

Joint ICTP-IAEA Workshop on Open-Source Nuclear Codes for Reactor Analysis 07 - 11 Aug 2023 Contact: <u>ONCORE@iaea.org</u>

Introduction to OFFBEAT

10 August 2023 Alessandro Scolaro - EPFL





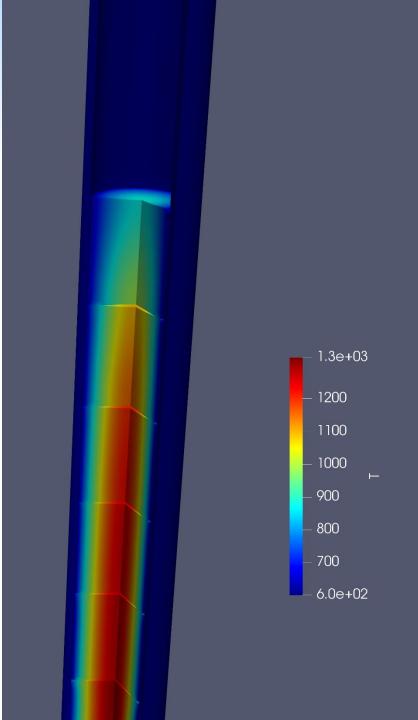
1. Introduce OFFBEAT main capabilities and features

2. Provide example of applications

3. Basic knowledge on how to approach OFFBEAT

OFFBEAT – OpenFOAM Fuel Behavior Analysis Tool

- Multi-dimensional fuel performance code:
 - 1D, 2D, 3D with arbitrary geometry & mesh
- Based on OpenFOAM® C++ library
- In development since 2017 at EPFL and PSI (Switzerland)
- Open-source at: <u>https://gitlab.com/foam-for-nuclear/offbeat</u>



Project prompted by a fuel failure in a Swiss NPP



8.2

Oxide Layer Thickness (µm)

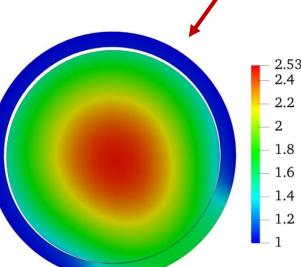
2017 - studies at PSI by I. Clifford et al., Ann. Nucl. En., 2019

Community would benefit from a readily available tool that:

- Enables *multi-dimensional* analysis.
- Clears the way to *multi-physics* and coupling.
- Allows straightforward tailoring.

_ 7 Not feasible with traditional tools 5 3 Normalised Temperature 2 2.2

Cladding oxide layer thickness under partial dryout



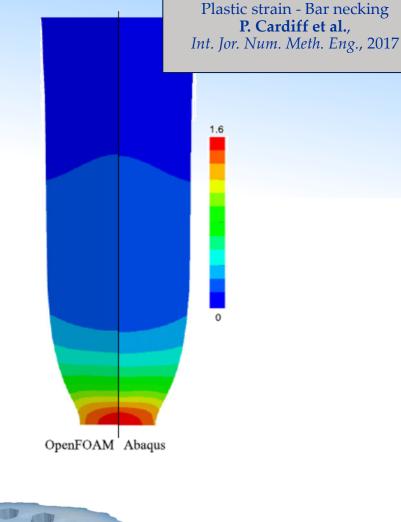
Temperature distribution for eccentric fuel under power peaking and partial dryout

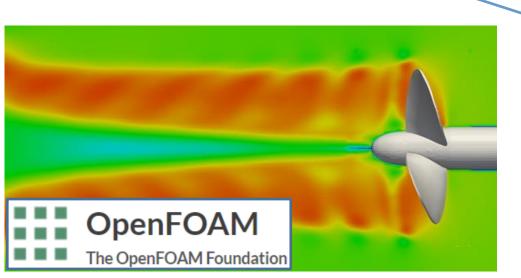
Solid mechanics & Finite Volume?

Extension of the FVM to **solid mechanics** in the last 30 years:

- Only simple linear elastic solver in standard OpenFOAM..
- ... but lots of great work done by the community!
 (e.g. foam-extend, *solids4Foam*)

Choice of OpenFOAM also motivated by EPFL-PSI experience for reactor analysis (e.g. *Gen-Foam* platform)









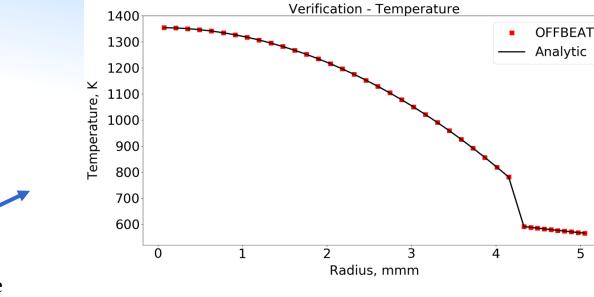
V&V status and past applications

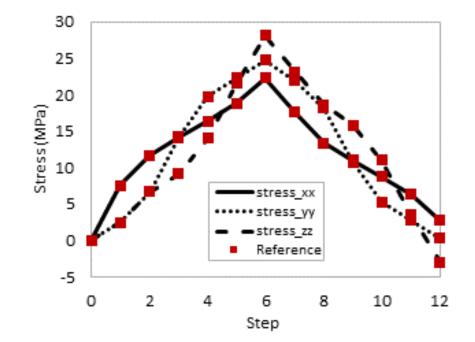
Verification

- Simple cases with focus on *single aspects*. 1.
- Useful for finding bugs. 2.

Main tests:

- Rod free volume ٠
- Heat transfer across the gap ٠
- Steady-state and transient temperature/stress profile •
- Rate-independent plasticity model •
- Corrosion layer thickness ٠
- Limbäck creep model and *plasticity* ٠
- Contact model(s) benchmark ٠
- Corrosion ٠
- **Neutronics** ٠
- Porosity ٠
- TRISO properties and IAEA benchmarks ٠





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Main focus on thermal analysis:

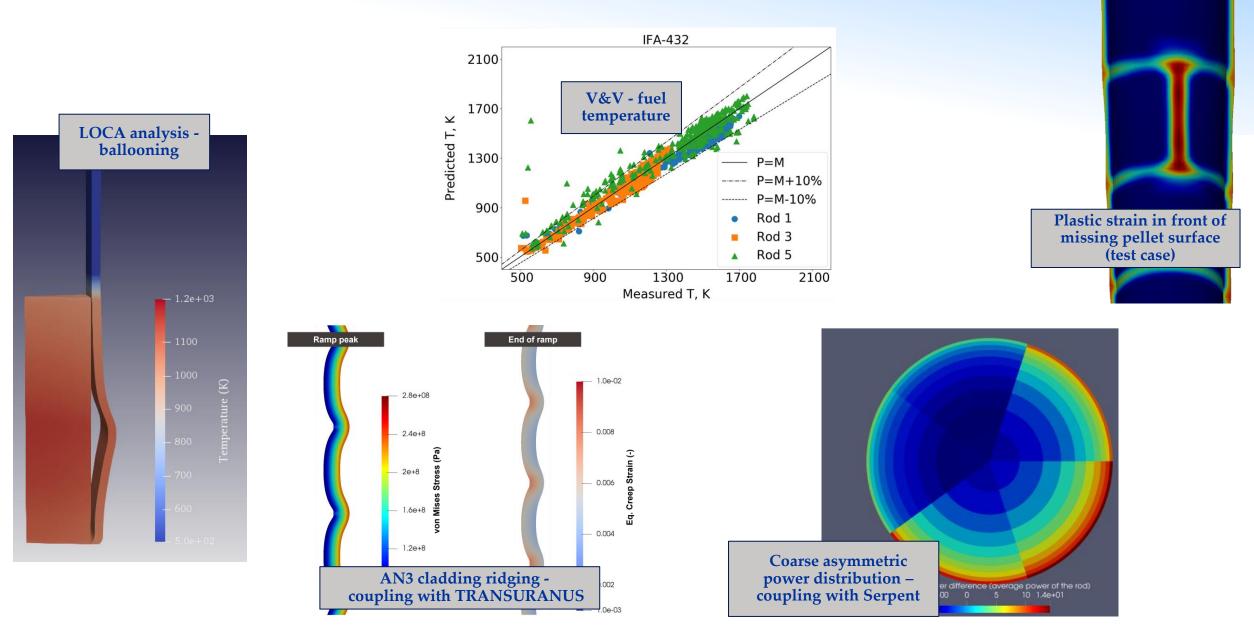
- Fuel Centerline Temperature (FCT)
- Fission Gas Release (FGR)

NOTE:

- Mechanics is indirectly embedded in thermal analysis (e.g. gap size)
- But validation for quantity such as elongation or cladding expansion is essential for future efforts.

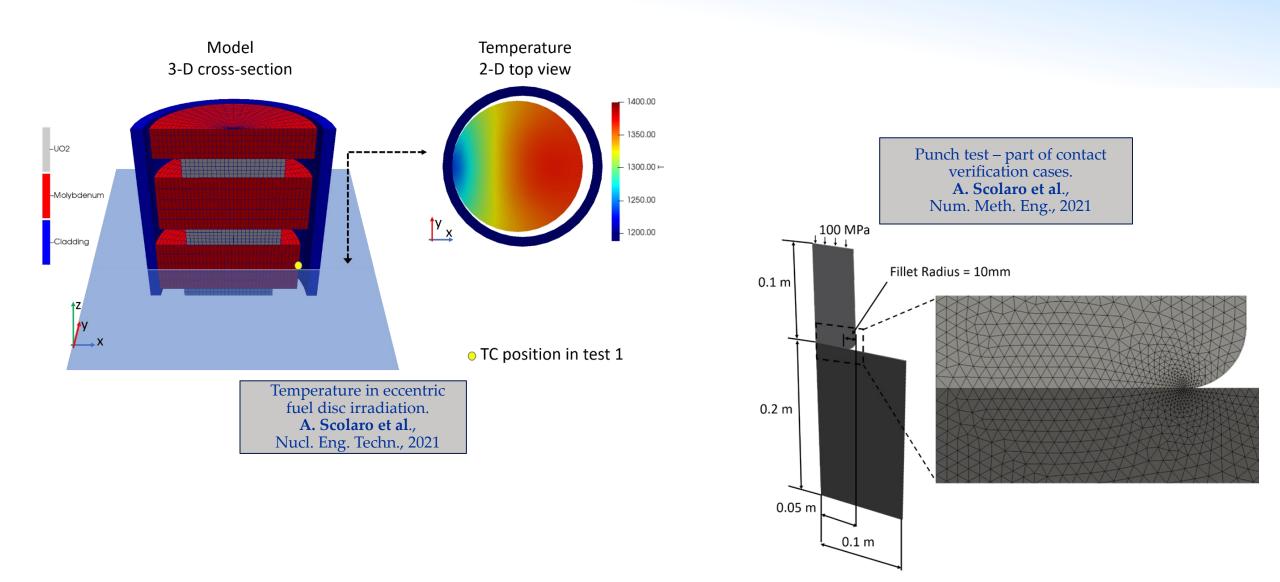
Experiment	Rod number/name		Burnup, MWd/kg	Quantity of interest	
IFA-562.1	Lower Cluster	1 2 3 4 5 6	~10	FCT	
IFA-302.1	Upper Cluster	7 8 9 10 11 12	~10		
IFA-432	13	5	~30/40	FCT	
	PW3	23		FGR	
	PK1	1234			
Sup or Domp	PK2	1 2 3 4 S	~40		
Super Ramp	PK4	1 2 3 S	~40		
	PK6	2 3 S			
	BK7	3 4 5 6			
	AN	1 2 3 4 8 10 11		FGR	
Risø-3	II	3 5	~30/40	(FCT for refabricated	
	GE	2467		rods)	

Main applications for LWR fuel (examples)



Not just standard configurations and materials!





