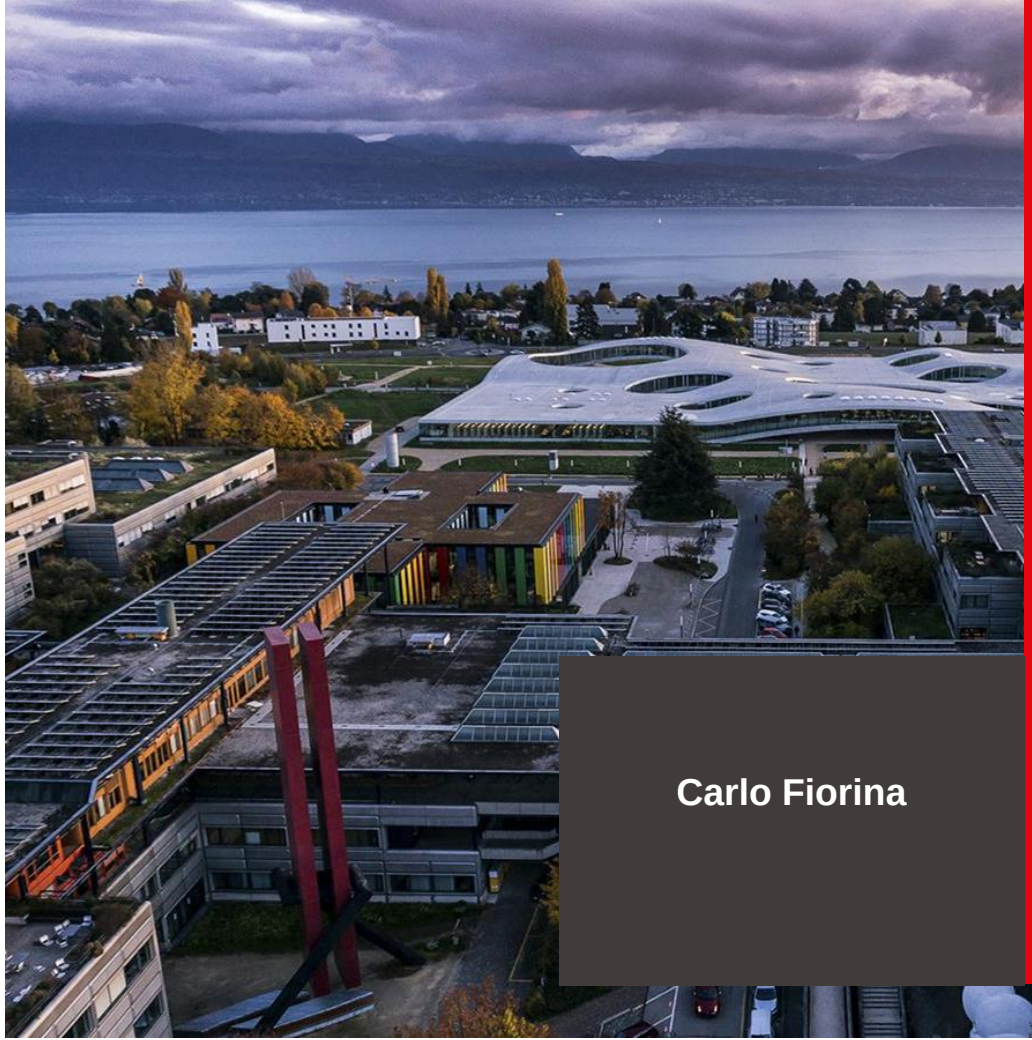


Approaching the “nuclear” solvers

Carlo Fiorina

École
polytechnique
fédérale
de Lausanne

Background: Some essential features of OpenFOAM

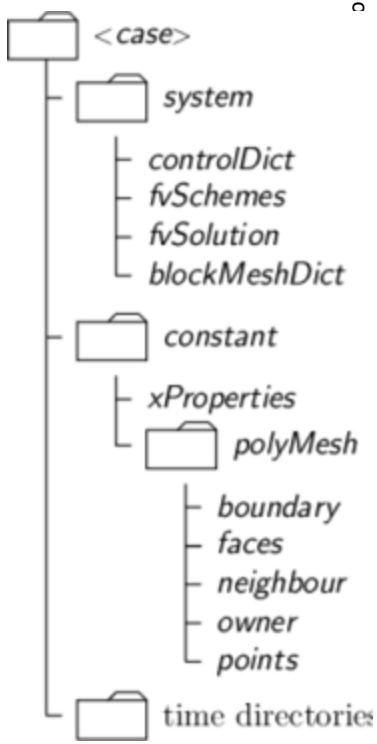
- Workflow divided in 4 distinct steps
  - Mesh creation
  - Input data and mesh are gathered inside a Case Folder
  - Running
  - Post-processing

Background: Some essential features of OpenFOAM - Mesh creation

- Don’t take it lightly:
  - one of the most time consuming steps
  - requires good understanding of methods to decide the type of mesh and its refinement
  - a bad mesh will give a bad solution (especially for CFD)
  - in some unlucky cases, a bad mesh will give a non-convergent solution
- Several available free tools: blockMesh (embedded in OpenFOAM), Salome, gmsh, cfMesh, snappyHexMesh…
- Complex geometries and situations where high-quality mesh are needed may require the use of commercial software
- Make sure that the tool you chose allows you to separate your mesh into zones (called cellZones in OpenFOAM). They are necessary to assign different physical properties to different materials!

Background: Some essential features of OpenFOAM - Input data

- All data (inlc. mesh) that OpenFOAM needs are collected into a Case Folder
- Inside a case folder you'll find at least 3 sub-folders
  - The folder "0", and possible other time directories, containing, for each field (viz., velocity, pressure, density):
    - Initial conditions
    - Boundary condition
  - The folder "constant" containing:
    - the mesh
    - all physical properties, gathered into "dictionaries"
    - the types of models (for instance k-epsilon or k-omega for turbulence), alse gathered into "dictionaries"
  - The folder "system" containing at least:
    - "controlDict" gathers main simulation parameters like initial time, time steps, final time, etc.
    - "fvSchemes" to set the type of discretization for various equations
    - "fvSolution" to set the parameters of the linear solvers

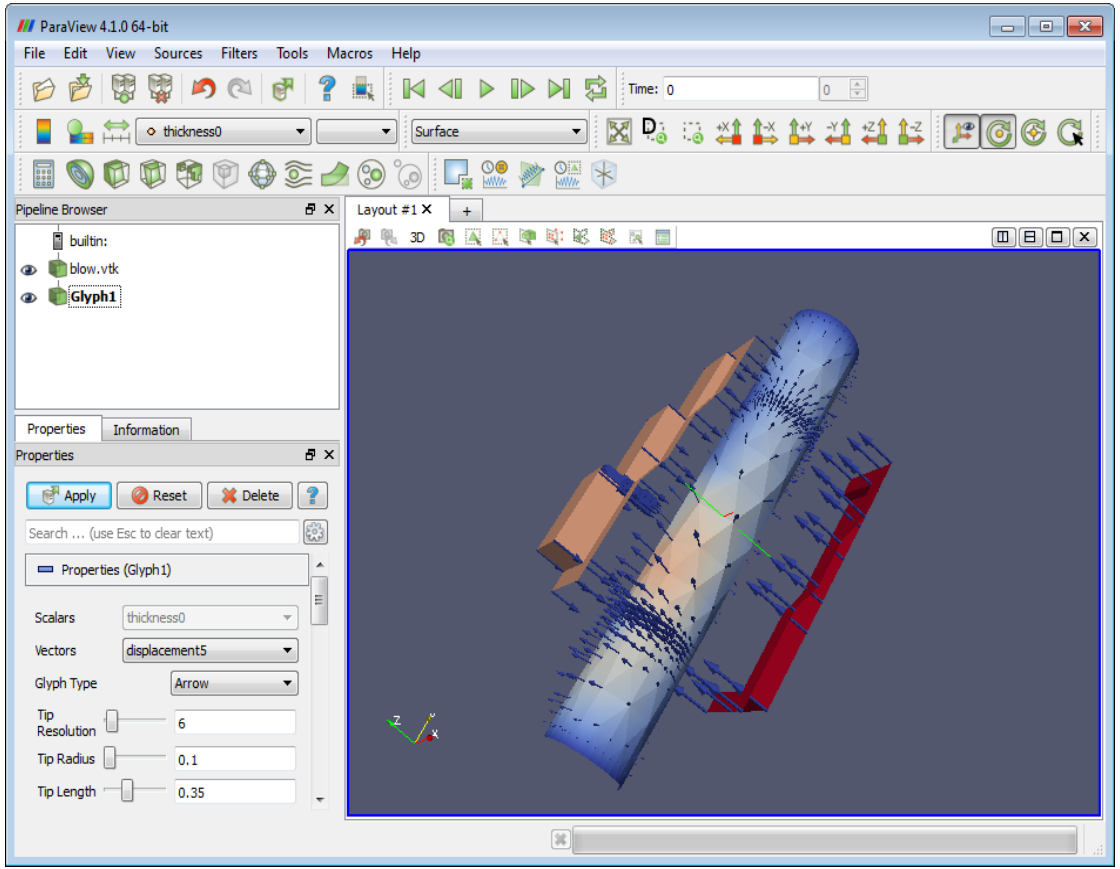


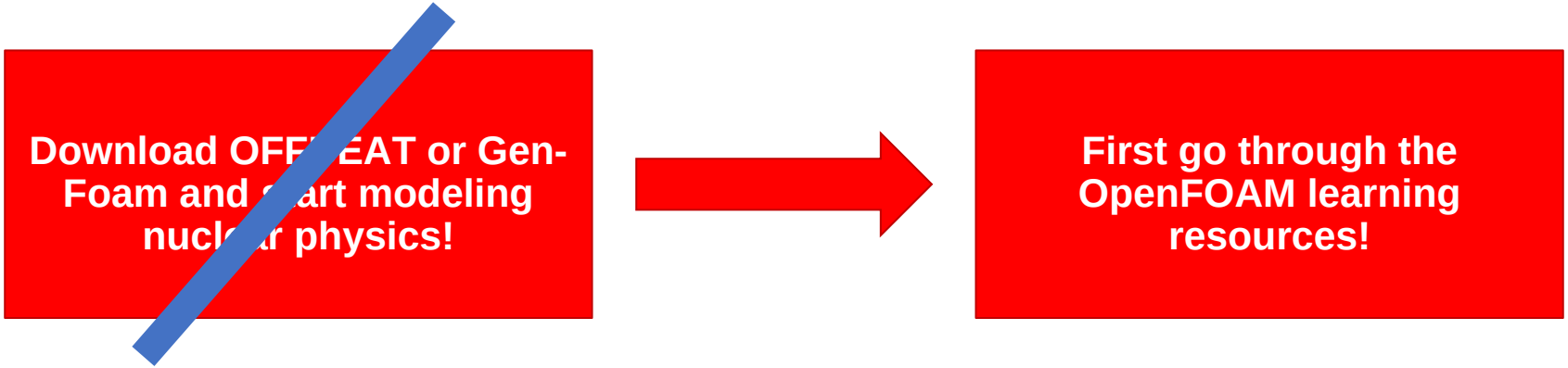
Background: Some essential features of OpenFOAM - Running

