IAEA
International Atomic Energy Agency

Multi-physics modelling and simulation of nuclear reactors using OpenFOAM
Lecture 0: What to expect from this course

30 August 2022

Stephan Kelm

Course Schedule – Lecture 1

- An overview on the use of OpenFOAM as a multi-physics library for nuclear reactor analysis
  - Lecture (August 30th by Ivor Clifford, PSI and Carlo Fiorina, EPF):
    - Introduction to OpenFOAM
    - A historical perspective of OpenFOAM usage for multi-physics nuclear reactor analysis
    - Main features, workflow, structure of the library, numerical aspects and code license
    - Overview of modeling capabilities, with reference to specific activities (reactor thermal-hydraulics, containment analysis, fuel behavior, neutronics)

Weaknesses

Strengths

Structure

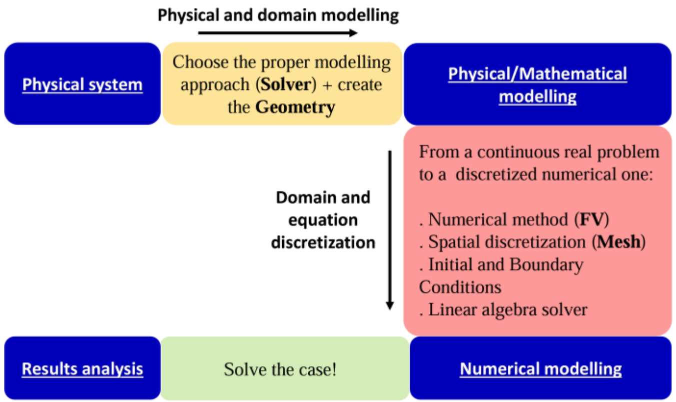
Capabilities

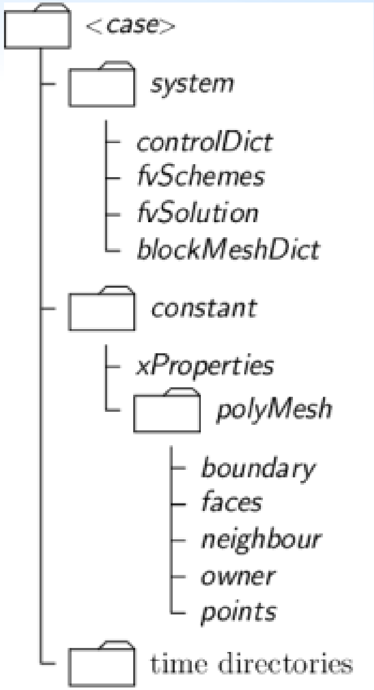
GPL 3 Free Software

Free as in Freedom

Course Schedule – Lecture 2, part A

- A practical introduction to OpenFOAM - Theory background and first steps
  - Lecture (Sept. 1th by Stefano Lorenzi, POLIMI):
    - Basic concepts about Partial Differential Equations (PDEs): from the physical system to the mathematical and numerical modeling to result analysis
    - Overview on Finite Volume discretization method and linear algebra solvers
    - First experience with OF: download, installation and case folder structure (where to find equations, parameters, boundary conditions, and initial conditions), running a case and post-process the results

