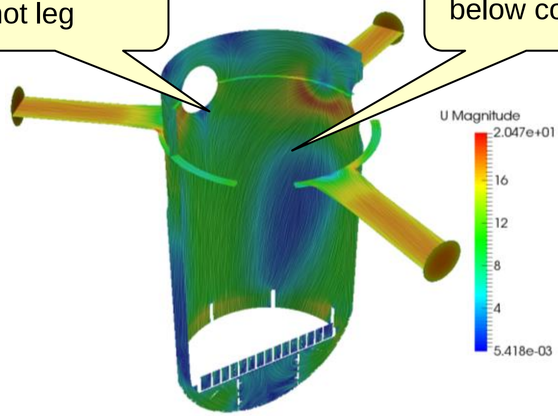




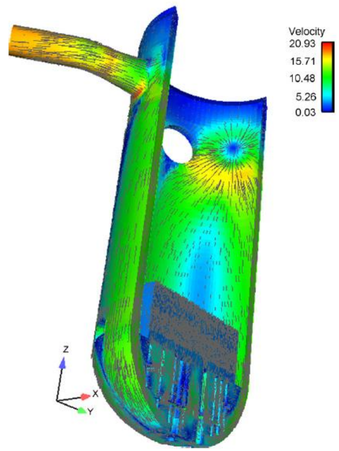
STARS CFD: PWR Reactor Operation and Flow Conditions

Flow separation from hot leg

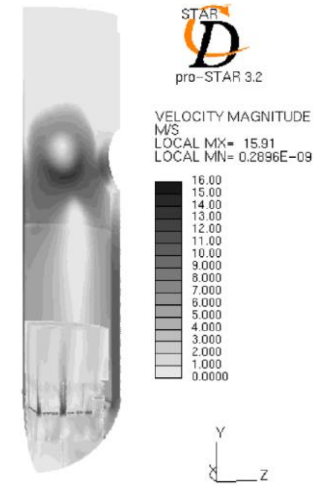
Stagnant zone below cold leg



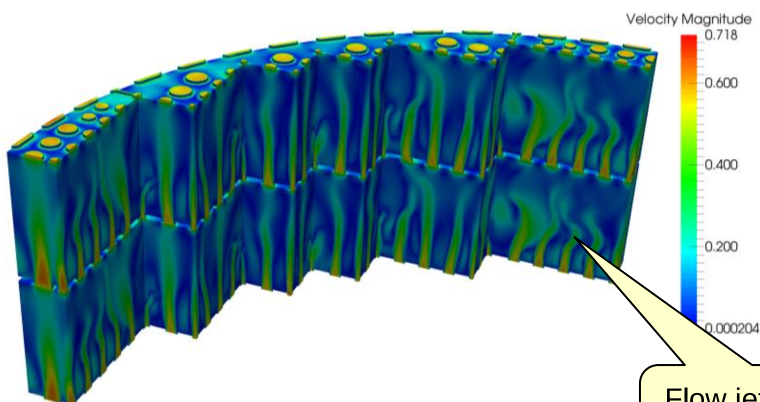
KKG Downcomer (Preliminary)



Fournier et al. (2007)

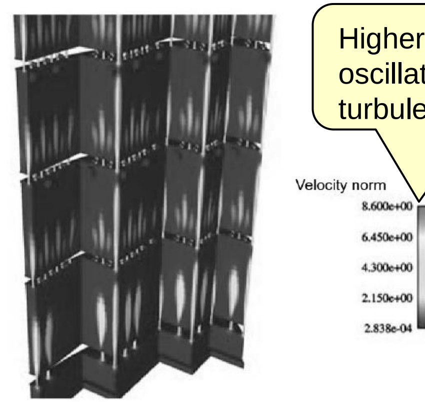


Jeong & Han (2008)



KKG Bypass (Preliminary)

Flow jets with vortex shedding



Higher velocity: oscillations damped by turbulence

Rupp et al. (2008)