Not *just* standard configurations and materials!



1 week ago

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🗅 timeHandling

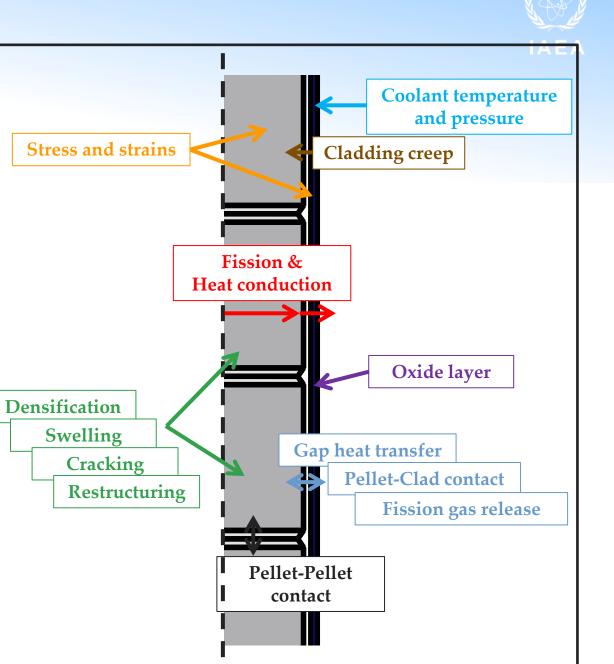
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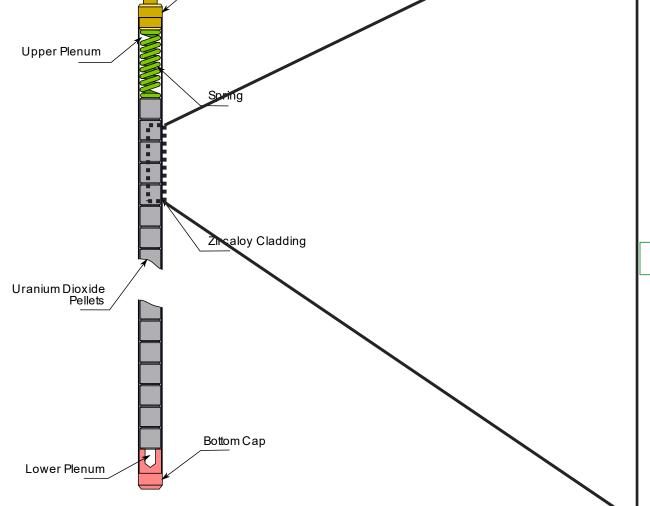


OFFBEAT Code structure

The complexity of fuel behavior: a brief recap

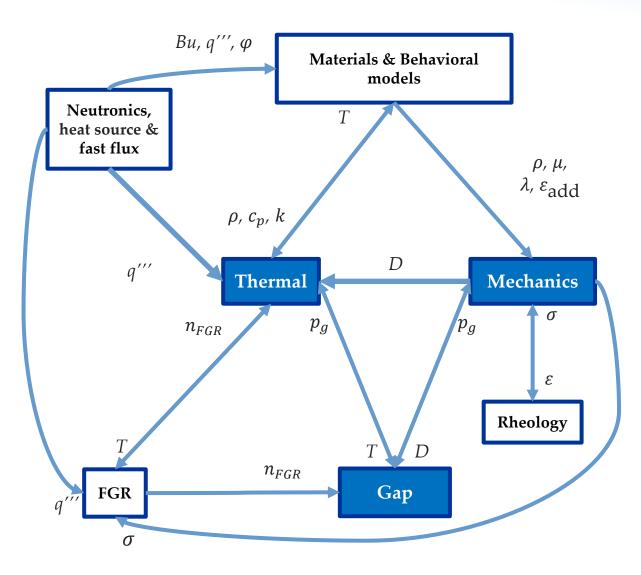
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Code structure (only main dependencies are shown)





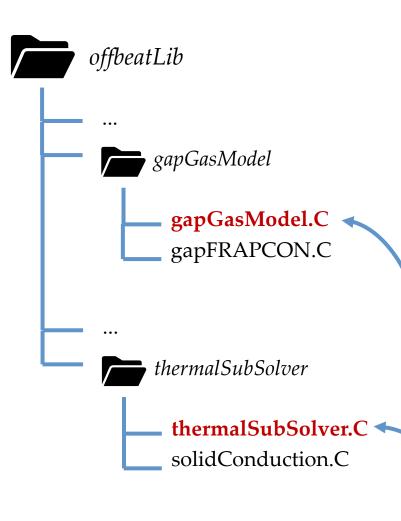
• Separate aspects of fuel behavior encapsulated in separate classes.

- Some physics are reproduced with models and correlations...
- ... others by solving governing equations.

• Fields and variables exchanged through functions or registry-lookup.

Switching on/off physics





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NOTE: most OFFBEAT options are in a single file, the *solverDict*.

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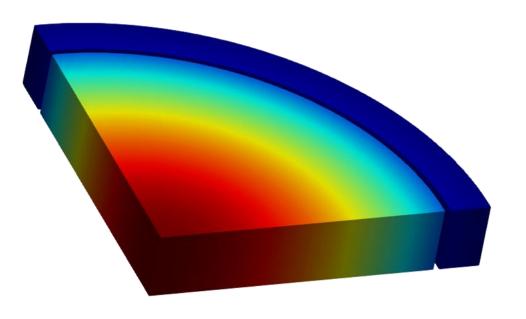
- Solvers/models are run-time selectable in the solverDict.
- Mother class selected to switch off the physics/model (e.g. for pure thermal analysis):
 - *none:* no additional field is created (e.g. for empty gap gas or fission gas release model)
 - *fromLatestTime:* the main field (e.g. temperature) is created but left unchanged to default/initial value.

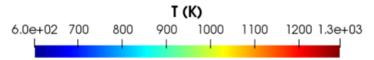


OFFBEAT Physics and solution strategy

Thermal solver - Heat diffusion equation

$$\int_{V} \frac{\partial \rho c_{p} T}{\partial t} dV = \oint_{S} \mathbf{n} \cdot \mathbf{k} \nabla T \, dS + \left(\int_{V} q^{\prime \prime \prime} dV \right)$$





Volumetric heat density q''' handled by heatSource class

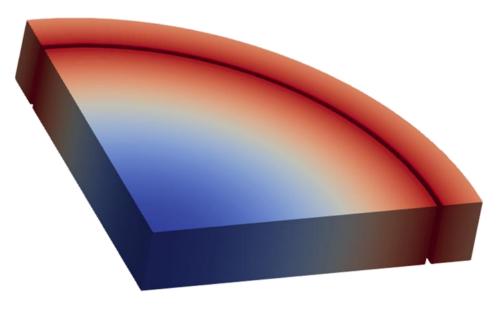
- 1. Through q'" file (e.g. mapped from separate neutronics code or calculated via fvOptions or codeStream).
- Providing (time-dependent) linear heat generation rate (*lhgr* or q') or volumetric heat generation rate (*vhgr* or q''')



Mechanics Solver – Momentum balance equation(s)









What needs to be decided:

- 1. Approach to momentum balance equations
 - Mesh updated or not
 - Total or incremental field
- 2. Definition of strainSmall-strain or finite strain
- 3. Constitutive law for mechanical behavior

Mechanics - selection of the solver

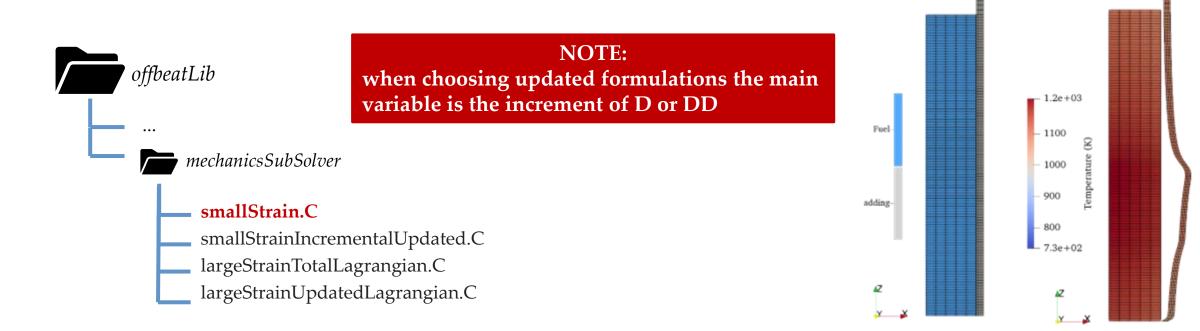


smallStrain is a good approximation for most scenarios:

$$\boldsymbol{\varepsilon} = \frac{1}{2} \left(\nabla \mathbf{D} + (\nabla \mathbf{D})^{\mathrm{T}} \right)$$

For finite strain scenarios (or when the change of the domain is relevant) the best options typically are updated formulations:

- *smallStrainIncrementalUpdated* → small strain but the mesh is updated (takes mostly care of geometric non-linearity).
- *lageStrainUpdatedLagrangian* → non-linear treatment of strains and compatible with non-linear constitutive laws.



Dedicated BCs

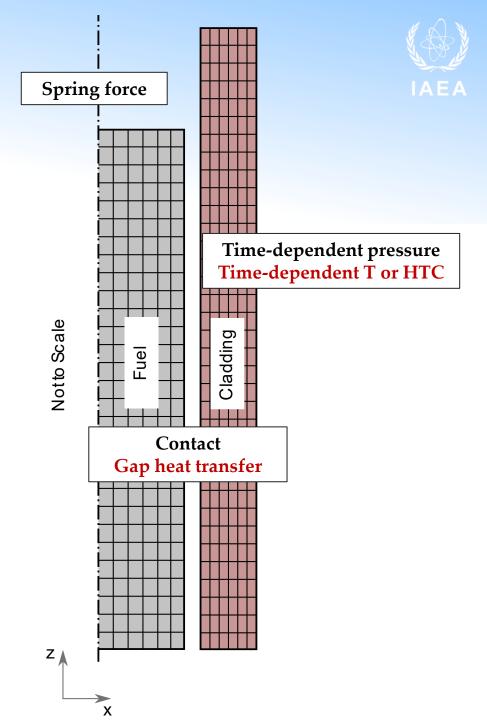
Thermo-mechanics solution obtained with a mix of standard (e.g. fixed-value) and dedicated BCs

Examples of dedicated BCs for mechanics:

- 1. Fixed or time-dependent pressure
- 2. Contact
- 3. Plenum spring pressure

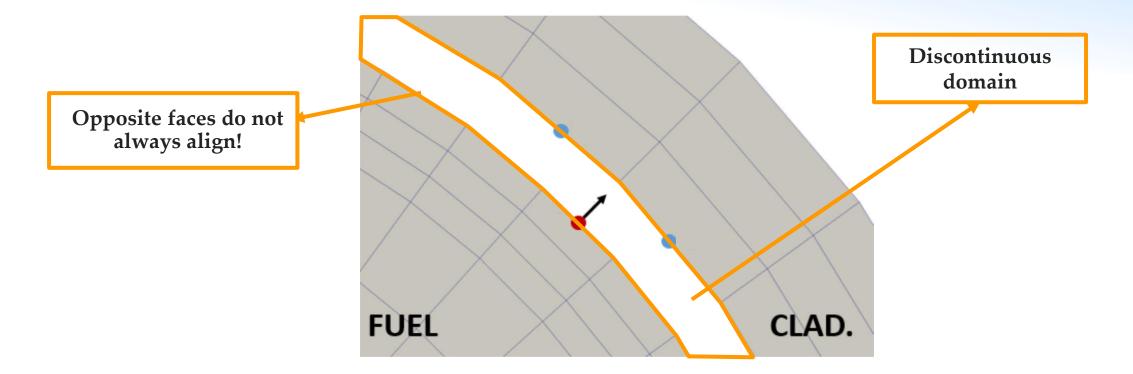
Examples of dedicated BCs for thermal analysis:

- **1.** Fixed or time-dependent temperature with axial profile
- 2. Fixed or time-dependent HTC with axial profile
- 3. Gap conductance heat transfer



Mapping methodology for non-conforming patches





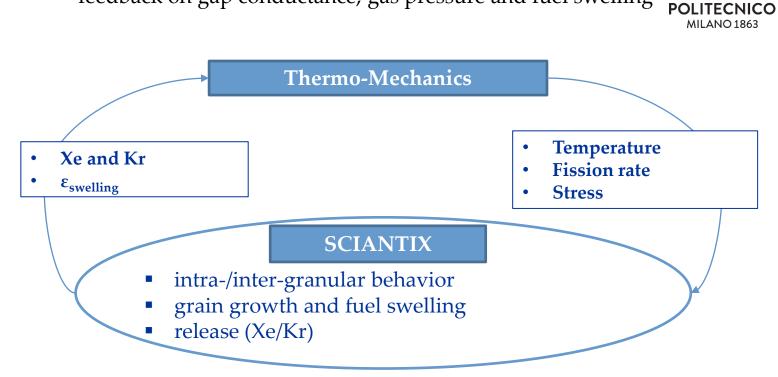
- Based on Arbitrary Mesh Interface (AMI) readapted to the presence of small gap.
- Heat transfer BC solved implicitly (i.e. using current value of the temperature field)

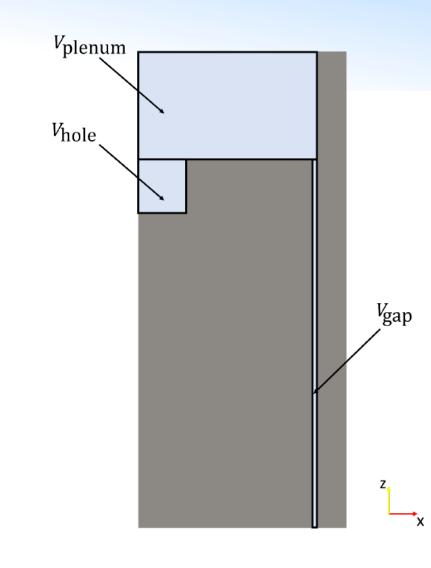
NOTE: the user must take care of defining master/slave patches as coupled!

Additional physics and models

• **Gap gas model**: keeps track of gas free volume, temperature, pressure and composition

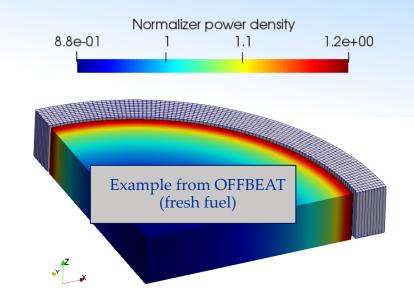
• **Fission gas release** with the SCIANTIX 0-D code: feedback on gap conductance, gas pressure and fuel swelling



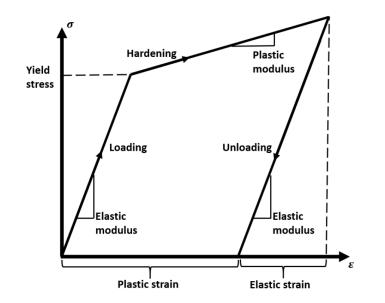


Additional physics and models





- **Burnup & neutronics** as capturing peaked power profile in fuel pellet is relevant for:
 - Rod's thermal response (lower maximum temperature).
 - Nuclide distribution: the source for advance models e.g. chemistry, plutonium redistribution etc
- Heat-source & fast-flux/fast-fluence classes

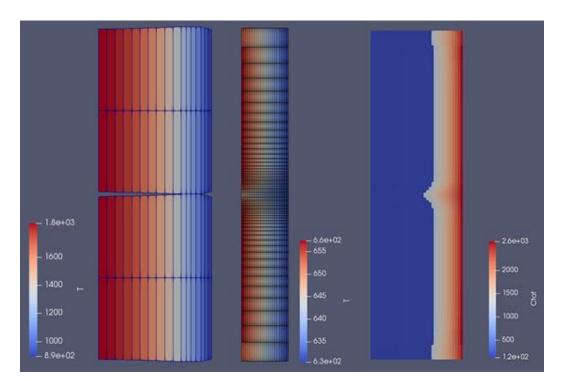


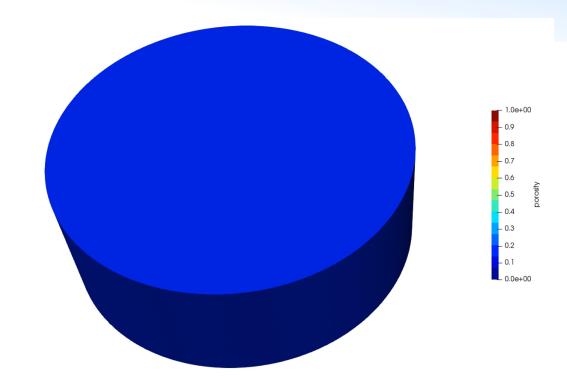
- Material properties and rheology class for capturing:
 - Evolution of material properties (e.g. conductivity, Young's modulus)
 - Constitutive mechanical behavior such as elasticity, plasticity or creep
 - Additional strain components due to behavioral models such as swelling or densification

Additional physics and models



- Element transport:
 - Porosity redistribution
 - Minor actinides redistribution
 - Hydrogen pickup
- Corrosion $Zr + H_2O \longrightarrow ZrO_2 + 2H_2$



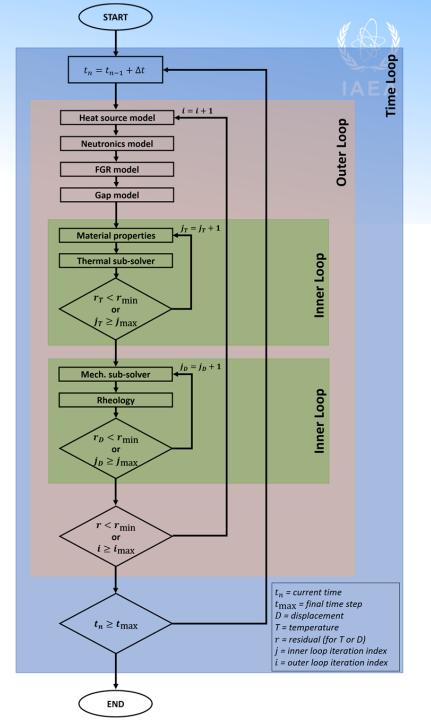


Segregated solution strategy

- Coupling through outer iterations within time step:
 - Each physics and each component solved sequentially.
 - Inner iteration for single main physics is possible.
- Convergence: user-defined residuals threshold.

$$r = \frac{1}{n} \sum |[\mathbf{b}_{\mathbf{u}}] - [\mathbf{A}_{\mathbf{u}}][\mathbf{u}]|$$

- Block-coupled approaches exist in the community (see solids4Foam or foamExtend)...
- ... potential developments for mechanics solver (i.e. solving x-, y- and z- direction in one matrix).





How to approach OFFBEAT Installation

Which OpenFOAM version?



Installation

OpenFOAM and *ParaView* can be simply installed for the first time using the **apt** package management tool. The user will need to provide superuser password authentication when executing the following commands with **sudo**

 Copy and paste the following in a terminal prompt (Applications → Accessories → Terminal) to add dl.openfoam.org to the list of software repositories for apt to search, and to add the public key (gpg.key) for the repository to enable package signatures to be verified.

Note: use secure https:// for the public key to ensure secure transfer, but use http:// for the repository, since https:// may not be supported and is not required since the key provides secure authentication of the package files.

sudo sh -c "wget -0 - https://dl.openfoam.org/gpg.key | apt-key add -"
sudo add-apt-repository http://dl.openfoam.org/ubuntu

**Note: This only needs to be done once for a given system

2. Update the apt package list to account for the new download repository location

sudo apt-get update

3. Install OpenFOAM (9 in the name refers to version 9) which also installs **paraviewopenfoam56** as a dependency.

sudo apt-get -y install openfoam9

OpenFOAM 9 and ParaView 5.6.3 are now installed in the /opt directory.

Main developments are compatible with **openfoam.org version 9** (simple installation following download page)

version 10 and 11 have abandoned AMI for mapping (relevant for gap/contact treatment)... porting to new version is in progress!

A recent branch (*develop_OF2212*) compiles both on **openfoam.org version 9** and **openfoam.com v2212**

How to get OFFBEAT



Open-source online at https://gitlab.com/foam-for-nuclear/offbeat

Open a terminal (typically inside the path OpenFOAM/<userName>-9/applications/solvers) and clone the repository:

git clone https://gitlab.com/foam-for-nuclear/offbeat.git offbeat

Move to the new folder and check the stable *master* (or the more advanced *develop*) branch

cd offbeat git checkout master

Clean (not always necessary) and install

make clean make



How to approach OFFBEAT Documentation

A quick look at the repository

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Access the documentation from main page

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IAEA

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OFFBEAT

README (appears in homepage)

OpenFOAM Fuel BEhavior Analysis Tool (OFFBEAT) is a three-dimensional finite-volume nuclear fuel performance code based on the OpenFOAM® C++ library. OFFBEAT is developed according to a cell-centered finite-volume framework solid mechanics. This is combined with a framework for thermal analysis and with numerical developments concerning the treatment of the gap heat transfer and contact, based on a mapping algorithm that allows the use of independent non-conformal meshes for fuel and cladding. The code considers the temperature and burnup dependence of the material properties, and it can model fuel densification, relocation, swelling, growth, fission gas release, creep, plasticity, and other relevant fuel behavior phenomena. OFFBEAT is a joint development by the Laboratory of Reactor Safety (LRS) at École Polytechnique Fédérale de Lausanne (EPFL) and Laboratory for Reactor Physics and Thermal-Hydraulics (LRT) at the Paul Scherrer Institut (PSI).

OpenFOAM version

The current version of OFFBEAT is based on OpenFOAM-9.0 from the OpenFOAM Foundation.

Documentation

Some useful documentation for the code usage is accessible at the following link: Doxygen documentation.

Forum

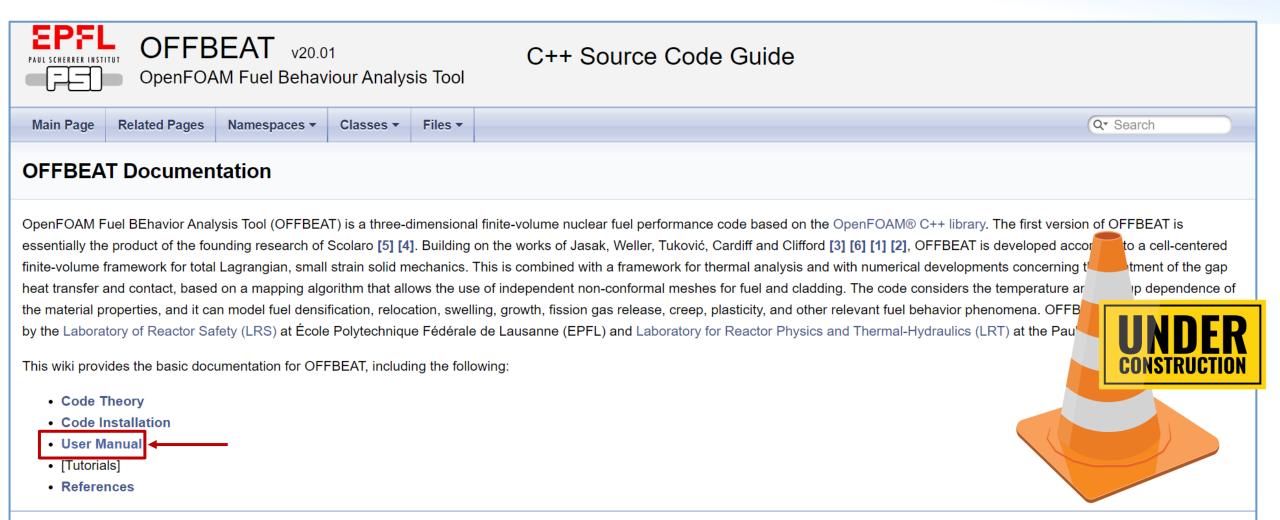
A forum to get support from the developers and the community is available at the following link : Forum

Documentation



Doxygen generated documentation at https://foam-for-nuclear.gitlab.io/offbeat/index.html

The documentation is constantly improving! Please report issues, typos or suggest corrections/new content!