- Via command line:
  - “name of the solver”, such as: icoFoam, pimpleFoam or… GeN-Foam
- If parallel
  - decomposePar
  - mpirun -np “number of mpi processes” “name of the solver” -parallel
  - reconstructPar

Background: Some essential features of OpenFOAM - Post-processing

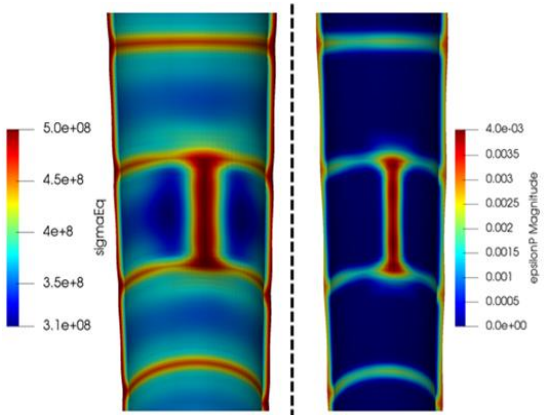
- Typically with paraview
- OpenFOAM also has some mechanisms to directly output, during or after simulation, specific quantities of interest




Download OFFBEAT or Gen-Foam and start modeling nuclear physics!
First go through the OpenFOAM learning resources!

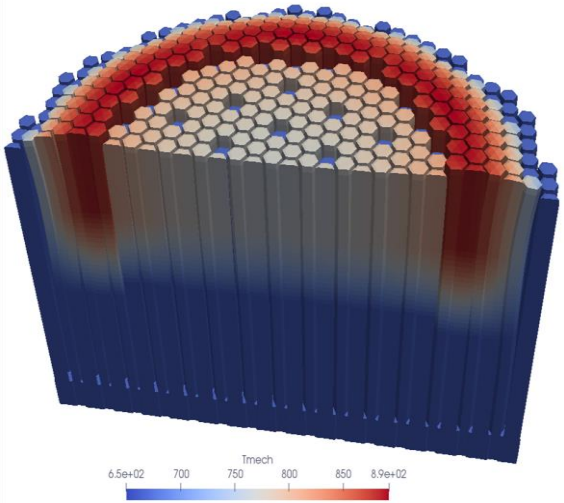
Use of OpenFOAM for nuclear multi-physics

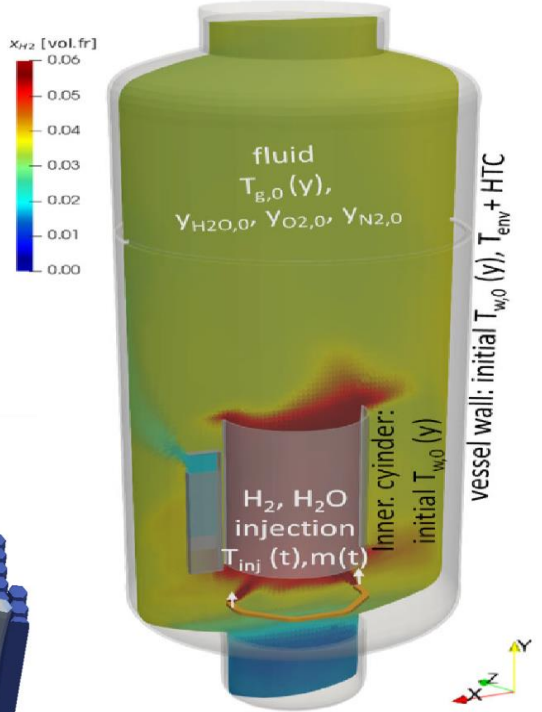
- Similar logic as other OpenFOAM solvers but
  - More complex
  - Typically multi-physics
  - Often multi-material
  - Some-times multi-mesh



OFFBEAT

GeN-Foam





containmentFoam

Carlo Fiorina

Use of OpenFOAM for nuclear multi-physics

Carlo Fiorina

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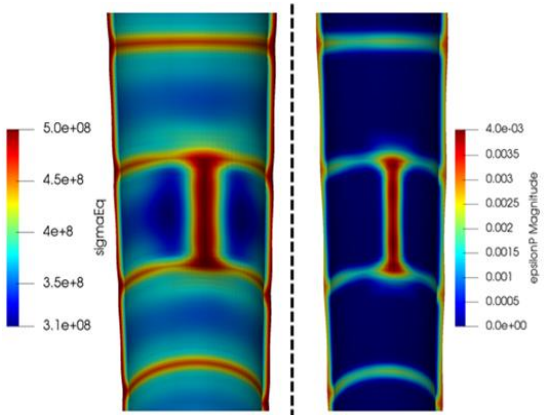
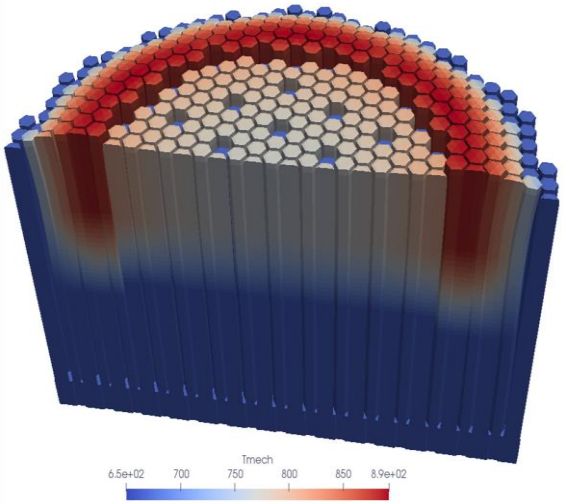
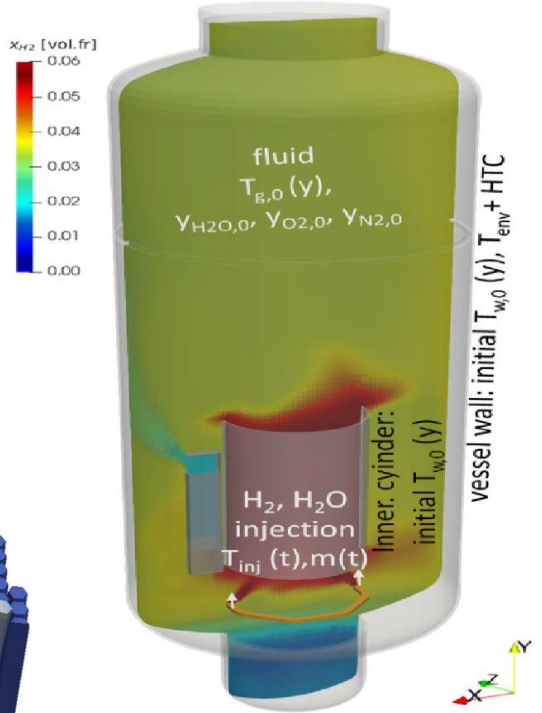
  - Typically multi-physics
  - **Often multi-material**
  - **Some-times multi-mesh**



OFFBEAT

GeN-Foam

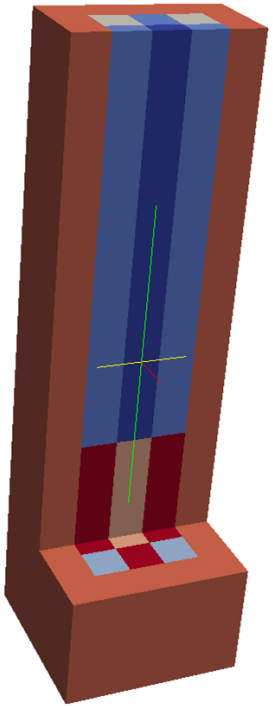




containmentFoam

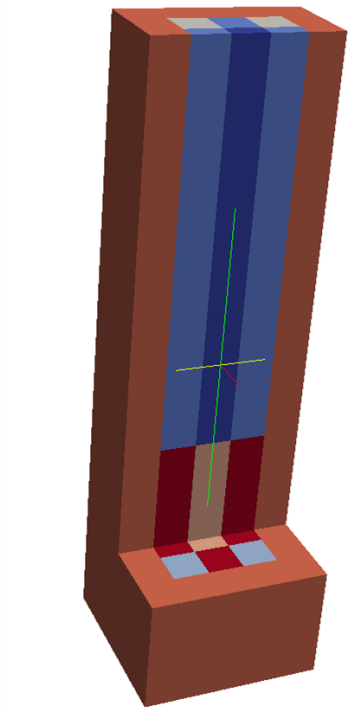
Multi-material in OpenFOAM

Carlo Fiorina



- Problem: one mesh, multiple material
- Solutions: cellZones
  - associate a label to each cell in polymesh/cellZones

```
FoamFile
{
    version     2.0;
    format      ascii;
    class       regIOobject;
    location    "constant/fluid/polyMesh";
    object      cellZones;
}
// * * * * * * * * * * * * * * * * * * * * * * * *

7
(
controlRod
{
    type cellZone;
cellLabels      List<label>
5994
(
0
1
2
```



- Then, for each physics, an input file (dictionary) is used that associates each of these labels with a set of properties. For instance in /constant/neutroRegion/nuclearData