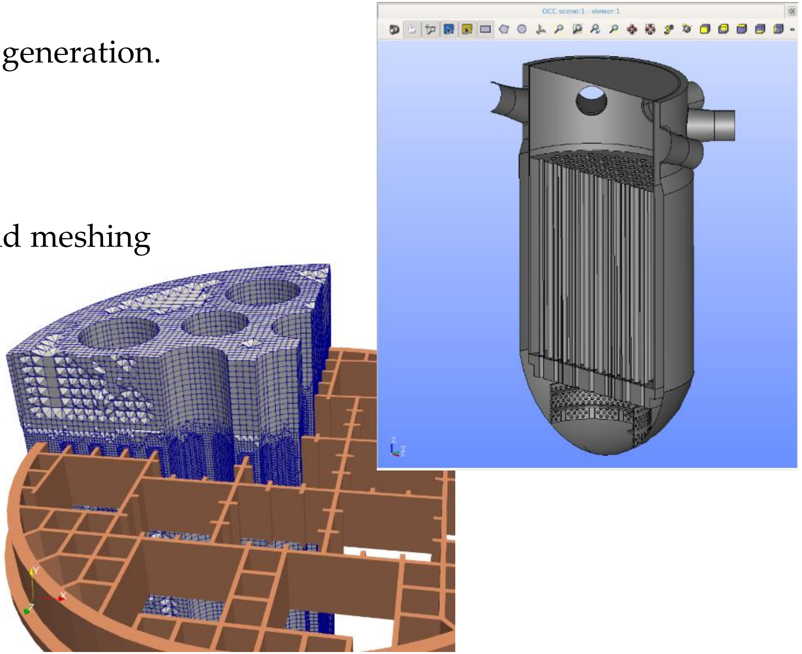




https://www.openfoam.com/documentation/userguide/img/user1x.png

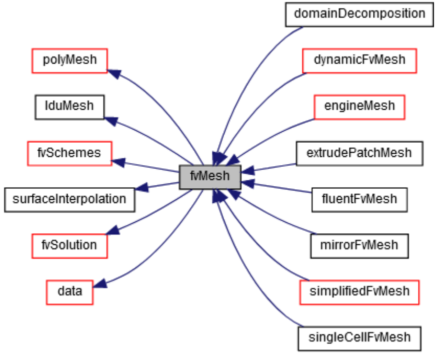
Course Schedule – Lecture 2, part B

- A practical introduction to OpenFOAM - Geometry Preparation and Meshing
  - Lecture (Sept. 6th by Ezequiel Oscar Fogliatto, PSI) :
    - Defining the computational domain
    - Finite volume meshing: What is a mesh? Mesh generation.
    - Aspects of mesh resolution and quality.
    - Grouping regions into zones
    - Dealing with multiple meshes
    - Open-source tools for geometry preparation and meshing



Course Schedule – Lecture 2, part C

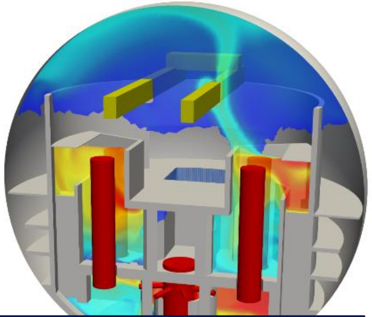
- A practical introduction to OpenFOAM – Source Code
  - Lecture (Sept. 8th by Ivor Clifford, PSI):
    - Structure of the OpenFOAM library
    - The basic classes of OpenFOAM (space and time, fields and solution variables, boundary conditions, sparse matrices, linear solvers, finite-volume discretization)
    - Structure of a typical solver
    - Beyond the basic classes (input/output, field and boundary mapping, moving meshes, dense matrices, ODE solvers, coupled boundaries, parallelization)




```
while (runTime.loop())
{
    Info<< "Time = " << runTime.timeName() << nl << endl;

    #include "CourantNo.H"

    // Momentum predictor

    fvVectorMatrix UEqn
    (
        fvm::ddt(U)
      + fvm::div(phi, U)
      - fvm::laplacian(nu, U)
    );

    if (piso.momentumPredictor())
    {
        solve(UEqn == -fvc::grad(p));
    }

    // --- PISO loop
    while (piso.correct())
    {
        volScalarField rAU(1.0/UEqn.A());
        volVectorField HbyA(constrainHbyA(rAU*UEqn.H(), U, p));
        surfaceScalarField phiHbyA
        (
            "phiHbyA",
            fvc::flux(HbyA)
          + fvc::interpolate(rAU)*fvc::ddtCorr(U, phi)
        );

        adjustPhi(phiHbyA, U, p);

        // Update the pressure BCs to ensure flux consistency
        constrainPressure(p, U, phiHbyA, rAU);

        // Non-orthogonal pressure corrector loop
        while (piso.correctNonOrthogonal())
        {
            // Pressure corrector

            fvScalarMatrix pEqn
            (
                fvm::laplacian(rAU, p) == fvc::div(phiHbyA)
            );
```

Course Schedule – Lecture 3

- Introduction to containment∇FOAM a tailored package for system scale CFD analysis of containment atmosphere pressurization, H_2/CO mixing and mitigation.
  - Theory (Sept. 13th by Stephan Kelm, FZJ):
    - Review of the containment phenomenology
    - Discussion of the baseline model strategy, theoretical background and implementation of the available models. (Condensation, thermal radiation, buoyancy turbulence etc.)
    - Outlook on Work-in-Progress: aerosol modeling, applications
  - Hands-on (Sept. 15th by Stephan Kelm, FZJ):
    - Modeling the International Standard Problem No°47 TOSQAN experiment (📖 J. Malet et al.: OECD International Standard Problem ISP-47 on containment thermal-hydraulics—Conclusions of the TOSQAN part, NED (240), 10, 2010 https://doi.org/10.1016/j.nucengdes.2010.05.061)
    - Using the Java based *cfGUI* – Templated Case Setup
    - Using the Java based *cfSolutionMonitor* for live analysis of the simulation progress
    - Basic validation and analysis of mass balance with Python3