OFFBEAT v20.01 C++ Source Code Guide OpenFOAM Fuel Behaviour Analysis Tool C++ Source Code Guide								
Main Page	Related Pages	Namespaces -	Classes -	Files -	Q- Search			
User Ma	nual							
-	-	uide assume that th tionary format for C		pasic understanding of OpenFOAM usage, including the basic workflow (mesh-generation, preprocessing, running solvers and post	processing). The user			
We recomme	nd that new users	work through the C)penFOAM v9	User Guide before attempting to use OFFBEAT.				
				enFOAM (e.g. icoFoam, pisoFoam, etc.) in that the user provides a mesh, control dictionary controlDict, solution parameters fvS ctionary solverDict, and with intial and boundary conditions for the main fields in the initial time step folder (e.g. the folder 0/).	olution and schemes			
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Heat source model

The heatSource class is used to enable the modeling of a heat source in OFFBEAT.

The power density or heat source density field is by default named ${f Q}$ and is in $W/m^3.$

Note on heat source modeling

Traditional 1D codes typically require as an input the radially averaged linear heat generation rate (lhgr) as a function of time, and often allow the user to provide a axial profile. For 3D codes with arbitrary geometries and unstructured meshes like OFFBEAT, it is less straightforward to define the heat source field or the power density field.

For scenarios where the power density field is not symmetric, the simplest way to define the heat source field is to couple OFFBEAT with a neutronics/multiphysics solver that directly provides the 3D field and use the **fromLatestTime** heat source model. Alternatively, one can define the power density field using OpenFOAM tools such as topoSet (e.g. for creating fields of heat source that can be modeled as mathematical functions).

On the other hand, for simulations (even in 3D) where the heat source is assumed to be uniform along the azimuthal angle, one can use the lhgr models developed specifically for OFFBEAT. These models are listed below.

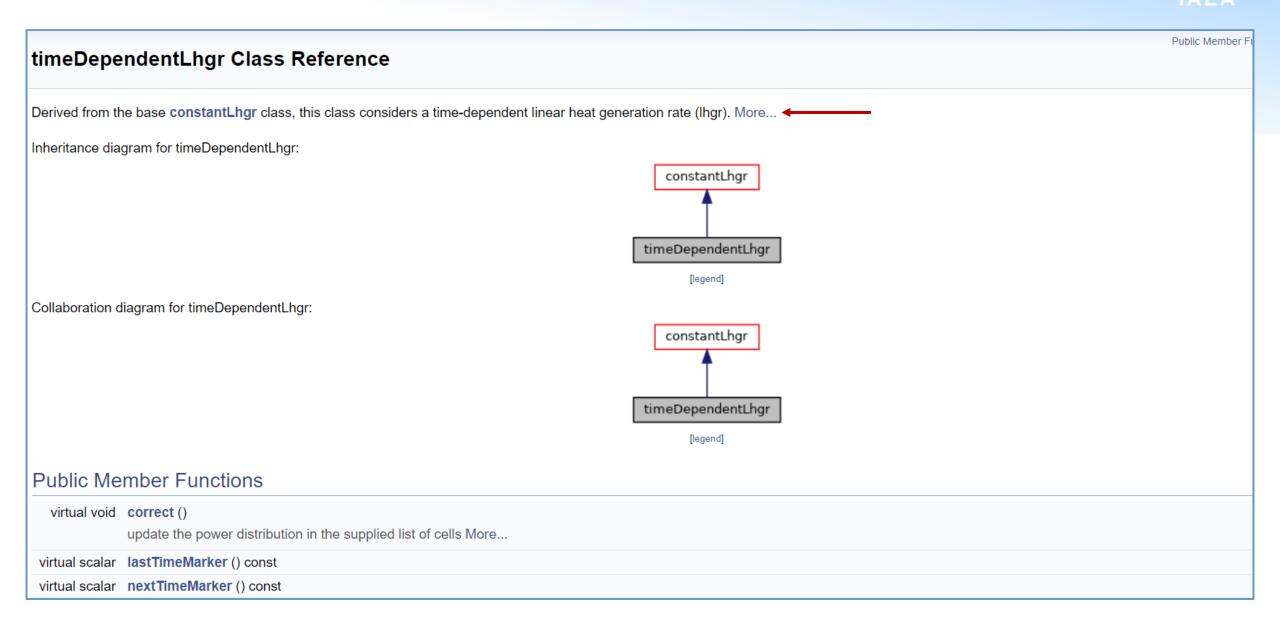
Usage

The heat source model must be selected with the heatSource keyword in the main dictionary of OFFBEAT (i.e. the solverDict dictionary, located in the constant folder).

Currently OFFBEAT supports the following heat source models:

- fromLatestTime, for a heat source field that is read from the Q file in the starting time folder
- <u>constantLhgr</u> for traditional fuel rod simulations where one needs to impose a constant linear heat generation rate (with the possibility of adding a time-dependent radial/axial profile)
- timeDependentLhgr, for traditional fuel rod simulations where one needs to impose a time-dependent linear heat generation rate (with the possibility of adding a time-dependent radial/axial profile)
- timeDependentVhgr, for traditional fuel rod and TRISO simulations where one needs to impose a time-dependent volumetric heat generation rate

Return to Setting the solverDict





Detailed Description

Derived from the base constantLhgr class, this class considers a time-dependent linear heat generation rate (lhgr).

User documentation for timeDependentLhgr heatSource class

For general instructions on the modeling of a heat source in OFFBEAT see here.

Similar to the constantLhgr heatSource class, the timeDependentLhgr class in OFFBEAT allows you to set a average **linear heat generation rate (lhgr)**. The main difference is that the lhgr provided by the user can vary over time. It is also possible to apply a radial and an axial profile to the lhgr. Note that even if the lhgr is constant over time, the axial and radial profile might change over time, depending on the profile type chosen by the user.

Formulation

The final volumetric heat source is derived as a combination of lhgr, radial and axial profiles, as follows:

$$Q(t, r, z) = Q_{avg}(t) \cdot f(r, t) \cdot g(z, t)$$

where:

- r is the relative radial position (0...1)
- *z* is the relative axial position (0...1)
- t is the current time
- f(r,t) and g(z,t) are the radial and axial profiles, respectively
- Q_{avg} is the average power density in W/m^3 .

The radial and axial profiles are expected to be normalized to 1, while the average power density is obtained from:

$$Q_{avg}(t) = rac{lhgr(t) \cdot h_{ref}}{rac{V_{model}}{lpha}}$$

where:

• href is the height of the rod in the reference, undeformed geometrY

Most physics and models have a page in the User Manual



Usage

To use the timeDependentLhgr heat source model in OFFBEAT, you will need to specify it in the solverDict dictionary using the following syntax:

heatSource timeDependentLhgr;

The timeDependentLhgr heat source model requires the user to specify a few additional parameters in the heatSourceOptions sub-dictionary:

- timePoints A list of time values at which the lhgr is provided. The time unit depend on the userTime selected by the user (seconds by default).
- 1hgr A list of lhgr values in W/m, one value per time-point.
- timeInterpolationMethod Select the time interpolation method for time steps that fall in between the time points indicated in the timePoints list.
- materials A list of material (or cellZones names) where the heat source model applies.
- axialProfile A sub-dictionary that specifies the type of axial profile.
- radialProfile A sub-dictionary that specifies the type of radial profile.

The timeDependentLhgr heat source model is designed to calculate the volumetric power density for a cylindrical rod with an initial reference height (i.e., in undeformed geometry) along a given axial direction. For simulations where there is an axis of symmetry, the class can take into consideration the angular fraction of the real rod that is being modeled.

Thus, the class requires the following additional parameters in the globalOptions sub-dictionary of the solverDict dictionary:

- pinDirection The vector of the axial direction (e.g. (0 0 1) for the z-axis).
- angularFraction The fraction of the 360 degree angle that is being modeled. NOTE: Remove this keyword for axisymmetric r-z models, as the angular fraction is automatically calculated from the wedge boundaries. Otherwise, it must be provided. For example, set it to 0.25 for quarter symmetry, to 0.5 for half-symmetry and to 1.0 for 3D simulations.

Most physics and models have a page in the User Manual



Examples

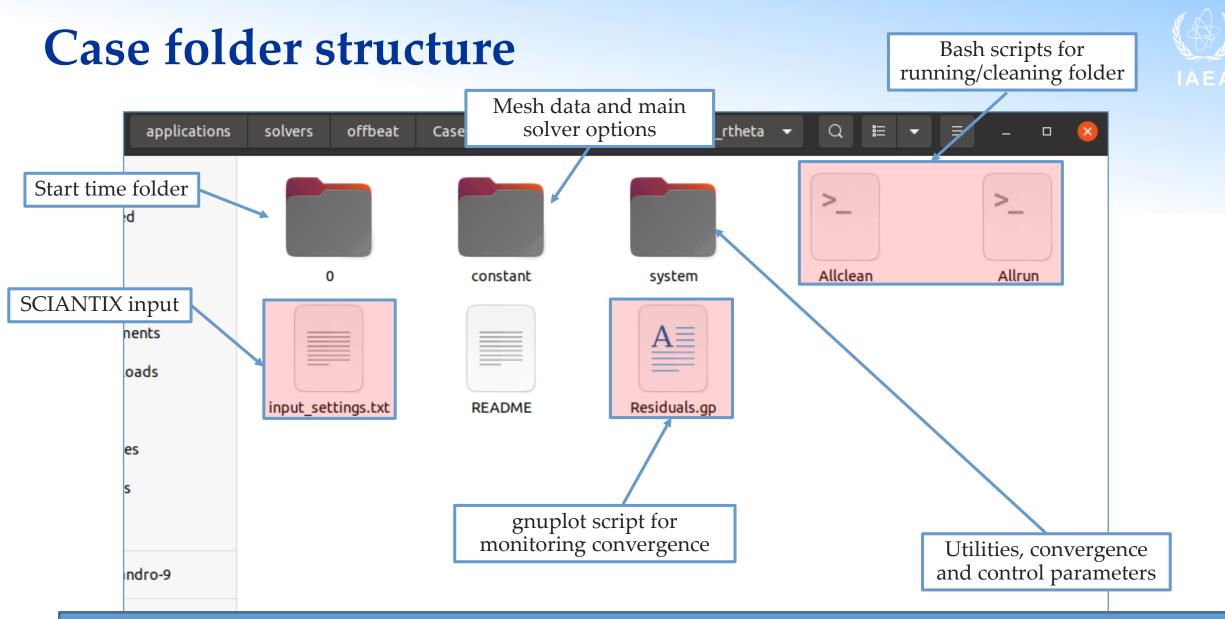
Here is an example of the solverDict to be used for the case of a lhgr that ramps to 10 kW/m in 1hr time, remains constant for a year, and then ramps down to 0 in 1 hr. This particular example considers fla axial and radial profiles, and a quarter of a fuel disc model.

```
heatSource timeDependentLhgr;
globalOptions
   angularFraction 0.25;
   pinDirection (0 0 1);
}
heatSourceOptions
 11
                                  1yr+1hr
              t0 1hr
                         1yr
 timePoints ( 0
                   3600
                        31536000 31539600);
             ( 0
                   100e2 100e2
                                           );
 lhgr
                                   0
 timeInterpolationMethod linear; //step;
   materials ( fuel );
   axialProfile
    ł
```

type flat.