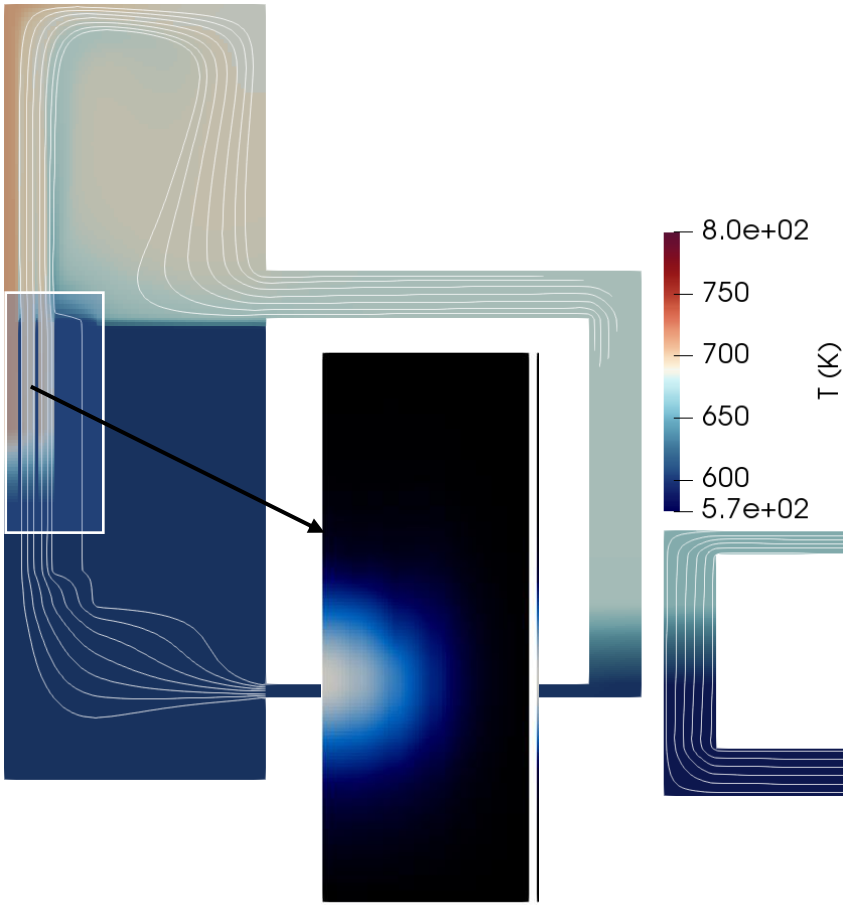
```
zones
 (

controlRod
{
 fuelFraction 1.000000e+00 ;
 IV nonuniform List<scalar> 1 (8.477550e-07  );
 D nonuniform List<scalar> 1 (1.562700e-02  );
 nuSigmaEff nonuniform List<scalar> 1 (0.000000e+00  );
 sigmaPow nonuniform List<scalar> 1 (0.000000e+00  );
 scatteringMatrix  1  1 (
 ( 2.509070e+01 )
 );
```

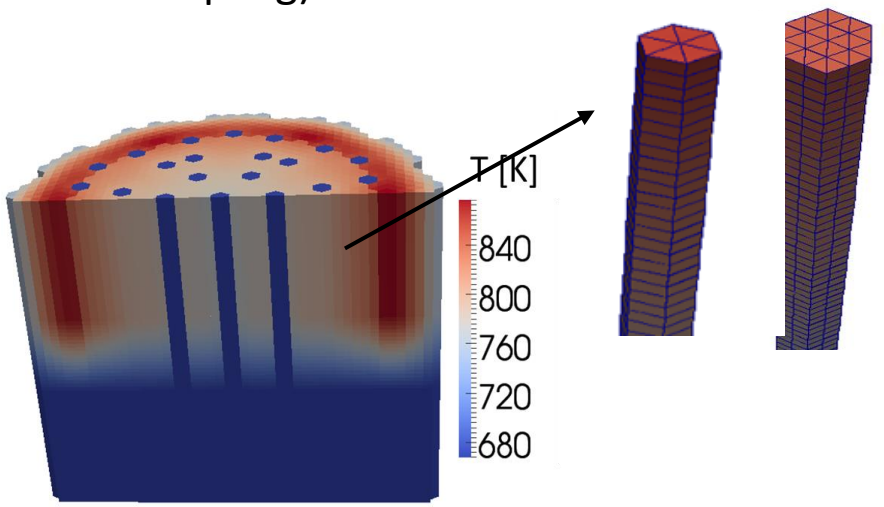
- **How to create a multi-zone mesh:**
  - All mesh generators allows for the option to generate “cellZones”
  - NB: cellZones are called in different ways (physical volumes in gmsh, groups in Salome, etc)
  - The mesh conversion tool (e.g., gmshToFoam) takes care of converting the format
- **Case folder:**
  - Polymesh folder including cellZones
  - Dictionaries that associates a cellZone to some value of a field or property

Multi-mesh in OpenFOAM

Carlo Fiorina

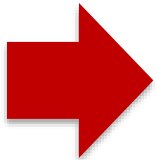
- Problem: different meshes for different “physics”
- Solution: multi-mesh (called multi-region in OpenFOAM)
- One mesh for each “physics”
- (Projection of fields from one mesh to the other for coupling)





Multi-mesh in OpenFOAM

- Case
  - 0
    - U
    - T
    - ...
  - constant
    - turbulenceProperties
    - ...
  - system
    - fvSolution
    - fvSchemes
    - controDict



- Case
  - 0
    - neutroRegion
      - Flux
      - ...
    - fluidRegion
      - U
      - ...
    - thermoMechanicalRegion
      - ...
  - constant
    - neutroRegion
    - fluidRegion
    - thermoMechanicalRegion
    - ...
  - system
    - neutroRegion
    - fluidRegion
    - thermoMechanicalRegion
    - ...

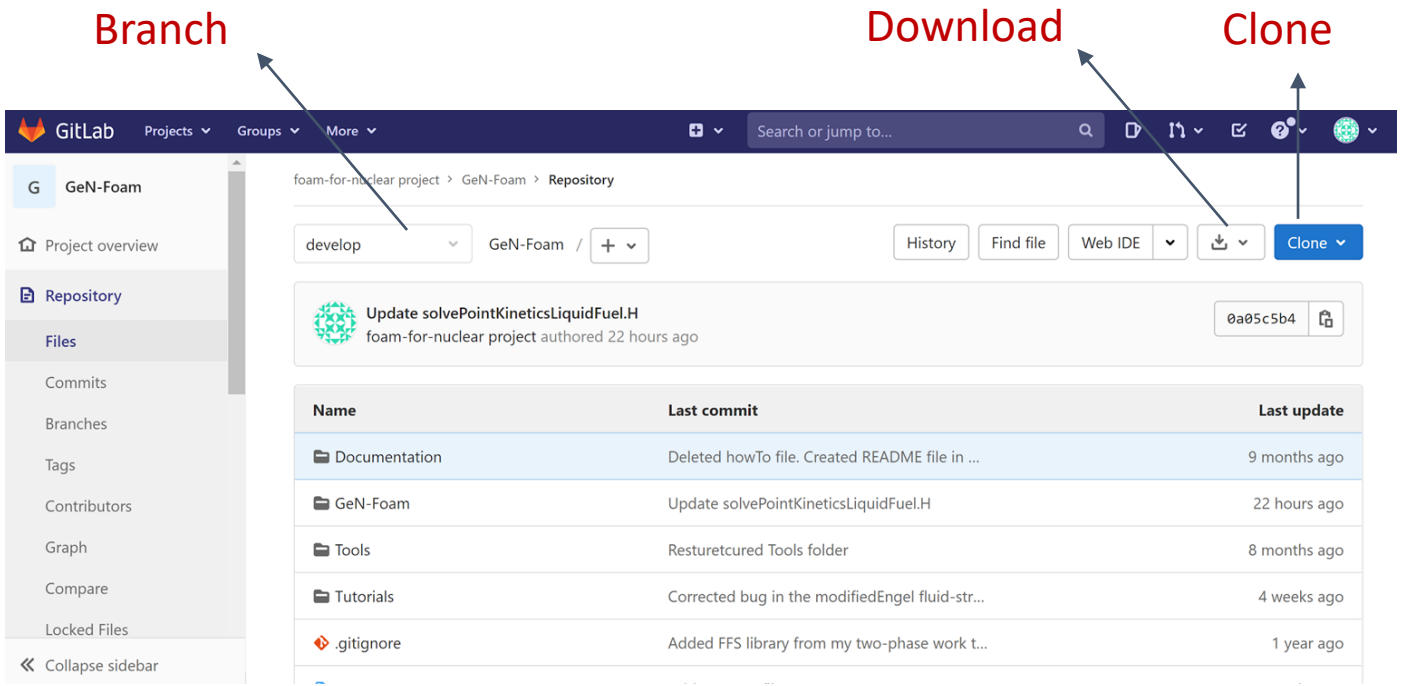
- Mesh-to-mesh projection to project from one mesh to the other

Carlo Fiorina

GeN-Foam: how to get it

- **Free, online at** https://gitlab.com/foam-for-nuclear/GeN-Foam/-/tree/develop
  - "Develop" branch or "Master" branch
  - Either
    - git clone https://gitlab.com/foam-for-nuclear/GeN-Foam.git"
    - or, simply download

GeN-Foam: how to get it



How to install it?

- Download OpenFOAM at
  - https://www.openfoam.com/download/
  - (Typically the latest release, but it may take us some few weeks to update to a new release each time)
- Install OpenFOAM and prepare the environment
  - https://www.openfoam.com/download/installation.php
- Download GeN-Foam
- Enter the GeN-Foam/GeN-Foam folder and run:
  - *Allwclean*
  - *Allwmake* (or *Allwmake -j*, to compile in parallel)
- Testing - enter any tutorial and run:
  - *Allrun*