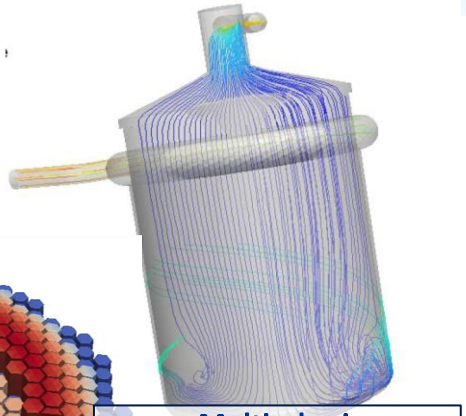


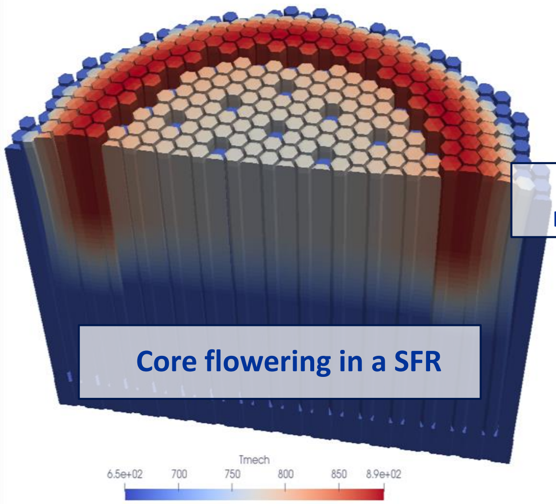
steam distribution inside the containment

Monitoring the solution progress

Course Schedule – Lecture 4

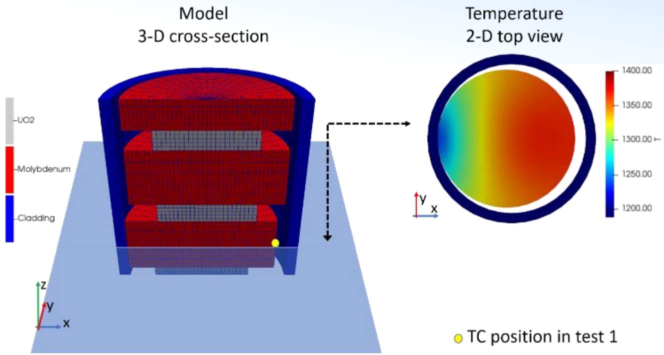
- Introduction to GeN-Foam: a multi-physics solver for the design and safety analysis of nuclear reactors, with a focus on advanced reactor concepts
  - Theory (Sept. 20th by Carlo Fiorina, EPFL):
    - Description of the various models available in GeN-Foam
    - Some details about their specific implementation using OpenFOAM
    - Description of the coupling strategy
  - Practice (Sept. 22th by Carlo Fiorina, EPFL):
    - Learning best practices and available resources
    - Setting up a model, running and post-processing
    - Basics of code tailoring



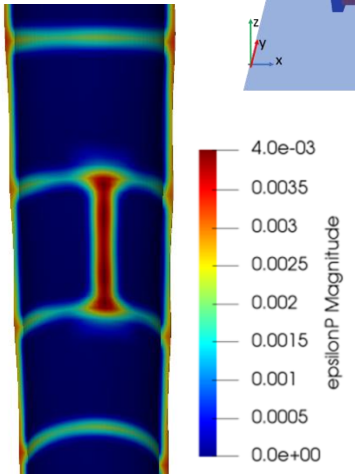


Course Schedule – Lecture 5

- Introduction to OFFBEAT: a finite-volume fuel performance solver for the multi-dimensional analysis of the nuclear fuel
  - Theory (Sept. 27th by Alessandro Scolaro, EPFL):
    - Review of fuel behavior and fuel modeling
    - Current status of OFFBEAT and description of the modeling strategy
    - Example of past applications and of current work-in-progress
  - Practice (Sept. 29th by Alessandro Scolaro, EPFL):
    - Learning about available resources (repository, documentation, tutorials etc.)
    - Overview of case folder structure and work-flow (mesh creation, boundary conditions etc.)
    - Analysis of a realistic 2-D fuel rod with basics of post-processing