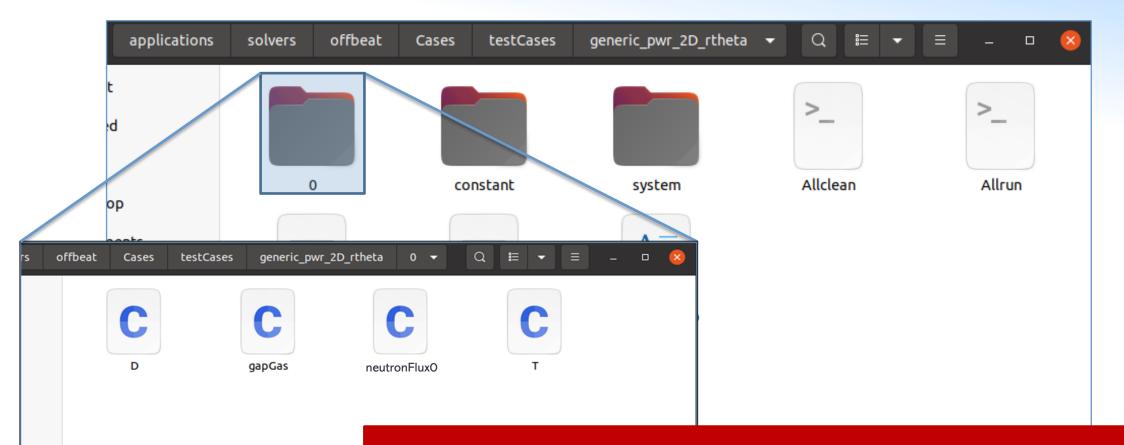
Case folder



The Allrun and Allclean bash scripts can be used to run the case or clean the folder... ... but in the next slides we will unpack each command from mesh creation to data post-processing!

Case folder structure: the initial time folder



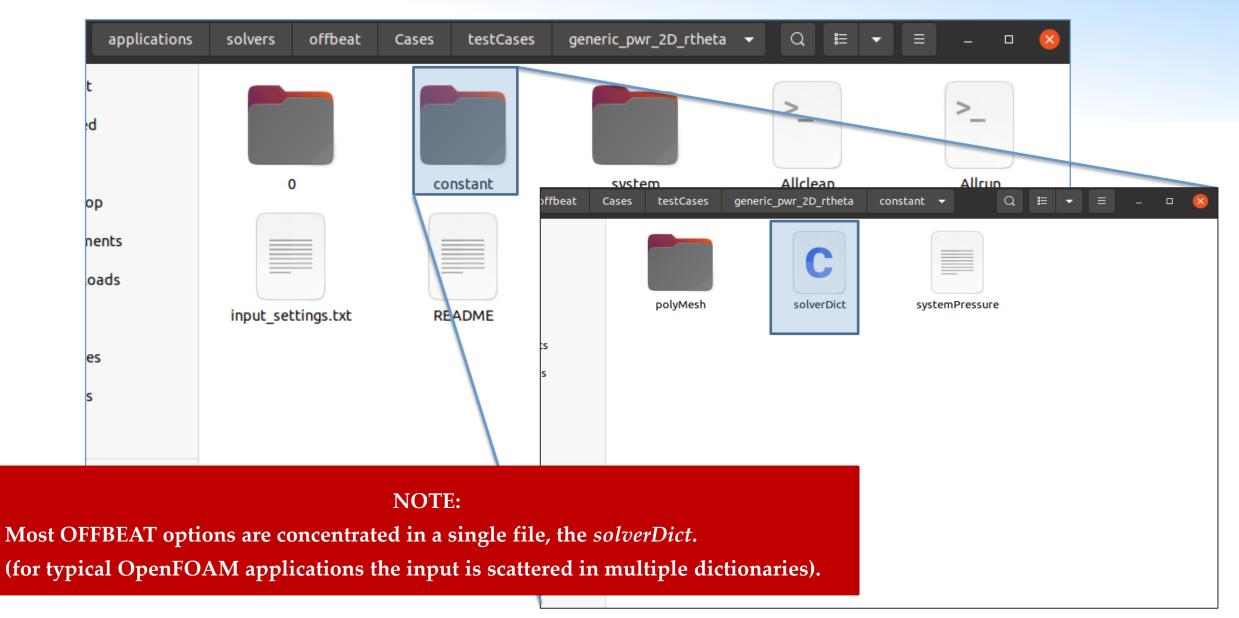


NOTE:

- It is fundamental to set meaningful and realistic boundary and initial conditions.
- The initial time step folder contains a separate file for each main field/quantity for which it is necessary to set initial and boundary conditions.

Case folder structure: the solverDict





Case folder structure: the solverDict

	IAEA
physics and models;	<pre>// Thermal and Mechanical solver selection: thermalSolver solidConduction; mechanicsSolver smallStrain; neutronicsSolver diffusion // Material and rhelogy treatment: materialProperties byZone;</pre>
st physics and models;	<pre> mechanicsSolverOptions { forceSummary on; }</pre>
aterial properties, rheology etc. 🔔	<pre>materials { fuel { } </pre>

3 main sections:

Global options for selecting •

• Separate dictionaries for mos

• A materials dictionary for ma

How to model multiple materials in a single mesh?





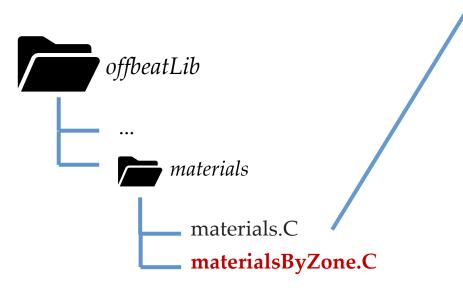
- Handles material properties and behavioral models.
- Stores material addressing (accessed by most other OFFBEAT classes).



collection of cell IDs with the same name (e.g. *fuel* or *cladding*)

IMPORTANT!

- Make sure that you can separate mesh into cellZones (might be called in different ways e.g. *groups* in Salome).
- The mesh creation utility (e.g. *gmshToFoam*) takes care of converting the format



How to select material properties?



Example (pseudo-input)

```
materials
{
     `fuel.*'
           material UO2;
            ...
     cladding
           material zircaloy;
            ...
     ...
```

Subdictionary inside *\$CASE/constant/solverDict*:

• One (and only one) subdictionary per zone.

cellZone naming:

- No specific rules (case sensitive).
- No specific order in the *materials* dictionary
- Collective **wild cards** are possible (e.g. several cellzones with identical portion of the name such as *fuel1*, *fuel2*, *fuel3* etc.).

Define a *constant* **material**

```
// List of materials, one per cellZone.
materials
{
    . . .
   cladding
       material constant;
                  rho [1-3000]
                                         6560;
       rho
                      [0 2 -2 -1 0]
                                        285;
       Ср
                  Ср
                        [1 1 3 -1 0]
                  k
       k
                                         21.5;
       emissivity emissivity [0 0 0 0 0]
                                         0.808642;
       Е
                  Е
                          [1 -1 -2 0 0]
                                        9.93e10;
                          [00000]
                                         0.37;
                  nu
       nu
                  G [1 -1 -2 0 0] 3.6241e+10;
       G
              alpha [00000]
       alpha
                                        6e-6;
                          [0 0 0 1 0]
       Tref
                  Tref
                                         300;
       . . .
    . . . .
```

- All thermo-mechanical properties must be provided.
- Material properties do not evolve over time.
- Behavioral models are not taken into account.



Select a preset material



Example (pseudo-input)

materials		
{		
fuel		
{		
	material UO2;	
	densityModel	UO2Constant;
	heatCapacityModel	UO2MATPRO;
	conductivityModel	UO2MATPRO;
	densificationModel	UO2FRAPCON;
	resinteringDensityCh	ange 0.1;
	swellingModel	none;
}		

- Available materials:
 - UO₂
 - MOX
 - Zircaloy
 - A few others (molybdenum, Inconel600)
- Specific correlations and models selected by default.
- Different correlations and models can be selected with the keyword '\$property_name\$Model'
- Often behavioral models (even if the default ones) might require additional input (relocation and densification in particular, check the documentation)
- Behavioral models can be switched off.



Test cases (check the develop branch)

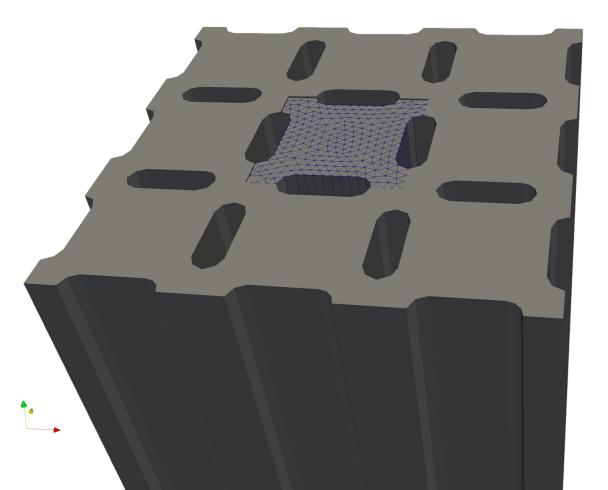
Graphite stringer - overview



- Complex shape derived from MSRE:
 - Fraction of power released in graphite
 - Interest to know temperature distribution
- Triangular prisms mesh form Salome (NETGEN algorithm)
- Transient simulation (from 0 to 100 s)

ddt	Schemes		
{			
	default	Euler;	
}			

• NOTE: power density increased 100x w.r.t MSRE



Graphite stringer - overview



• Purely thermal case (in **constant/solverDict**)

thermalSolver	solidConduction;			
mechanicsSolver	fromLatestTime;			
neutronicsSolver	fromLatestTime;			
elementTransport	fromLatestTime;			
materialProperties	byZone;			
rheology	byMaterial;			
<pre>// With fromLatestTime the power Q will be read // directly from the 0/ folder heatSource fromLatestTime;</pre>				

• Constant graphite properties (in **constant/solverDict**)

materia {	ls					
str	ringer					
{						
	material		C	constant;		
	// Values f					
	// At https	://doi.or	rg/10.	1016/j.pnu	cene.2015.02.014	
	rho	rho	[1 -3	8000]	1874;	
	Ср	Ср	[0 2	-2 -1 0]	1772;	
	k	k	[1 1	3 -1 0]	53;	

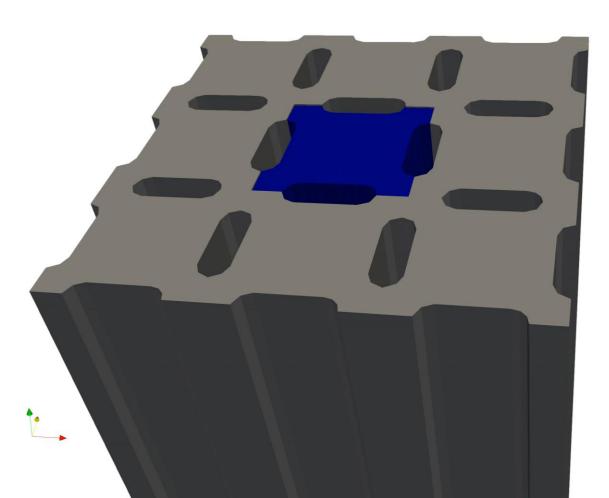
• Non-uniform **Q** field (in **0**/ folder) with **codeStream**

```
internalField #codeStream
{
    code
    #{
        const IOdictionary& d = static_cast<const IOdictionary&>(dict);
        const fvMesh& mesh = refCast<const fvMesh>(d.db());
        scalarField fld(mesh.nCells(), 2.5e7);
        const vectorField& C(mesh.C());
        scalar pi(Foam::constant::mathematical::pi);
        forAll(fld, i)
        {
            scalar Cz(C[i].z());
            fld[i] *= cos((Cz-1)*pi/2 );
        }
        writeEntry(os, "", fld);
    #};
```