What's inside

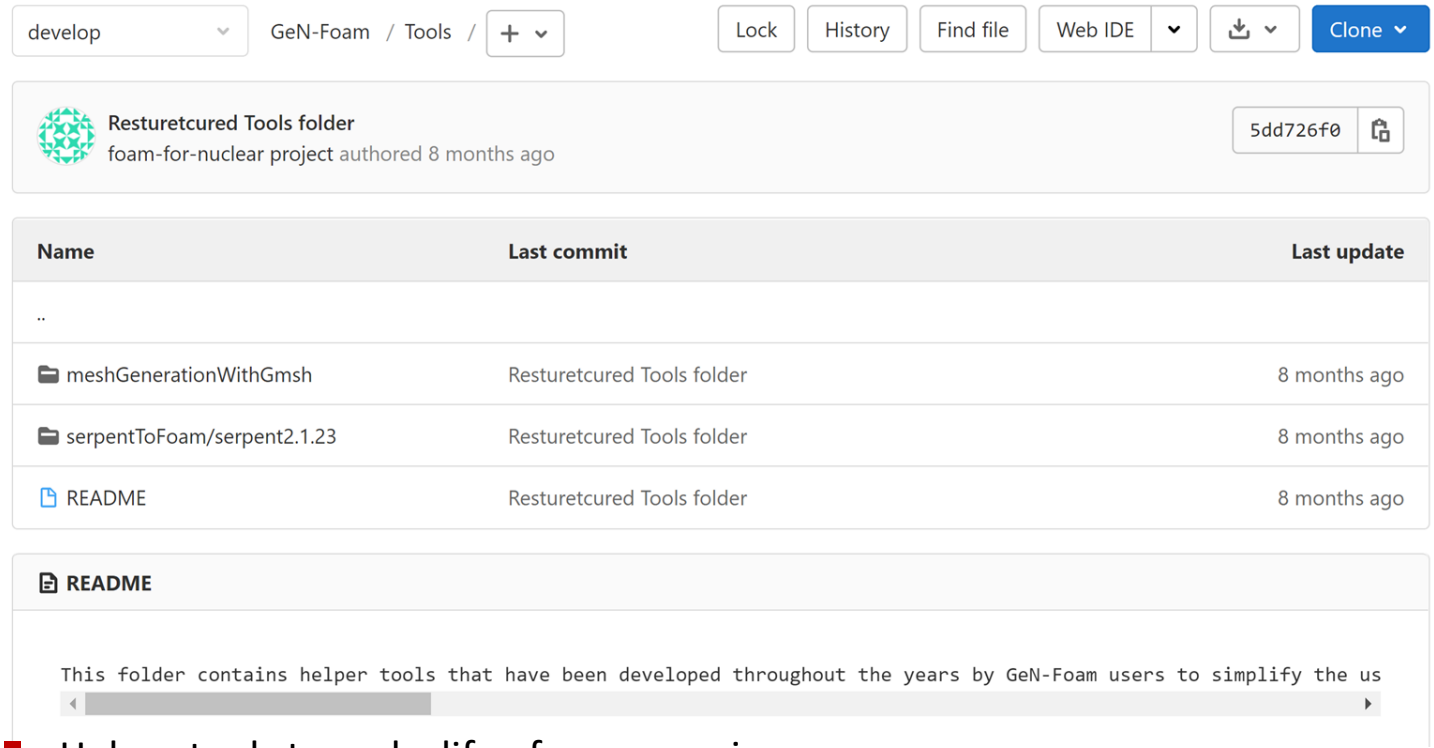
develop | GeN-Foam / + | History | Find file | Web IDE | Clone

Update solvePointKineticsLiquidFuel.H
foam-for-nuclear project authored 22 hours ago — 0a05c5b4

Name	Last commit	Last update
Documentation	Deleted howTo file. Created README file in ...	9 months ago
GeN-Foam	Update solvePointKineticsLiquidFuel.H	22 hours ago
Tools	Resturetcured Tools folder	8 months ago
Tutorials	Corrected bug in the modifiedEngel fluid-str...	4 weeks ago
.gitignore	Added FFS library from my two-phase work t...	1 year ago
LICENSE	Add LICENSE file	3 months ago
README	Update README	3 months ago

- README file often present to describe what's in a subfolder

What's inside: Tools



- Helper tools to make life of a user easier
  - Example of a mesh creation with gmsh
  - Script to convert an output of Serpent into an input for GeN-Foam

What's inside: Documentation

GeN-Foam is an unusually complex OpenFOAM solver. For this reason, some documentation (in the form of an online Doxygen-generated documentation has been prepared to facilitate its use. In addition, several commented tutorials have been prepared to showcase use and capabilities of the solver. An EMPTY case is also provided that can be used for step-by-step building one's own case. It is recommended to start from the EMPTY case to build each new case, as it already includes a consistent minimum set of (dummy) files that have to be present independent of the physics that are solved for. Beside this documentation, users ar encouraged to make use of the typical OpenFOAM ways:

- the high-level C++-based object-oriented language of OpenFOAM, which normally allows to easily understand the logic of a solver;
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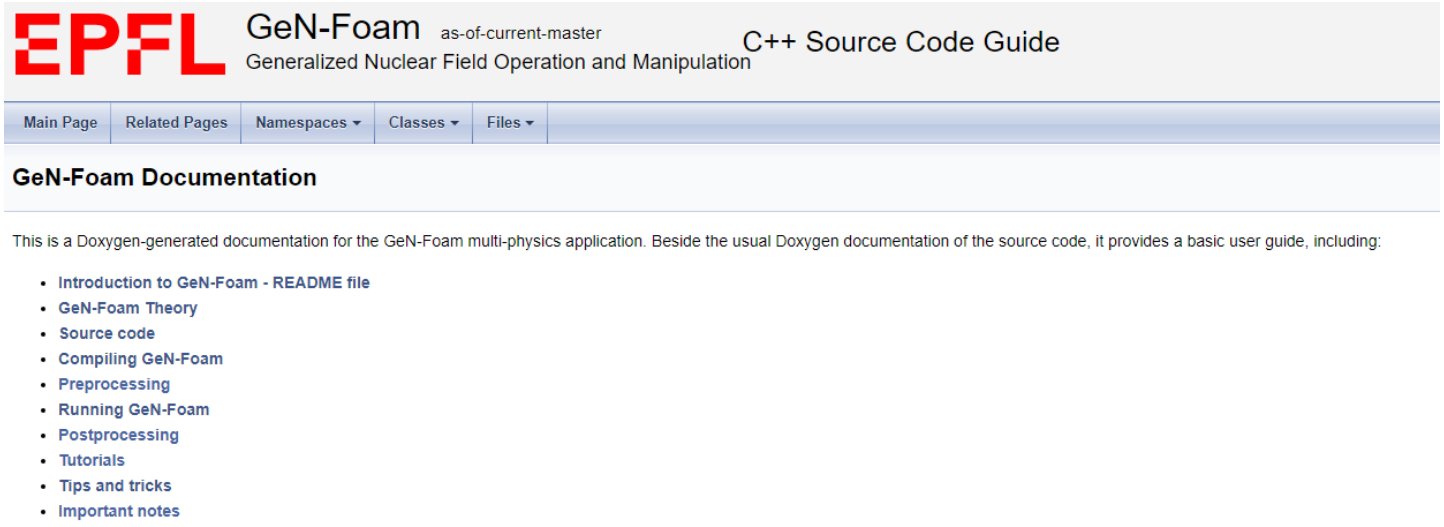
- the support of the community.



https://foam-for-nuclear.gitlab.io/GeN-Foam/index.html

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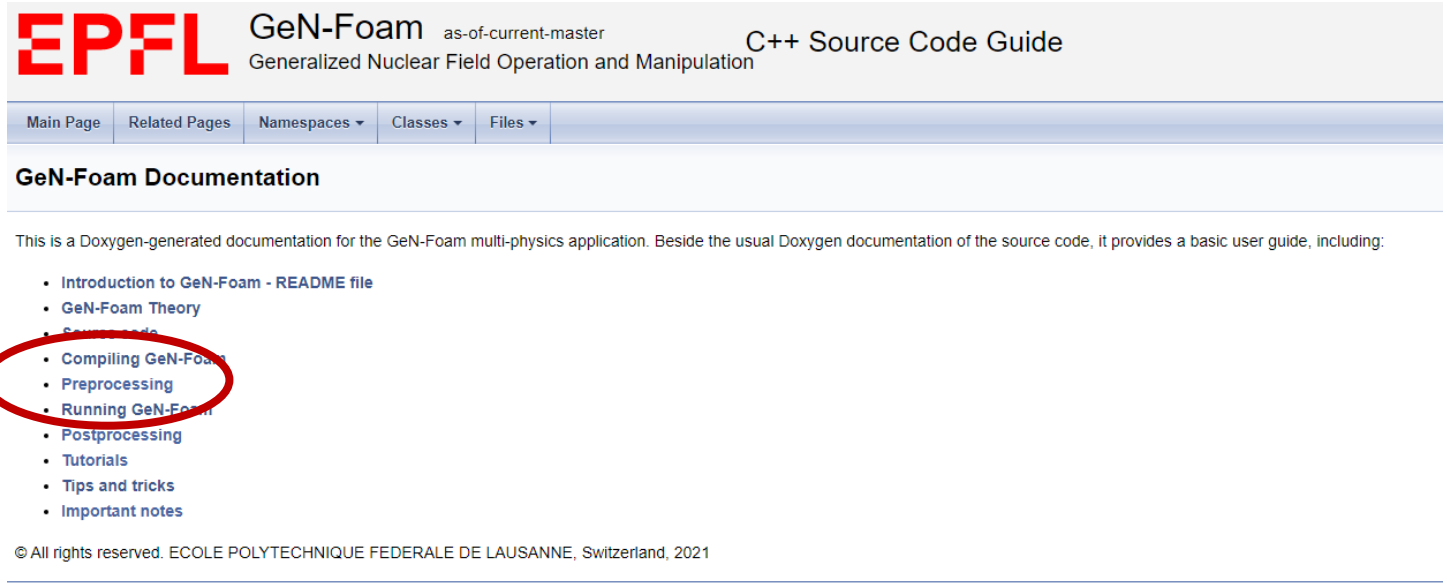

EPFL GeN-Foam as-of-current-master C++ Source Code Guide

Generalized Nuclear Field Operation and Manipulation

Main Page | Related Pages | Namespaces | Classes | Files

GeN-Foam Documentation

This is a Doxygen-generated documentation for the GeN-Foam multi-physics application. Beside the usual Doxygen documentation of the source code, it provides a basic user guide, including:

- Introduction to GeN-Foam - README file
- GeN-Foam Theory
- Source code
- Compiling GeN-Foam
- Preprocessing
- Running GeN-Foam
- Postprocessing
- Tutorials
- Tips and tricks
- Important notes

https://foam-for-nuclear.gitlab.io/GeN-Foam/index.html

What's inside: Documentation

Physical properties

The data for the GeN-Foam simulations can be filled in the following input files (dictionaries):