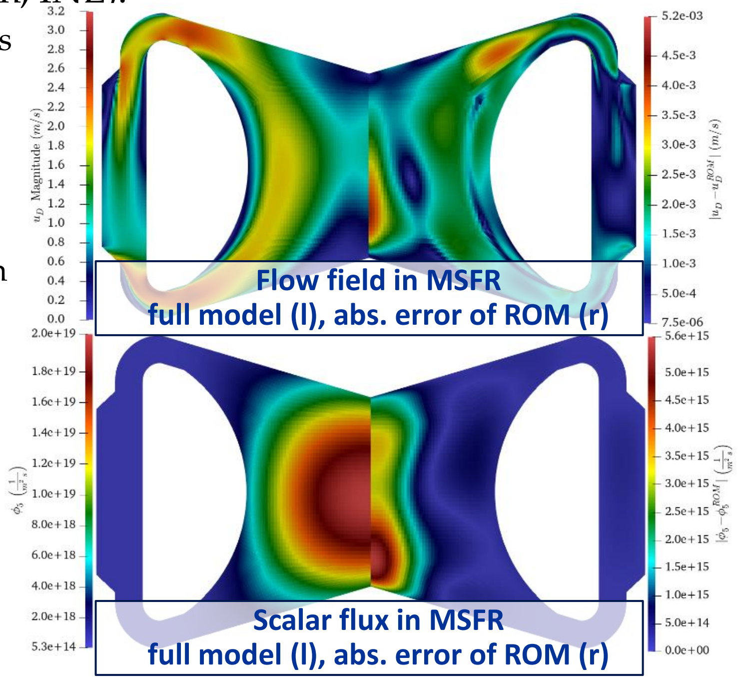
Eccentric fuel disc and asymmetric temperature distribution



Cumulative plastic strain in front of MPS

Course Schedule – Lecture 6

- Introduction to GeN-ROM: an OpenFOAM®-based Reduced-Order Modeling (ROM) framework for the simulation of nuclear reactors (mainly MSRs)
  - Theory (Oct. 4th by Jean Ragusa, TAMU and Peter German, INL):
    - Overview of projection-based ROMs for parametric problems
    - Overview of subspace-discovery for linear and nonlinear problems [1]
    - Brief introduction to GeN-ROM
  - Practice (Oct. 6th by Peter German, INL):
    - Hands-on exercise: creating a ROM for a multigroup neutron diffusion k-eigenvalue problem (quasi-linear problem)
    - Hands-on exercise: creating a ROM for a coupled neutronics and fluid dynamics problem in a Molten Salt Reactor (nonlinear problem)



Flow field in MSFR
full model (l), abs. error of ROM (r)

Scalar flux in MSFR
full model (l), abs. error of ROM (r)

[1] Chaturantabut, Saifon, and Danny C. Sorensen. "Nonlinear model reduction via discrete empirical interpolation." *SIAM Journal on Scientific Computing* 32.5 (2010): 2737-2764.

Q&A

- https://foam-for-nuclear.org/phpBB/

phpBB forum software

foam-for-nuclear

A forum to support the use of OpenFOAM for nuclear applications

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It is currently Tue Jul 05, 2022 8:33 am

FORUM	TOPICS	POSTS	LAST POST
Source code / programming / API	0	0	No posts
Pre-processing and meshing in OpenFOAM (non application-specific)	0	0	No posts
Post-processing in OpenFOAM (non application-specific)	0	0	No posts
Miscellanea	0	0	No posts
GeN-Foam Subforums: Compiling, Pre-processing, Running, Post-processing, Documentation, Source code	2	4	**Re: Reactivity insertion** by CarloF Sat Feb 12, 2022 8:54 pm
OFFBEAT Subforums: Compiling, Pre-processing, Running, Post-processing, Documentation, Source code	2	4	**Re: Radial power profile** by AlessandroS Sun Jan 23, 2022 6:26 pm
containmentFOAM Subforums: Compiling, Pre-processing / cfGUI, Running / cfSolutionMonitor, Post-processing, Models and Documentation, Source code	1	1	**Getting containmentFOAM** by stephankelm Thu Mar 24, 2022 2:31 pm

Prerequisites

- The following software installation is needed:
  - Installation of OpenFOAM
    - Introduction to OpenFOAM → any version (www.openfoam.com or www.openfoam.org)
    - containmentFOAM → OpenFOAM-v9 (https://openfoam.org/download/9-linux)
    - GeN-FOAM → OpenFOAM 2206 (https://www.openfoam.com/news/main-news/openfoam-v2206)
    - OFFBEAT → OpenFOAM-v9 (https://openfoam.org/download/9-linux)
    - GeN-ROM → OpenFOAM 2206 (https://www.openfoam.com/)
  - Installation of Python3, incl. Pandas, Numpy, OS
  - Installation of the packages:
    - https://go.fzj.de/containmentFOAM
    - https://gitlab.com/foam-for-nuclear/GeN-Foam
    - https://gitlab.com/foam-for-nuclear/OFFBEAT
    - https://gitlab.com/peter.german/gen-rom
- Direct installation on a Linux Operating System (preferably Ubuntu) is strongly reccomended