• Fixed-value BC could be changed for more realistic BCs or coupling with TH

Graphite stringer - result





Copy folder from Cases/testCases/graphite_stringer

Use **Allrun** script or

- 9.8e+02

- 970

- 960

950

940

- 930

9.2e+02

- Create mesh with:
 ideasUnvToFoam stringer.unv
- Run the case with:
 offbeat

Check results with:

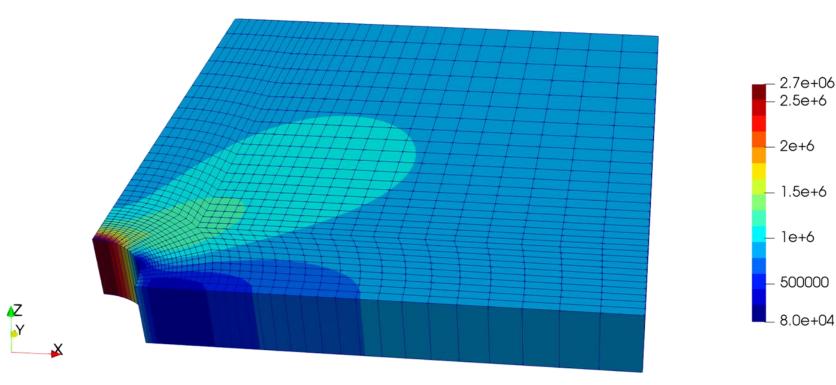
paraFoam

Mechanics-only cases



sigmaEq

- For mechanics-only test cases check the folder **Cases/Verification**:
- multiMaterial/multiMaterialBlock and multiMaterial/multiMaterialCylinder
- thickCylinderExpansion
- plateHole



Hot bi-material cylinder - overview

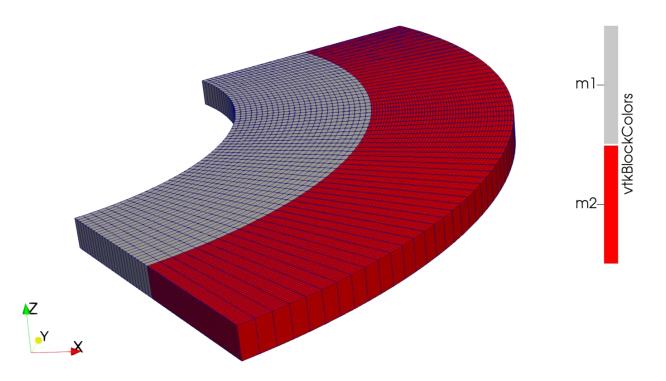
IAEA

- Bi-material cylinder subjected to temperature and pressure gradient from inner (800 K, 1e7 Pa) to outer surface (300 K, 1e5 Pa).
- Thermo-mechanical case (in **constant/solverDict**)

//- Select the physics	to solve for		
thermalSolver	<pre>solidConduction;</pre>		
mechanicsSolver	smallStrain;		
neutronicsSolver	fromLatestTime;		
elementTransport	fromLatestTime;		

٠

Two cellzones with different material properties defined in constant/solverDict.materials



Hot bi-material cylinder - overview

- Bi-material cylinder subjected to temperature and pressure gradient from inner (800 K, 1e7 Pa) to outer surface (300 K, 1e5 Pa).
- Thermo-mechanical case (in **constant/solverDict**)

//- Select the physics	to solve for		
thermalSolver	<pre>solidConduction;</pre>		
mechanicsSolver	<pre>smallStrain;</pre>		
neutronicsSolver	fromLatestTime;		
elementTransport	<pre>fromLatestTime;</pre>		

•

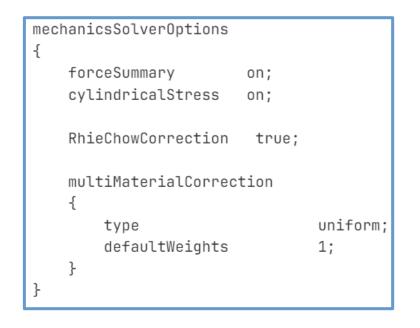
Two cellzones with different material properties defined in **constant/solverDict.materials**

```
materials
{
    inner
        material
                    constant;
                    "rho" [1 -3 0 0 0] 8000.0;
        rho
                    "Cp" [0 0 0 0 0] 1000.0;
        Сp
                    "k" [0 0 0 0 0] 50;
        k
                    "alpha" [0 0 0 -1 0] 5e-6;
        alpha
        emissivity "emissivity" [0 0 0 0 0] 0.7;
                    "E" [0 0 0 0 0] 200e9;
        F
                    "nu" [0 0 0 0 0] 0.3;
        nu
                    "Tref" [0 0 0 1 0] 300;
        Tref
        rheologyModel
                                    elasticity;
    }
    outer
                    constant;
        material
                    "rho" [1 -3 0 0 0] 8000.0;
        rho
                    "Cp" [0 0 0 0 0] 1000.0;
        Cр
                    "k" [0 0 0 0 0] 20;
        k
                    "alpha" [0 0 0 -1 0] 5e-6;
        alpha
        emissivity "emissivity" [0 0 0 0 0] 0.7;
                    "E" [0 0 0 0 0] 50e9;
        Е
                    "nu" [0 0 0 0 0] 0.35;
        nu
                    "Tref" [0 0 0 1 0] 300;
        Tref
        rheologyModel
                                    elasticity;
```

Hot bi-material cylinder – multiMaterialCorrection

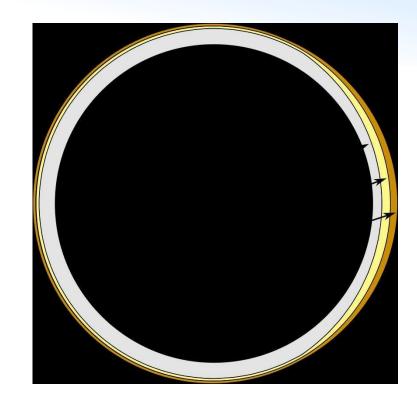


 multiMaterialCorrection must be activated (in constant/solverDict)



- Why? Only displacement and normal stress must be *continuous* at the interface...
 - ... but material properties (E, μ , ν) and gradient of displacement *not necessarily!*

• Interest for coated fuels, clad with liners, oxide layers

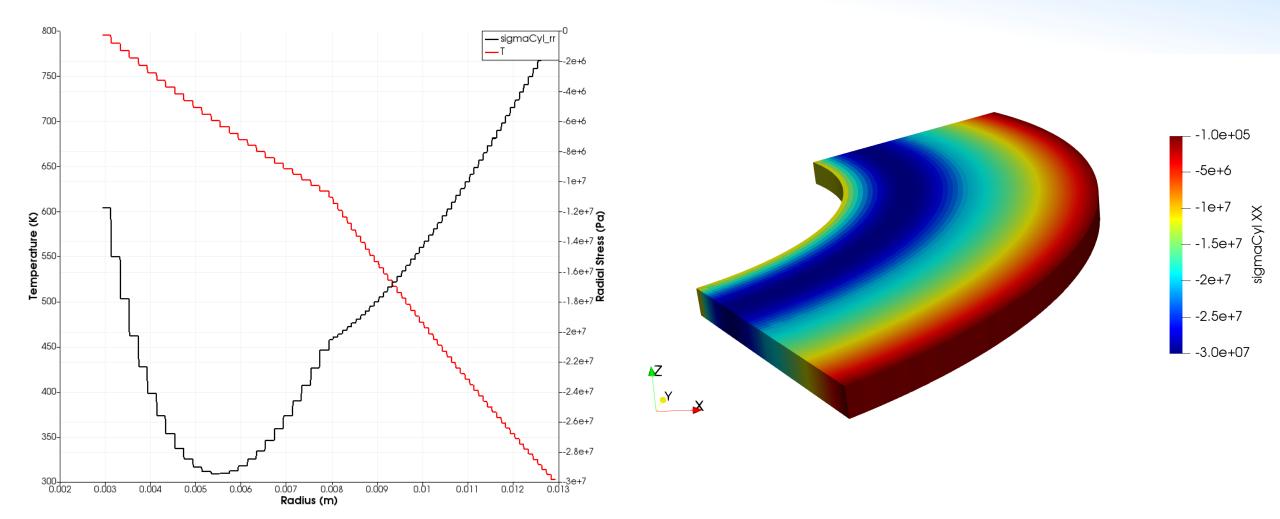


NOTE:

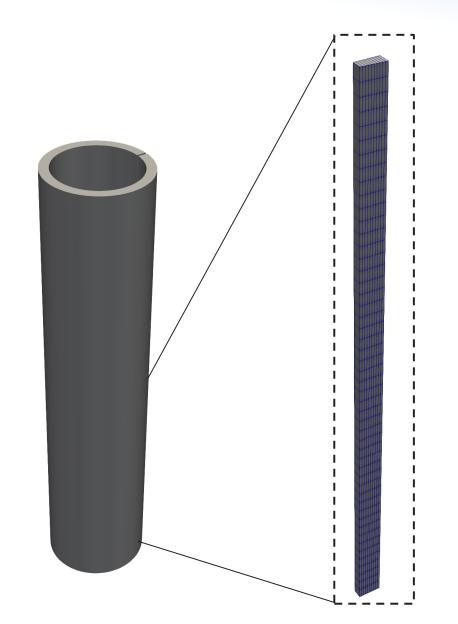
- Similar situation when modeling coarse meshes with high gradients in temperature or strains.
- We find benefit from applying this correction even in the abscence of actual multi-material bodies.

Hot bi-material cylinder - results





Generic PUZRY - overview





- Experiments performed to study clad burst during LOCA
- Short Zircaloy segments (5cm) internally pressurized until failure:
 - Different pressure ramp rates
 - Different temperature levels
- Half-symmetry model created with blockMesh
- Thermo-mechanics case (constant/solverDict) with incremental mesh-updated solver

thermalSolver	solidConduction;
mechanicsSolver	smallStrainIncrementalUpdated;
neutronicsSolver	fromLatestTime;
elementTransport	fromLatestTime;

Generic PUZRY – Time-dependent BCs



Time-dependent inner pressure (0/DD.boundaryField)

```
inner
{
                    tractionDisplacement;
   type
   pressureList
    {
                        table;
        type
                        "$FOAM_CASE/constant/data/p_PUZRY";
       file
       format
                        foam;
        outOfBounds
                        clamp;
        interpolationScheme linear;
   traction
                    uniform (000);
   relax
                    1;
                    $internalField;
   value
```

Time-dependent outer temperature (**0/T.boundaryField**)

```
outer
{
   type timeDependentAxialProfileT;
   axialProfileDict
   {
      axialLocations ( 0 0.005 0.01 0.015 0.02 0.025 );
      #include "$F0AM_CASE/constant/data/Tprofile_PUZRY";
   }
   value $internalField;
}
```

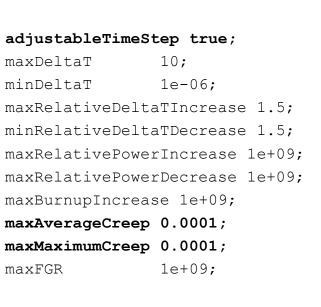
Generic PUZRY – LOCA creep model



Creep (LOCA) rheological model for cladding in (constant/solverDict.materials)



Creep increment dictate time-step size (system/controlDict)



runTimeModifiable true;

NOTE:

- Creep might need relaxation (sometimes as low as 0.1).
- For most simulations relax can be set to 1 (and for some other simulations not under-relaxing creep even improves stability...)