- *constant/thermoMechanicalRegion/thermoMechanicalProperties* - thermo-mechanical properties of structures, subdivided according to the cellZones of the thermoMechanicalRegion mesh. One can find a detailed, commented example in the tutorial 3D_SmallESFR.
- *constant/fluidRegion/g* - gravitational acceleration.
- *constant/fluidRegion/turbulenceProperties* - standard OpenFOAM dictionary to define the turbulence model to be used. One can find a detailed, commented example in the tutorial 3D_SmallESFR.
- *constant/fluidRegion/thermophysicalProperties* (for single-phase simulations) - standard OpenFOAM dictionary to define the thermo-physical properties of the coolant. One can find a detailed, commented example in tutorial 3D_SmallESFR (single phase)
- *constant/fluidRegion/thermophysicalProperties.(name of fluid)* (for two-phase simulations) - standard OpenFOAM dictionaries to define the thermo-physical properties of various phases. The name of fluid is defined in *constant/fluidRegion/phaseProperties*. One can find a detailed, commented example in the tutorial 1D_boiling (liquid), (vapour).
- *constant/fluidRegion/phaseProperties* - large dictionary that can be used to: determined whether the simulation is single-phase or two-phase; set various properties of the phases (beside the thermo-physical properties defined in *constant/fluidRegion/thermophysicalProperties*); set the properties of the sub-scale structures (fuel pins, heat exchangers, etc) in the porous zones, including the possibility to assign a *powerModel* for power production (e.g., nuclear fuel, or constant power) and the *passiveProperties* of another sub-structure that interacts thermally with the fluid (for instance the wrappers in sodium fast reactors). The name of the porous zones must coincide with that of the cellZones of the fluidRegion mesh. Anisotropic pressure drops can be set by using the keywords *transverseDragModel* (Blasius, GunterShaw, same) and *principalAxis*(localX, localY, localZ) in the sub-dictionary *dragModels.(nameOfPhase).structure.(nameOfCellZones)*. *principalAxis* sets the axis on which the nominal dragModel is used. *transverseDragModel* sets the model to be used on the two directions that are perpendicular to *principalAxis*. If *same* is chosen as *transverseDragModel*, the code will use the nominal model in all directions, but with the possibility of an anisotropic hydraulic diameter. The anisotropy of the hydraulic diameter can be set using the keyword *localDhAnisotrpy* and assign to it a vector of 3 scaling factors (one for each local directions). One can find detailed, commented examples in the tutorials 3D_SmallESFR (single phase) and 1D_boiling (two phases).
- *constant/neutroRegion/neutronicsProperties* - dictionary to control how neutronics is solved (point kinetics, diffusion, SP3 or SN), and if it's an eigenvalue calculation or a transient. One can find detailed, commented examples in most tutorials. See for instance 3D_SmallESFR (single phase).
- *constant/neutroRegion/reactorState* – contains the target power (pTarget) for eigenvalue calculations, the keff that results from the eigenvalue calculations and the external reactivity (i.e., the extra reactivity one can add for instance to simulate a reactivity step). N.B.: keff has no effect on pointKinetics. You can find detailed, commented examples in most tutorials. N.B.2: In point kinetics, pTarget is the initial value used by the point kinetics solver to plot results, but the solver actually scale the powerDensity and flux fields provided by the user. It is up to the user to make sure that pTarget is consistent with the powerDensity and flux fields. A commented reactorState can be found in 3D_SmallESFR (single phase). Please note that eigenvalue calculations will update the keff value in this dictionary. In parallel calculations, the updated value can be found in *processor0/constant/neutroRegion/reactorState*.
- *constant/neutroRegion/nuclearData* - contains all basic nuclear properties for the reference reactor state. The other *nuclearData...* files in *constant/neutronics/* should include the cross-sections for perturbed reactor states. In addition, these files include information about the perturbed and reference (*nuclearData*) reactor state. For instance, *nuclearDataFuelTemp* must include *TfuelRef* and *TfuelPerturbed*, which represent the temperatures at which the reference (*nuclearData*) and perturbed (*nuclearDataFuelTemp*) cross sections have been calculated, respectively. Linear interpolation is performed by GeN-Foam between reference and perturbed reactor states, except for fuel temperature, for which a logarithmic or square root interpolation is provided (depending on the spectrum, which in turns is defined by the keyword *fastNeutrons*). If no data are provided, the reference cross sections are used. Nuclear data can be generated using any nuclear code. The serpentToFoam routines provided with GeN-Foam (in the *Tools* folder) is an Octave script that automatically converts Serpent output files into the nuclear data files employed by GeN-Foam. The entry *discFactor* is used only if discontinuity factors have to be used. The term *integralFlux*, is used only if the automatic adjustment of discontinuity factors is performed **[3]**. Nonetheless, these entries should always be present. One can find detailed, commented examples of nuclearData in the tutorials 3D_SmallESFR (for diffusion or SP3), Godiva_SN (for discrete ordinates) and 2D_onePhaseAndPointKineticsCoupling (for point kinetics). One can find examples of the *nuclearData...* files in the tutorial 3D_SmallESFR

- All descriptions of dictionaries contain a link to a tutorials where that dictionary is extensively commented!

- Compiling GeN-Foam
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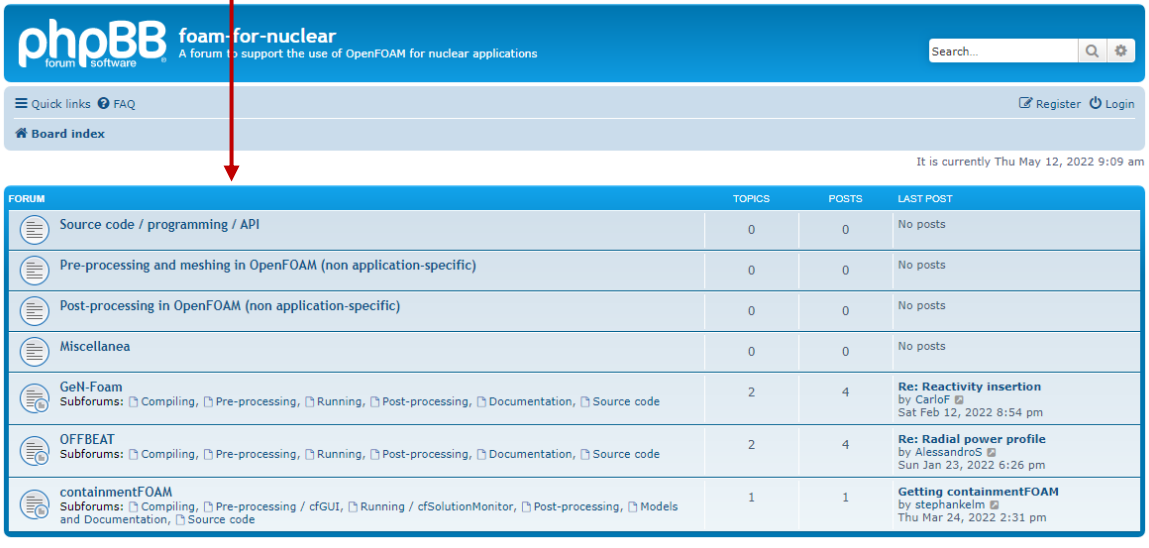

https://foam-for-nuclear.org/phpBB/

What's inside: Documentation

GeN-Foam as-of-current-master
Generalized Nuclear Field Operation and Manipulation
C++ Source Code Guide

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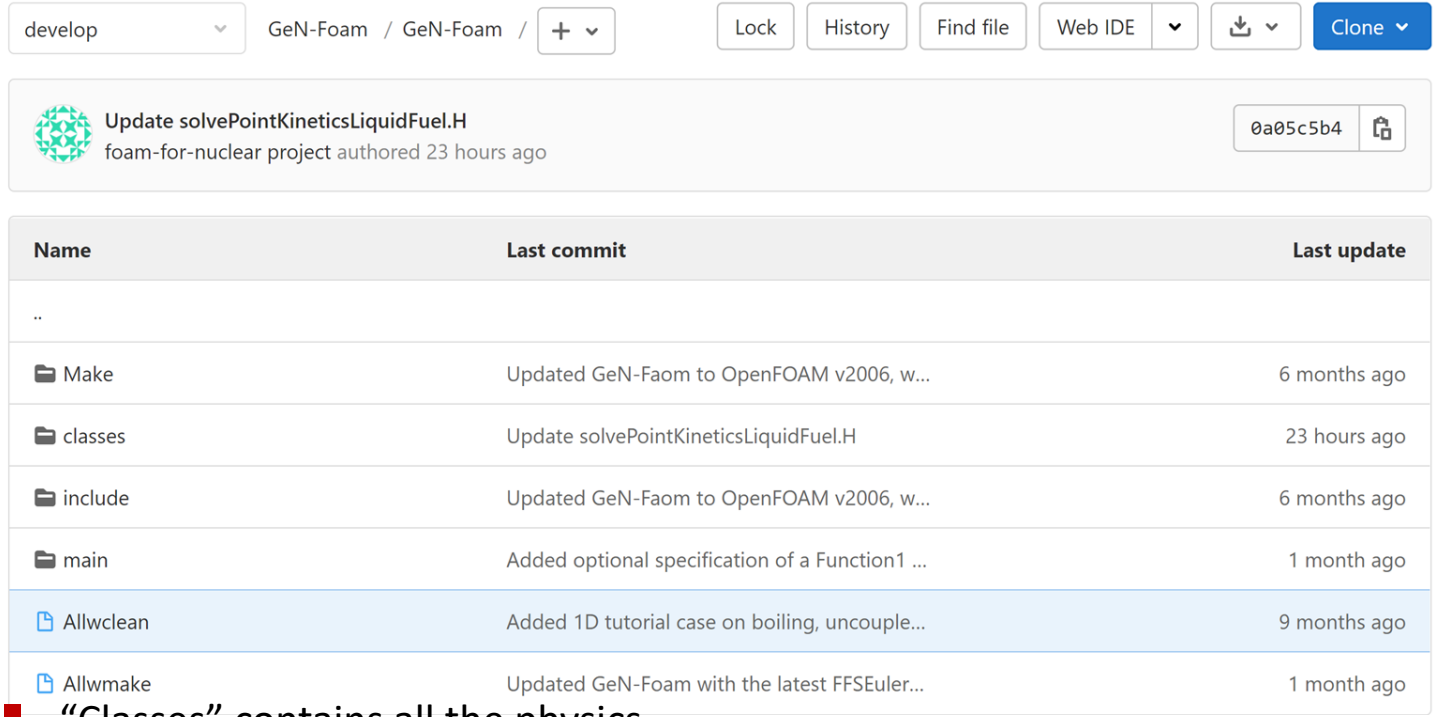
https://foam-for-nuclear.gitlab.io/GeN-Foam/citelist.html

What's inside: Source code



- "Classes" contains all the physics
- "main" contains what glues them together
- "include" are folders that mainly contain chunks of code that perform specific tasks and that are included (#include) in the code

https://gitlab.com/foam-for-nuclear/GeN-Foam/-/tree/develop/GeN-Foam

What's inside: Tutorials

develop / GeN-Foam / Tutorials / + | Lock | History | Find file | Web IDE | Clone

Corrected bug in the modifiedEngel fluid-structure drag model (thanks to...
Stefan Radman authored 4 weeks ago