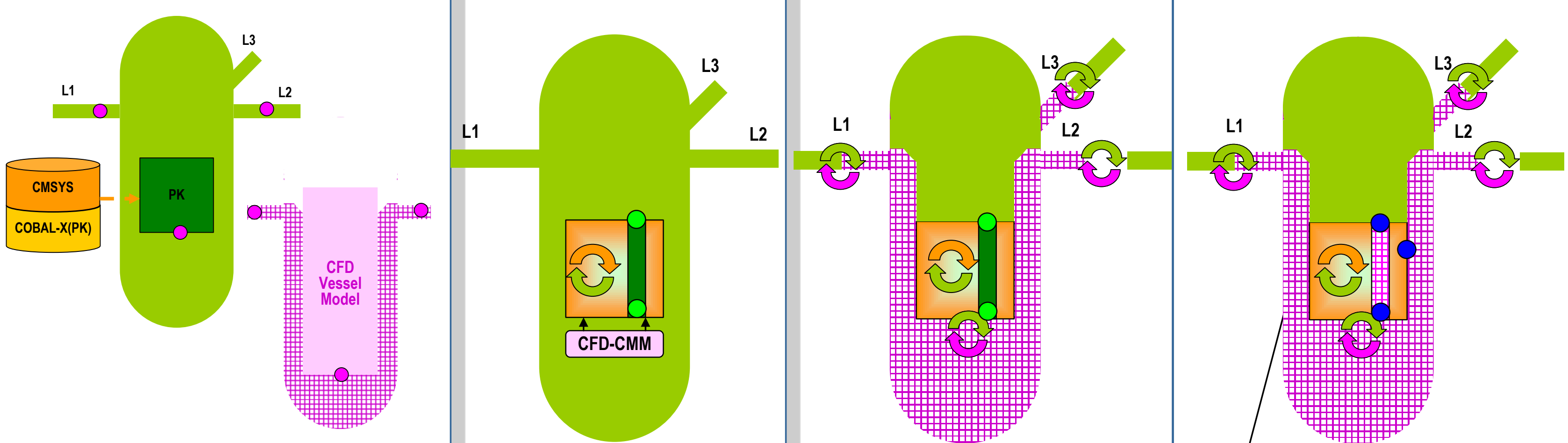
Development CFD-TRACE/S3K-COBRA-TF Coupling for KKG MSLB

STEP 1
TRACE PK for BC
CFD for Coolant Mixing Matrices (CMM)

STEP 2
TRACE/S3K + COBRA-TF
with CMM

STEP 3
TRACE/S3K + COBRA-TF
with TRACE/CFD Coupling

STEP 4
TRACE/S3K + COBRA-TF
with TRACE/CFD Coupling

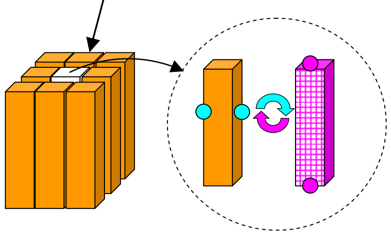


- BC Coupling TRACE→CFD
- BC Coupling TRACE/S3K→COBRA-TF
- BC Coupling TRACE/S3K→CFD
- BC Coupling S3K →Higher-Order Transport (NHO)

Dynamic Coupling: TRACE/S3K, TRACE/CFD, NHO/CFD

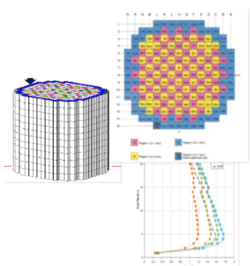
STEP 5
Zoom Analysis for Hot-Assembly (HA)
with Higher-Order Transport/CFD Coupling

Coordination with Participation to NURESAFE



STARS — RPV Fluence, Activation and Ageing

Development and Validation of **CORE** Models for the **Swiss** Reactors



Neutron Source $S(\vec{r},t)\big|_{Core}$

SN Projects

RADAR – Fluence/Activation

CF-DYNAMO - Coupling MCNP/CFD

MCNP
Neutron/Radiation Transport from core to vessel

Temperatures/Densities of Coolant/Structures

Heat Sources to Coolant/Structures

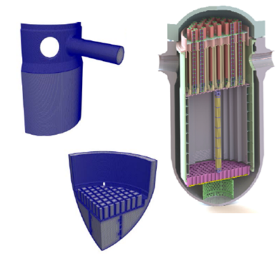
CFD
Flow/Heat Transfer in Bypass and Downcomer

$\varphi(\vec{r},E,t)\big|_{RPV}$

$T(\vec{r},t)\big|_{RPV}$

PREVENT
RPV Embrittlement

Development and Verification of **Solid CAD and CFD Models** for the **Swiss** Reactors



Other nuclear-related development efforts (that I know about)

- Politecnico di Milano (Manuele Aufiero et al.)
  - Molten salt reactors
    - Transport of delayed neutron precursors
  - Coupled CFD / Monte Carlo simulations
- FAST group at PSI (Carlo Fiorina et al.)
  - Sodium-cooled fast reactors
  - Discrete ordinates neutron transport
- GRS (Joachim Herb)
  - Coupled CFD / system code (ATHLET) simulations for LWRs
- KTH Sweden (Klas Jarateg)
  - Multigroup neutron diffusion for LWRs
  - Discrete ordinates neutron transport for LWRs
- Other: Have a look at

  http://openfoamwiki.net/index.php/SIG_Nuclear_/_Publications

Summary and Outlook

- OpenFOAM is a free software, available to all at no charge: GNU Public License
- Object-oriented approach facilitates model implementation
- Equation mimicking opens new grounds in Computational Continuum Mechanics
  - Far more than simply a set of CFD solvers and tools
  - A comprehensive multi-physics framework for solving sets of PDEs
- Extensive capabilities already implemented (mostly CFD-related); open design for easy customisation
- Nuclear-related developments are still at an early stage
  - Existing examples demonstrate that ground-breaking developments are possible
  - Development time for new solvers and physical models can be surprisingly short

PAUL SCHERRER INSTITUT