Generic PUZRY - result





1.5e+08

- 1.4e+8

- 1.3e+8

- 1.2e+8 - 1.1e+8

1e+8

-9e+7 5

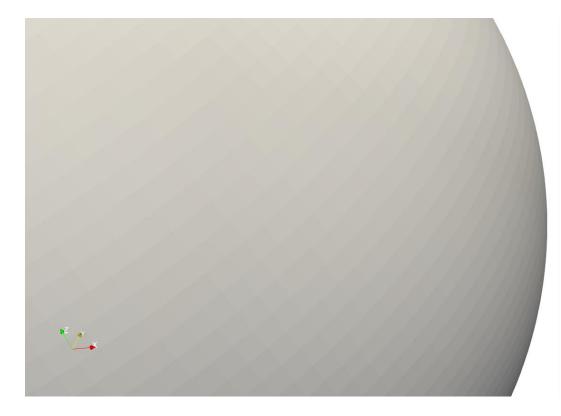
- 8e+7

– 7e+7 – 6e+7 – 5e+7 – 4.1e+07

- Copy folder from Cases/testCases/generic_PUZRY
- Use **Allrun** script or
 - Create mesh with:
 blockMesh
 - Run the case with:offbeat
- Check results with: **paraFoam**
- Failure takes place at 1118.16 seconds ... lots of time-step are needed due to high creep-rate!

Generic TRISO - overview

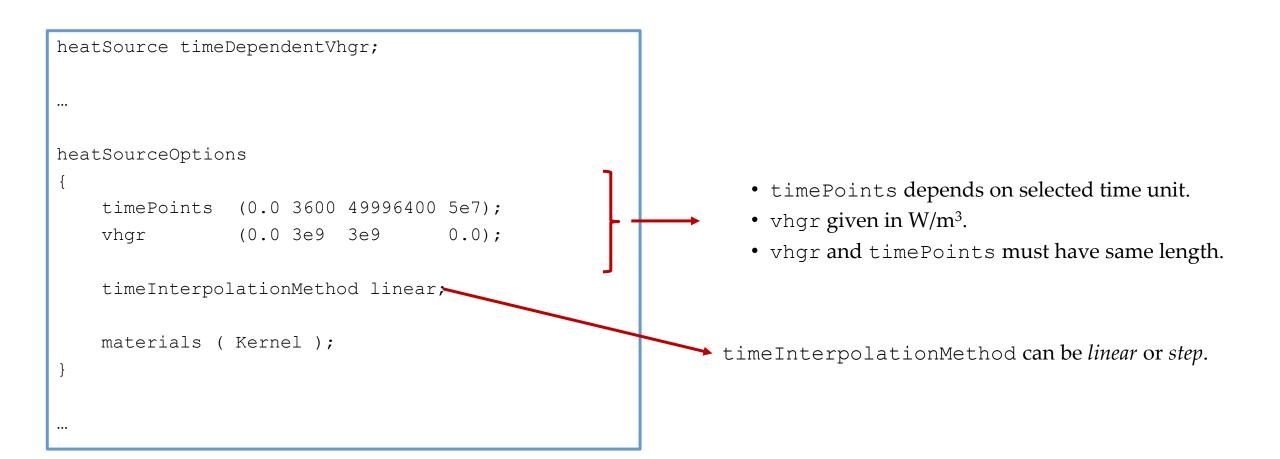




- TRISO fuel case derived from IAEA benchmark
- Double wedge geometry for spherical symmetry (1D case)
- Multiple layers: kernel, **buffer**, **IPyc**, **SiC** and **OPyC**
- Material models for each layer defined in **solverDict**
- Multi-material correction necessary
- Buffer and IPyC start already detached (automatic debonding is on its way...)

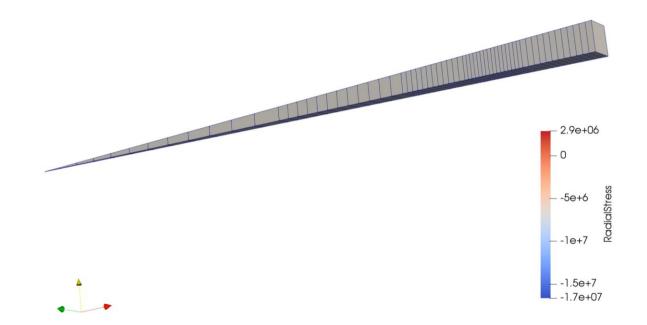
Generic TRISO – time-dependent heat source

A time dependent heat source can be set in **constant/solverDict/heatSourceOptions** (Similar syntax for setting a linear heat rate or lhgr for rod cases)



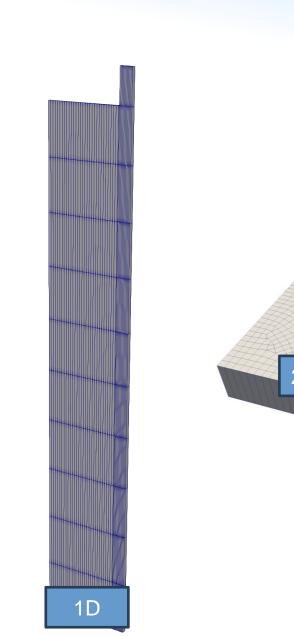
Generic TRISO - result



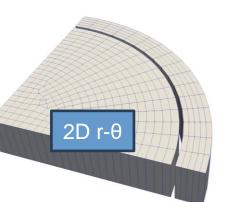


- Copy folder from Cases/testCases/generic_TRISO
- Use **Allrun** script or
 - Create mesh with **blockMesh**
 - Run the case with **offbeat**
- Check results with **paraFoam**

Generic PWR - overview



2D r-z

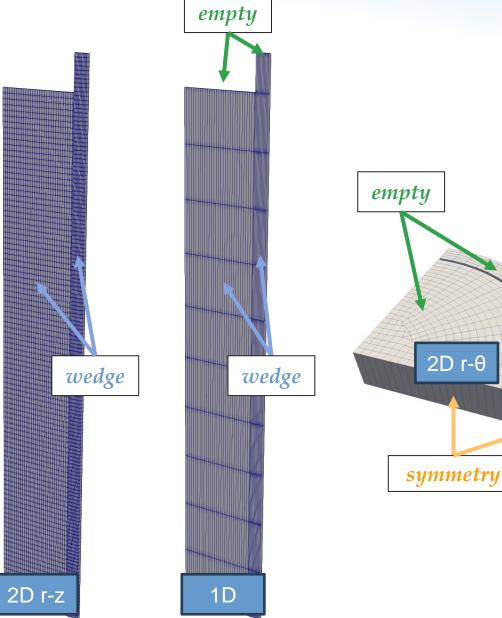


- Generic PWR rod irradiated for 1 year
- *More complex case*! Most models are activated:
 - Gap gas model
 - Burnup
 - Axial profile linear heat source
 - Contact, gap heat transfer etc...
- 3 versions available:
 - 1D coarse mesh
 - 2D r-z fine mesh (smeared column)
 - 2D r- θ (disc)



Generic PWR - setting the geometry





• *wedge* type patches makes the case axisymmetric 2D: OFFBEAT neglects solution along y (i.e. azimuthal direction).

• The addition of *empty* type patches on top and bottom makes the case 1D (we need to activate the switch *modifiedPlaneStrain*)

• Alternatively, 1-cell-thick disc with *empty* patches makes the case 2D in the r-theta plane

Tools for mesh generation

- *blockMesh* good tool for axisymmetric geometries (1D and 2D r-z).
- *rodMaker.py* available in the *tools*/ folder.
- A similar script can be found in the TRISO tutorial and verification cases for TRISO 1D geometries

Name	Last commit	Last update
 P README	Initial commit (14.09.2022)	1 week ago
	Initial commit (14.09.2022)	1 week ago
🕒 rodDict	Initial commit (14.09.2022)	
🔶 rodMaker.py	Initial commit (14.09.2022)	rodMaker is not You can use dire

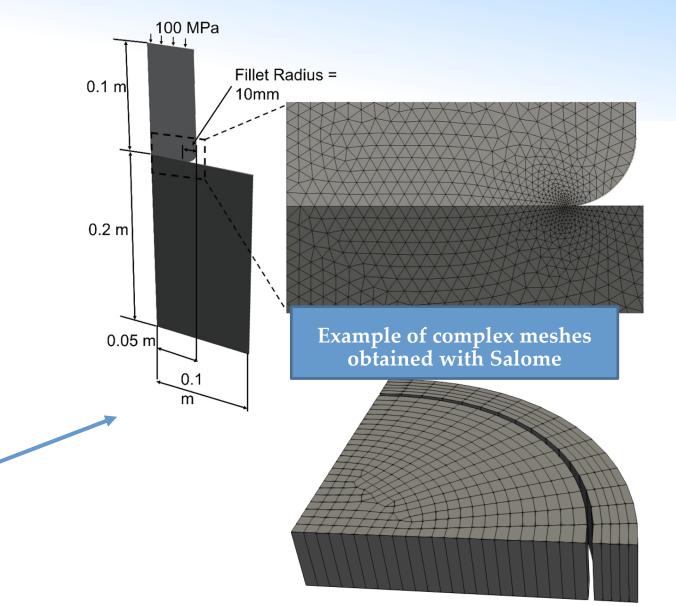
######################################	JT SECTION ####################################
{	
# Either '1D', '2Dsmeared', '2D' 'geometryType':	Ddiscrete' '1D',
<pre># Angle of the wedge, degrees 'wedgeAngle':</pre>	0.25,
<pre># Unit conversion (e.g. 0.001 f 'convertToMeters':</pre>	for units in mm) 0.001,
· · · · · · · · · · · · · · · · · · ·	f the rodDict input file the rodMaker.py
<pre># Block names (one per block) 'blockNameFuel': 'blockNameClad':</pre>	['fuel'], ['cladding', 'cladding'],
# Inner radii (one per block) 'rInnerFuel': 'rInnerClad':	[0.0], [4.565, 4.565],
<pre># Outer radii (one per block) 'rOuterFuel': 'rOuterClad':</pre>	[4.5], [5.315, 5.315],
<pre># Height (or lenght) of each bl # (e.g. [1500, 1500] for a 3000 'heightFuel': 'heightClad':</pre>	· · · · · · · · · · · · · · · · · · ·
<pre># Starting vertical offset 'offsetFuel':</pre>	0.0.
NOTE:	
necessary to create OFFI	BEAT geometries!

Tools for mesh generation



• *blockMesh* good tool for axisymmetric geometries (1D and 2D r-z).