424e122b

Name	Last commit	Last update
..		
1D_HX	Corrected bug in the modifiedEngel fluid-str...	4 weeks ago
1D_boiling	Updated GeN-Foam with the latest FFSEuler...	1 month ago
2D_FFTF	updated regression test	1 month ago
2D_MSFR	Added expected keff to Allrun.	2 months ago
2D_cavityBoussinesq	Added optional specification of a Function1 ...	1 month ago
2D_onePhaseAndPointKineticsCo...	Added novel feature to the pointKinetics mo...	1 month ago
2D_voidMotionNoPhaseChange	Updated GeN-Foam with the latest FFSEuler...	3 months ago

- Cover essentially all functionalities of GeN-Foam
- They include a README file, an Allrun file (sometimes Allrun_parallel), an Allclean file, and some extensively commented inputs

Carlo Fiorina

An example: 1D_MSR_pointKinetics

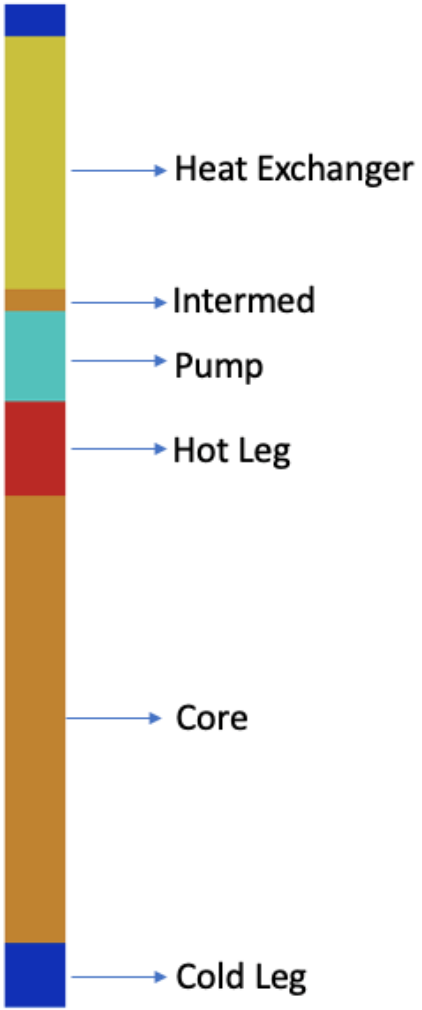
- https://gitlab.com/foam-for-nuclear/GeN-Foam/-/tree/develop/Tutorials/1D_MSR_pointKinetics
- Understanding the tutorial:
  - README file
  - Case folder
  - Allrun file
  - Run it and use paraview to see what happens

An example: 1D_MSR_pointKinetics

- Start from the README file (https://gitlab.com/foam-for-nuclear/GeN-Foam/-/tree/develop/Tutorials/1D_MSR_pointKinetics/README)

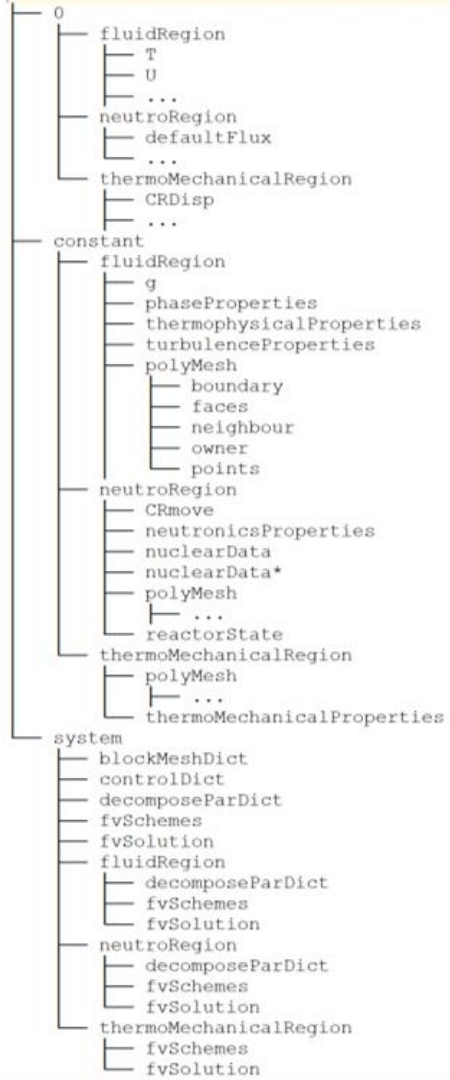
```
DESCRIPTION
This tutorial displays how to use the point kinetics module of
GeN-Foam for MSRs. It is a simple 1-D case with core, hot leg,
pump, heat exchanger and cold leg. The geometry is one
dimensional and salt recirculation is simulated by making use
of a cyclic boundary condition between top and bottom
boundaries.

Three simulations are performed:
- energy and fluid dynamics to obtain a steady state
- energy, fluid dynamics and point kinetics to simulate a loss
  of-flow
- recalculate the reactivity  loss due to recirculation of the
  delayed neutron precursors.
```



An example: 1D_MSR_pointKinetics

- Look at the case folder
  - *0* folder with three subfolder containing the fields for each physics
  - *constant* folder with 3 subfolders
    - 3 meshes (*polyMesh* folders)
    - 3 sets of dictionaries
  - *system* folder with:
    - 3 subfolders with dedicated *fvScheme* and *fvSolution* for each physics
    - 1 *controlDict*
    - 1 common *fvSolution* with some multi-physics controls



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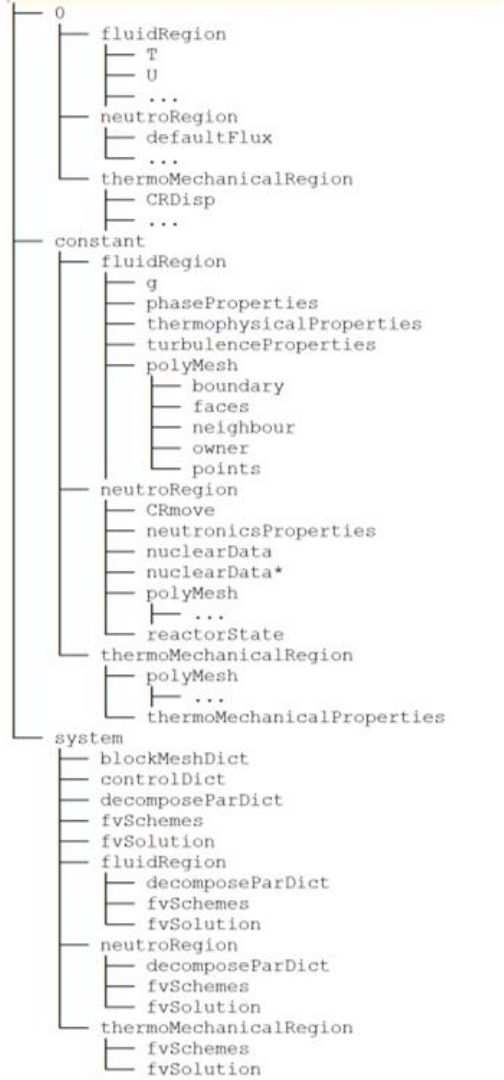
An example: 1D_MSR_pointKinetics

- Look at the dictionaries
  - All the dictionaries are extensively commented in at least one of the tutorials
  - Which tutorial to look at for every dictionary? Look in the Prepreprocessing section of the documentation https://foam-for-nuclear.gitlab.io/GeN-Foam/PREPROCESSING.html
  - In our case, the tutorial is mainly dedicated to the point kinetics model. Look at constant/neutroRegion/nuclearData https://gitlab.com/foam-for-nuclear/GeN-Foam/-/blob/master/Tutorials/2D_onePhaseAndPointKineticsCoupling/rootCase/constant/neutroRegion/nuclearData



An example: 1D_MSR_pointKinetics

- Look at the Allrun file

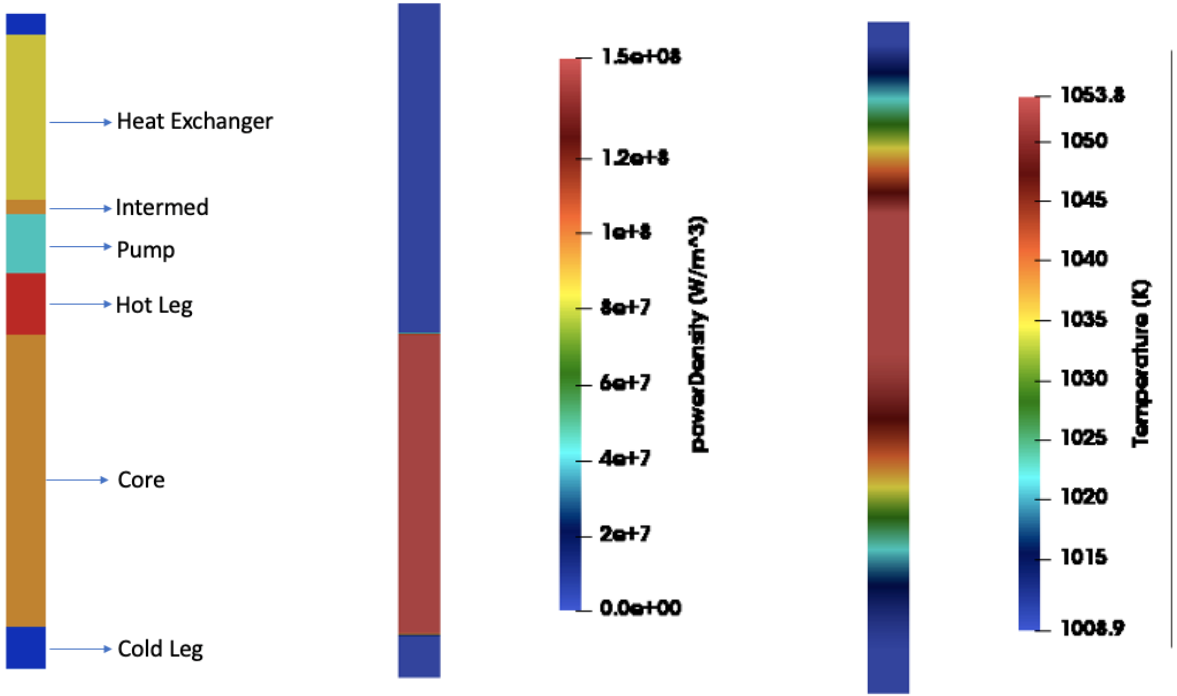
```
cases="steadyState  transient  transientEnd "
...
setSteadyState()
{
          runCloneCase $1 $2
          foamDictionary steadyState/system/fvSolution -entry tightlyCoupled -set false
          foamDictionary steadyState/system/controlDict -entry startTime -set 0
          foamDictionary steadyState/system/controlDict -entry endTime -set 100
          foamDictionary steadyState/system/controlDict -entry adjustTimeStep -set true
          foamDictionary steadyState/system/controlDict -entry solveFluidMechanics -set true
          foamDictionary steadyState/system/controlDict -entry solveEnergy -set true
          foamDictionary steadyState/system/controlDict -entry solveNeutronics -set false
          foamDictionary steadyState/system/controlDict -entry solveThermalMechanics -set false    =
...
setTransient()
{
          foamDictionary transient/system/controlDict -entry startTime -set 100
          foamDictionary transient/system/controlDict -entry endTime -set 400
          foamDictionary transient/system/controlDict -entry solveNeutronics -set true

...
```