Prerequisites

- To follow the lectures, the participants should have fundamental knowledge of
  - Computational fluid & solid mechanics
  - Thermodynamics
  - Reactor physics and technologies
  - Numerical mathematics

- and first practical experience with
  - Linux / bash
  - Computer Aided Design
  - OpenFOAM
  - paraview
  - Programming: Python, git, ideally C++

Recommended Reading (1)

- Overview:
  - C. Fiorina, I. Clifford, S. Kelm, S. Lorenzi: On the development of multi-physics tools for nuclear reactor analysis based on OpenFOAM®: state of the art, lessons learned and perspectives, Nuclear Engineering and Design 387 (2022) 111604, https://doi.org/10.1016/j.nucengdes.2021.111604

- Introduction to OpenFOAM:
  - OpenFOAM tutorials - 3 weeks series, https://wiki.openfoam.com/%223_weeks%22_series
  - J. Guerero: Introduction to OpenFOAM, training materials, http://www.wolfdynamics.com/tutorials.html
  - H. Jasak: OpenFOAM: Introduction and Basic Class Layout, OpenFOAM in Industrial Combustion Simulations, Pohang University Feb, 2015
  - H. Jasak, H. Rusche: Five Basic Classes in OpenFOAM, OpenFOAM Workshop 2010, Gothenborg, Sweden http://www.personal.psu.edu/dab143/OFW6/Training/jasak2_slides.pdf
  - F. Moukalled, L. Mangani, M. Darwish: The Finite Volume Method in Computational Fluid Dynamics, Springer, 2016 https://link.springer.com/book/10.1007/978-3-319-16874-6
  - https://github.com/UnnamedMoose/BasicOpenFOAMProgrammingTutorials

Recommended Reading (2)

- containmentFOAM:
  - S. Kelm, et al.: The Tailored CFD Package 'containmentFOAM' for Analysis of Containment Atmosphere Mixing, H_2/CO Mitigation and Aerosol Transport, Fluids 2021, 6(3), 100 https://doi.org/10.3390/fluids6030100
  - X. Liu et al.: Monte Carlo method with SNBCK nongray gas model for thermal radiation in containment flows, Nuclear Engineering and Design (390), 111689, 2022 https://doi.org/10.1016/j.nucengdes.2022.111689
- GeN-FOAM:
  - C. Fiorina et al.: GeN-Foam: A novel OpenFOAM® based multi-physics solver for 2D/3D transient analysis of nuclear reactors, Nuclear Engineering and Design (294),24-37, https://doi.org/10.1016/j.nucengdes.2015.05.035
  - S. Radman et al.: Development of a point-kinetics model in OpenFOAM, integration in GeN-Foam, and validation against FFTF experimental data, Annals of Nuclear Energy (168), 108891, 2022, https://doi.org/10.1016/j.anucene.2021.108891

Recommended Reading (3)

- OFFBEAT:
  - A. Scolaro et al.: The OFFBEAT multi-dimensional fuel behavior solver, Nuclear Engineering and Design (358), 110416, 2020, https://doi.org/10.1016/j.nucengdes.2019.110416
- GeN-ROM:
  - P. German et al.: GeN-ROM—An OpenFOAM®-based multiphysics reduced-order modeling framework for the analysis of Molten Salt Reactors, Progress in Nuclear Energy (146), 104148, 2022, https://doi.org/10.1016/j.pnucene.2022.104148

Outlook

- What to expect and what not:
  - Specific introduction to multi-physics modelling and simulation of nuclear reactors using OpenFOAM, but no basic / generic training on OpenFOAM
  - Starting point for the use of the tailored packages in R&D or E&T projects. To become an ‚application-ready' user or even developer, further continuous training, learning and comprehensive V&V is required
  - Personal experiences, perspectives and opinions of productive OpenFOAM users and developers but by no means claiming completeness and general validity

- Disclaimer:
  "This offering is not approved or endorsed by the OpenFOAM Foundation or OpenCFD Limited, the producer of the OpenFOAM software and owner of the OPENFOAM® and OpenCFD® trade marks."

Thank you!

Contact: ONCORE@iaea.org

Course Enrollment : Multi-physics modelling and simulation of nuclear reactors using OpenFOAM

ONCORE: Open-source Nuclear Codes for Reactor Analysis