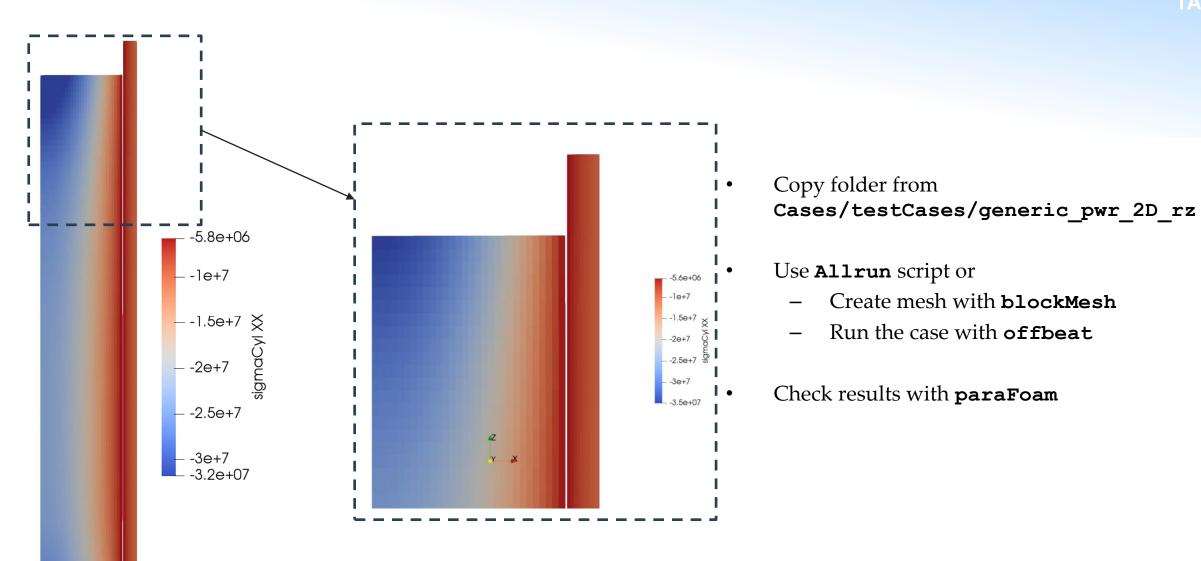
- *rodMaker.py* available in the *tools*/ folder.
- A similar script can be found in the TRISO tutorial and verification cases for TRISO 1D geometries



Limited to structured meshes!

Difficult to extend to complex 3D cases!

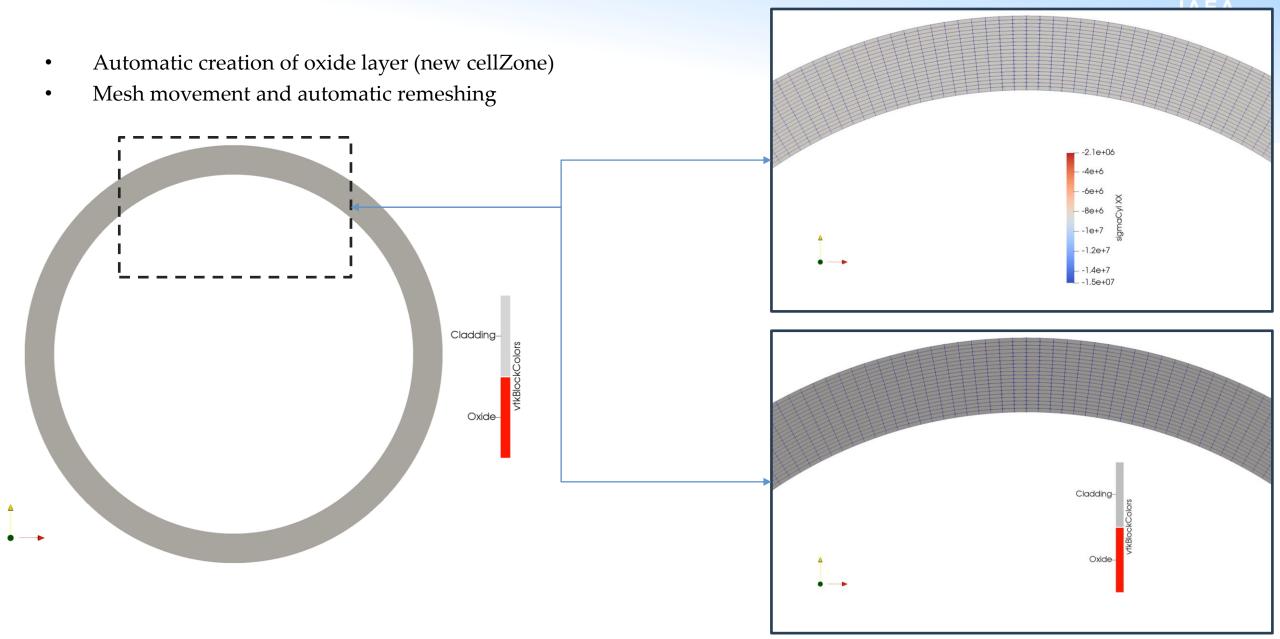
Generic PWR - results





Cladding corrosion – coming soon!







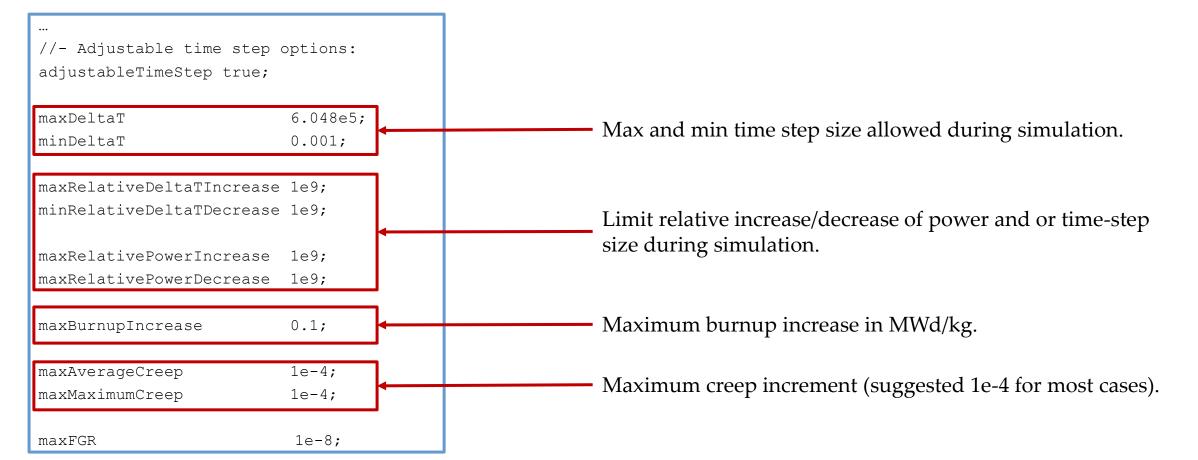
Tips & tricks

Time stepping

A dynamic time-step size is often fundamental to:

- Manage the computing time (e.g. avoid too long simulations).
- Improve convergence (e.g. when creep is activated and time steps need to adapt to creep rate).

Dynamic time step size can be activated in the *controlDict* file in the *system*/ folder:





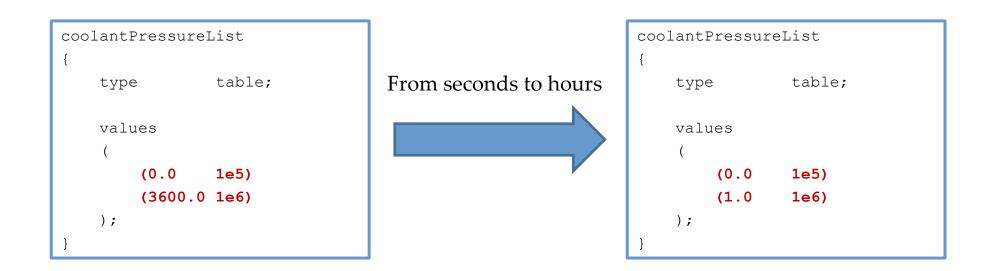
Time unit

- OpenFOAM time unit is seconds.
- Not always convenient for fuel performance simulations.
- In OFFBEAT the time step unit can be changed in the *controlDict* file.

userTime
{
<pre>// type is seconds by default</pre>
<pre>type seconds;//hours;//days;</pre>
}

NOTE:

When changing time unit all time-dependent input must be changed accordingly!





Simulation control

Main controls are in *fvSolution* file inside *system*/ folder

- nCorrectors: number of inner iterations for main physics (neutronics, thermal, mechanics).
- maxOuterIter: maximum number of outer iterations before end of time step (if not converged yet).
- D, T, neutronFlux0: are the residual thresholds. Values between 1e-6 and 1e-5 work best.
- relaxationFactors: relax main fields such as D and T. Values between 0.8 and 1 work best.
- It is also possible to relax the equations and not the fields, but typically it has worse convergence properties.

master	~	offbeat / Cases	/ testCases / gene	eric_pwr_2D_rTheta / system / fvSolutio
		o Scolaro authored	1 week ago	
🕒 fvSolutio	on la	5 1.73 KiB		Main controls
45	str	essAnalysis		
46	{	-		
47		nCorrectors	1;	
48		maxOuterIter	1000;	
49		referencePairs	() .	
50 51		reterencePairs	();	
52		D	(1e-5 1 1e-5	5):
53		T	1e-5;	- , ,
54		neutronFlux0	1e-5;	
55				
56		relD	1e-6;	
57		relT	1e-6;	
58 59	}	relneutronFlux0	1e-6;	
60	ſ			
61	rel	axationFactors		
62	{			-
63		fields		
64		{		
65		D 0.8;		
66 67		// T 0.8;		
68		// neutronF ા	lux0 0.9;	
69		/*		
70		, equations		

Simulation control

Other three important relaxation parameters:

- Relax the heat transfer coefficient in fuelRodGap in the thermal BCs.
- Relax interface pressure in gapContact in the mechanics BCs.
- Relax creep in the rheologcal model dictionary for a specific material.

ШψС/10Ц/0/1.	
fuelOuter	
{	
type	fuelRodGap;
patchType	regionCoupledOFFBEAT;
kappa	k;
coupled	true;
alpha	uniform 5000;
roughness	uniform 2.2e-6;
value	<pre>\$internalField;</pre>
relax	1;
}	

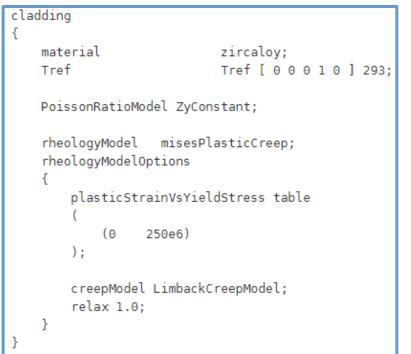
In *\$CASE/0/D*:

"fuelOuter|cladInner"

gapContact; type patchType regionCoupledOFFBEAT; penaltyFactor 0.1; frictionCoefficient 0; relax 1.0; relaxInterfacePressure 0.1: traction uniform (0 0 0); pressure uniform 15.5e5; value \$internalField;



In *\$CASE/constant/solverDict:*



In *\$CASE/0/T*:

Troubleshooting



Sometimes the simulation might fail or might have problems converging.

- 1. Always checks the residuals: the simulation might go on but the residual might not properly converge.
- 2. Check the mesh: is it valid? Are the patch name assigned correctly?
- 3. Check the BC conditions: is the body properly fixed? Are the BC for the top cladding and fuel surfaces correct?
- 4. Check the solverDict: start from the main solvers and then focus on the finer options.
- 5. Check the relaxation factors:
 - fuelRodGap relaxation and gapContact tend to be activated most of the time (down to 0.1).
 - Fields relaxation often helps too (0.9 is a typical value).
 - Creep as a last resource might help the simulation to converge.
- 6. Check the time step size: is the initial time step too large for the creep to converge? Does the creep time-stepping criterion need to be tighter?

Conclusions



- OFFBEAT is open-source!
 - Download it from: <u>https://gitlab.com/foam-for-nuclear/offbeat</u>
 - It consists of a thermo-mechanics library for application in nuclear engineering.
 - Documentation has recently improved significantly and will continue to grow!
- Extensive verification and ongoing validation for several different conditions
- Large scope of possible applications (even beyond the fuel rod)!
- Interesting features are coming soon, such as:
 - Mesh movement/modification capabilities for corrosion, porosity, layer detachment.
 - More tutorials e.g. for RIA, LOCA.
 - Examples of coupling with TH (or integration with GeN-Foam in a unified library).
- Contributions, comments, suggestions, bug reports etc. are more than welcomed!
- Get in touch with us if you want to participate to the project

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Thank you!

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