An example: 1D_MSR_pointKinetics

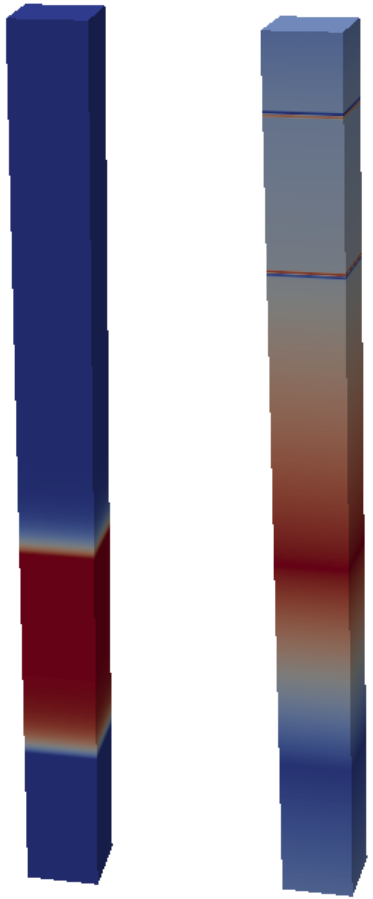
- Run the tutorial -> ./Allrun
- Check the results:
  - Choose a folder: steadyState, transientNoDriveline, transientWithDriveline
  - Use:
    - paraFoam
    - ./log.GeN-Foam: standard OpenFOAM log
    - ./GeN-Foam.dat: quick overview of time behavior of main quantities (power, keff, min/max/average fuel and clad temp.)
    - ./constant/neutroRegion/reactorState for keff
    - in some tutorials, a python script to extract info from log file

An example: 1D_MSR_pointKinetics

- paraFoam



Precursors, group 0 and 7



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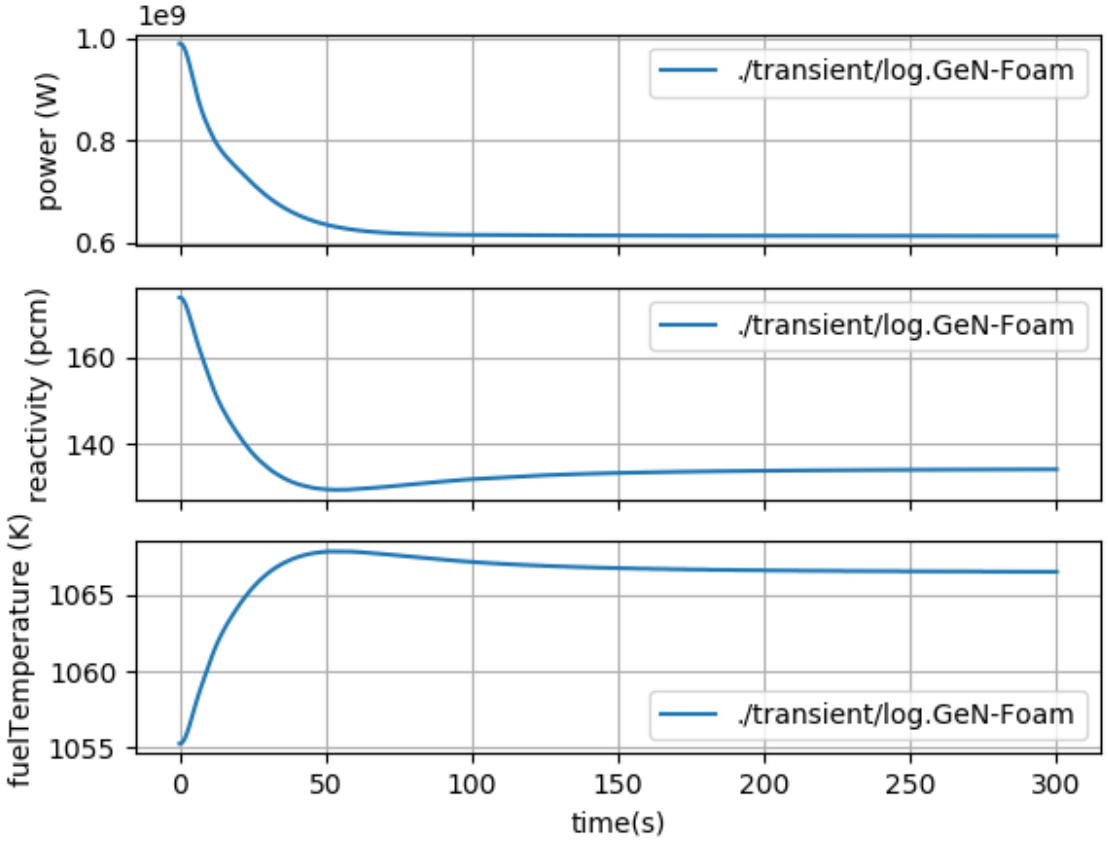
An example: 1D_MSR_pointKinetics

- python script (extract data from log)
- Type in terminal:

```
Python3 plotPKlin.py
./transient/log.GeN-Foam
```



Other tutorials: 1D_HX

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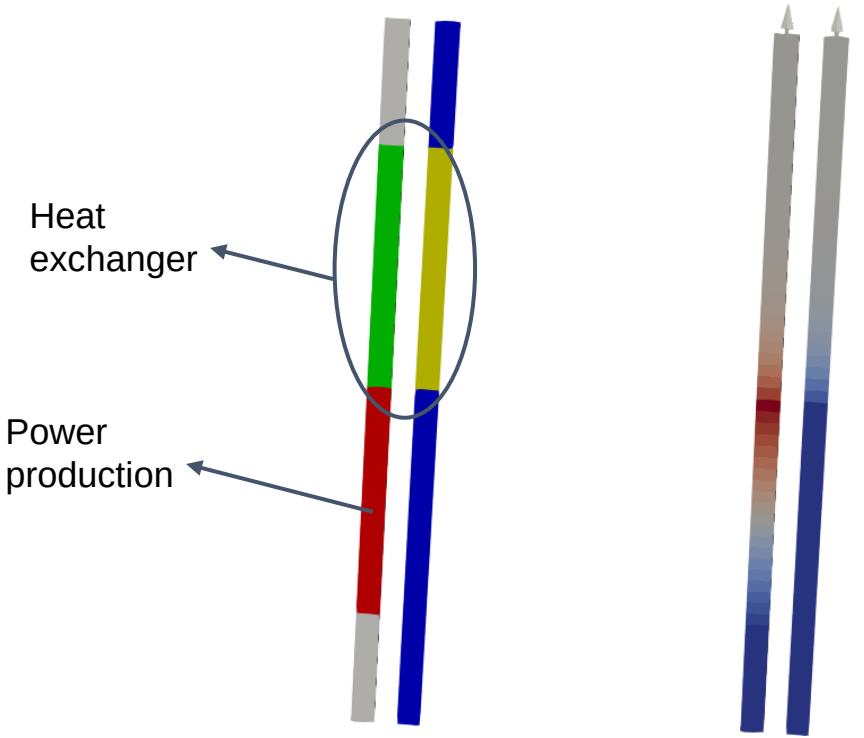
Example on how to set up a heat exchanger

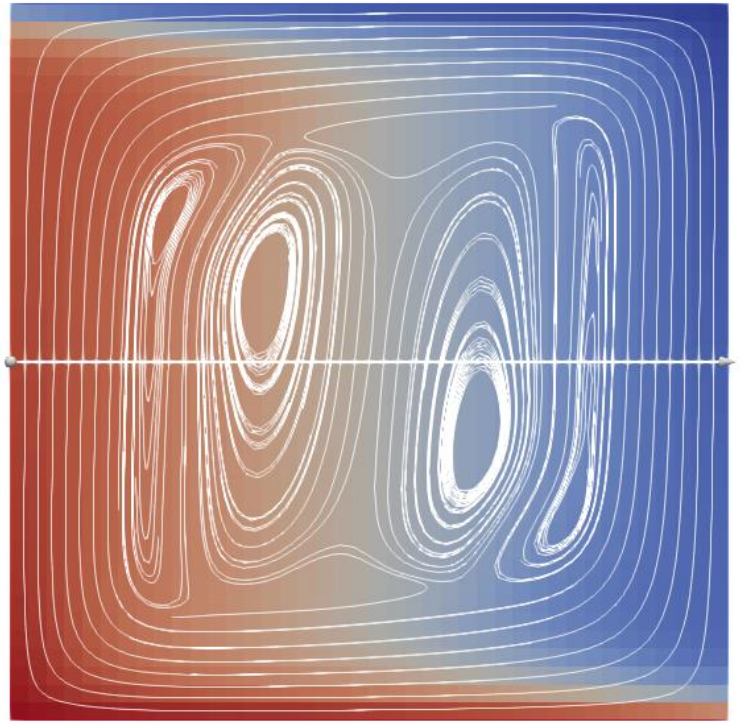


Other tutorials: 1D_boiling

Example of two-phase simulation. 1D channel with a pressure-driven flow of liquid sodium, with power source turned on at time 0, eventually leading to boiling. After a certain time the power is turned off

Other tutorials: 2D_cavityBoussinesq

Example of how to use of the Boussinesq approximation for buoyancy based on the standard buoyancy-driven cavity

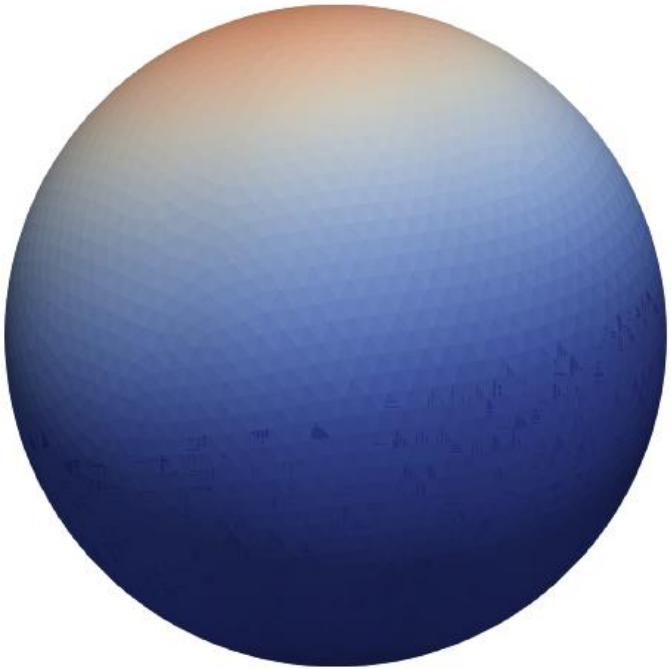


Other tutorials: 2D_voidMotionNoPhaseChange

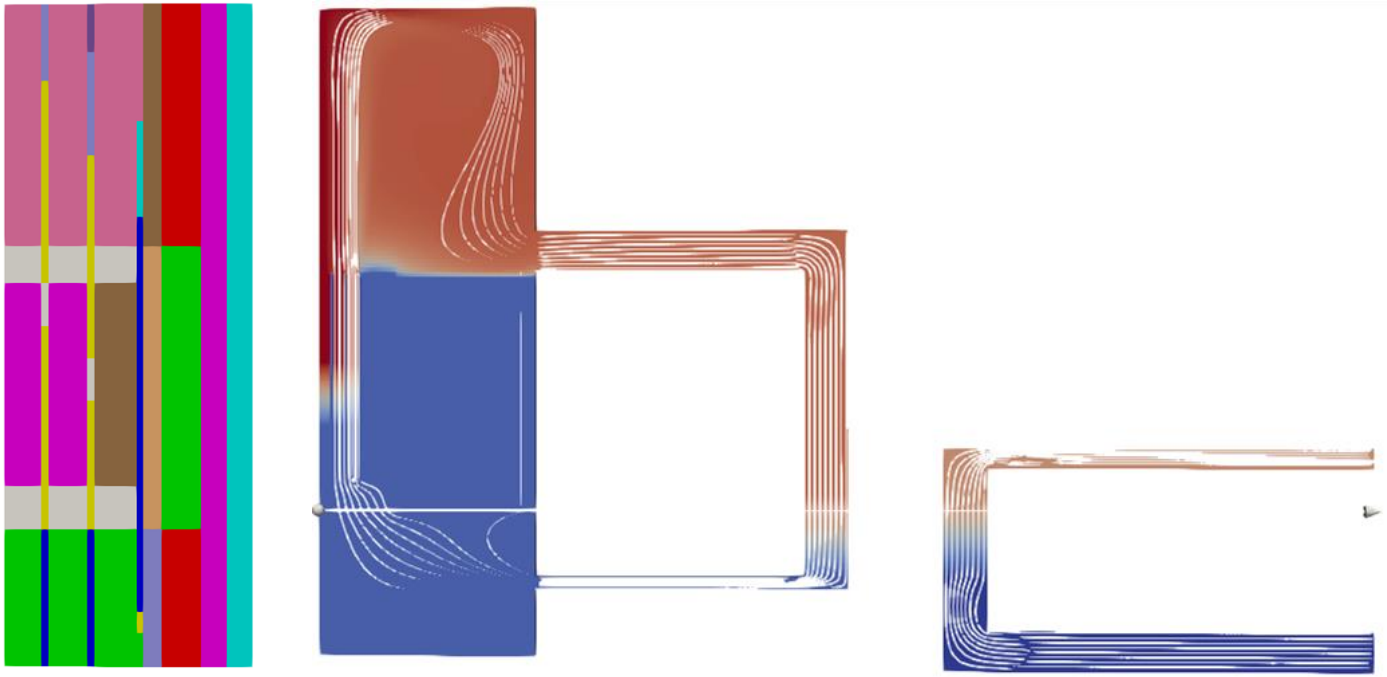
Simple two-phase case without mass transfer between phases

Other tutorials: Godiva_SN

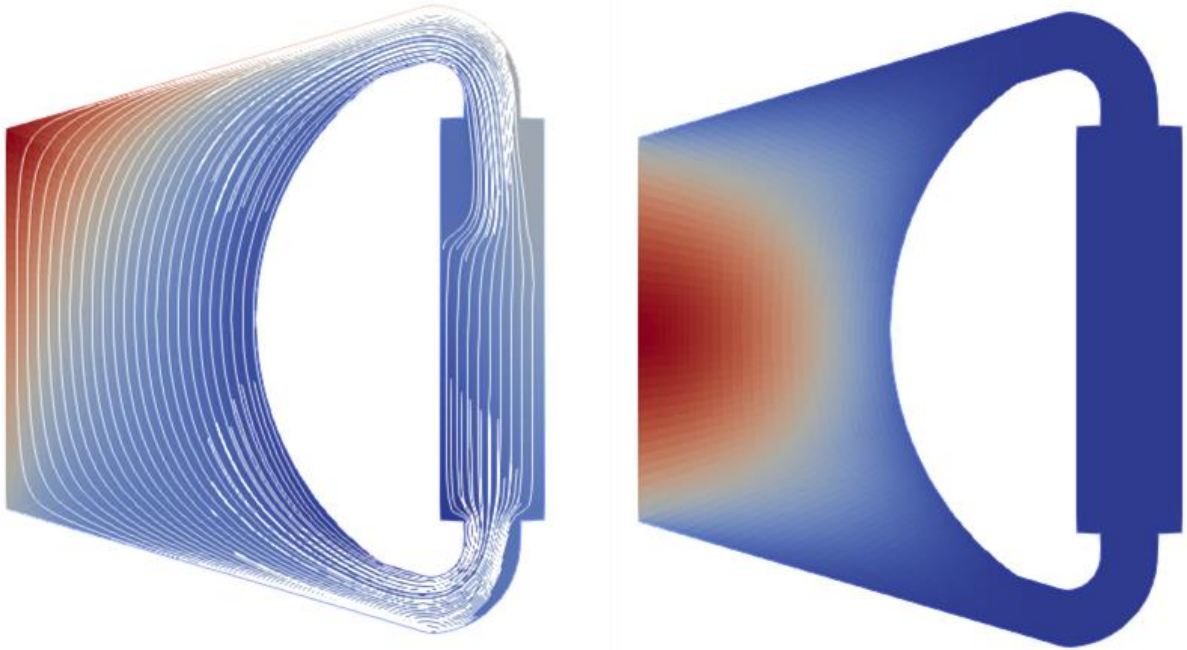
Example of a discrete ordinate calculation of Godiva



2-D model of the FFTF. Simulation of a ULOF

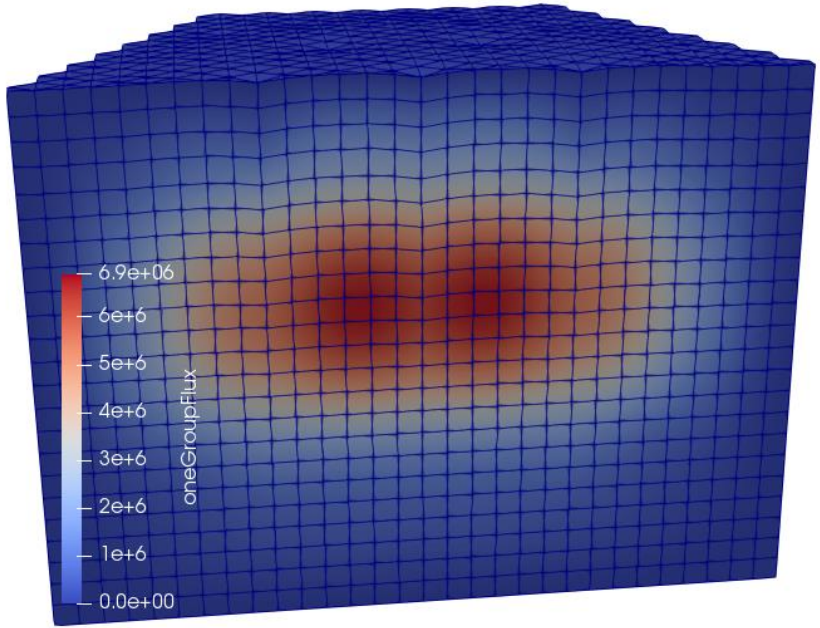


2-D model of the MSFR



Other tutorials: 3D_SmallESFR

- Slightly smaller version of the European Sodium Fast Reactor
- Example of a 3D full multi-physics simulation, including core deformation



GeN-Foam: what's next?

- User manual…
- Validation for water
- Further validation for MSRs

Thank you

Carlo Fiorina

How to install it - paraview

- Requires separate installation in the openfoam.com version of OpenFOAM
- Just install the latest version from paraview.org

Why isn't ParaView included in the precompiled packages? This would be much more convenient than having to compile it myself!
Some more details are given in modules/visualization, but essentially the paraview version distributed with the operating system or a newer binary package is likelyfully adequate for your needs. We would prefer to focus on extending and improving the OpenFOAM support in ParaView/VTK directly since this provides the best long-term and most universal solution

The source code of the GeN-Foam multi-physics solver

- All sub-solvers are organized into C++ classes
  - Easier to understand its coding
  - Possible to easily extract sub-solvers for use in other solvers
    - ✓ You have complete freedom to freely use and modify
    - ✓ (Does not mean that copyright does not exists: acknowledgment of previous the work of other authors is always good practice and consistent with ethics in open-source development)

What is a C++ class

- C++ is object oriented
- Object-oriented roughly means that you can organize you code into classes
- Classes are a set of data, and functions that operate on those data
- For instance, in GeN-Foam, classes for:
  - neutronics
  - cross-sections
  - thermal-hydraulics
  - thermal-mechanics
  - other “functional classes” e.g. for handling multi-physics simulations
- For instance, the neutronics class contains:
  - neutronics quantities, such as keff, power field, etc.
  - functions that manipulate these quantities

What is a C++ class

- Classes can have *derived classes*, i.e., classes that can “see” everything in the original class, but that contains additional data and functions
- In GeN-Foam, this is used to “specialize” solver classes into sub-solvers
- For instance, from the neutronic class, we derive classes for:
  - diffusion
  - Sp3
  - SN
  - point-kinetics
- For instance, the “diffusion” derived class contains:
  - all data and functions from the neutronics class
  - additional data (e.g., multi-group fluxes)
  - additional functions, the most important being the function that solves for the fluxes at every time step