The development of the 3D fuel behavior code OFFBEAT

A. Scolaro, EPFL
I. Clifford, PSI
C. Fiorina, EPFL
A. Pautz, EPFL - PSI
Motivations for a novel fuel performance code

- **OpenFOAM Fuel BEhavior Analysis Tool (OFFBEAT):**
  - developed since 2 years at the LRS-EPFL and at the PSI.
  - main focus are local **multi-physics** and **multi-dimensional** aspects of fuel behavior.

- Recent fuel failure (Swiss NPP) and followup analysis at PSI.
  - need for higher-fidelity tools.

- Existing 2D/3D codes (BISON, ALCYONE, DIONISIO etc.) not easily accessible.

- Lab expertise with OpenFOAM® C++ library
Not "just" CFD! OpenFOAM is a toolbox for PDEs solution and multi-physics problems.

Many applications outside of CFD, e.g.:
- Chemistry and combustion or fluid-structure Interaction.
- Nuclear Reactor Analysis (GeN-Foam at EPFL-PSI).


OpenFOAM as a toolbox for engineering applications

- OpenFOAM comes with useful features:
  - inherently 3D library, but 2D and 1D is also possible;
  - unstructured meshes and arbitrary geometry;
  - data pre- and post-processing;
  - equation discretization, meshing and parallel solution.

- No need to modify underlying numerics!

- Open-source code
  - EPFL now collaborating center on a new IAEA project.
Finite Volume Method and segregated approach

- OpenFOAM based on the **FVM**:
  - simple problem definition and implementation.
  - strongly conservative.

- FVM and FEM share a number of features\(^1\).

- FVM is gaining momentum for solid mechanics applications\(^2\).

- **Segregated** approach: each physics or component solved separately.

- Iterations take care of explicit terms: **solution is still implicit!**

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\(^1\) Idelsohn, Onate, *Finite volumes and finite elements: Two ‘good friends’*, 1994

\(^2\) P. Cardif, *Thirty years of the finite volume method for solid mechanics*, 2018
Outline

- Motivations and main features
- OFFBEAT structure
- OFFBEAT development summary
- Coupling and interaction possibilities
- Conclusions
OFFBEAT - Structure

- Modular approach: independent C++ classes.
- Classes exchange fields and communicate via functions.

**Material properties**
- Density
- Conductivity
- Heat capacity
- Emissivity
- Poisson’s ratio
- Young’s modulus

For UO2 and Zr.

**Gap/Plena gas model**
- FRAPCON 1.5D

**FGR models**
- Forsberg-Massih

**Thermal sub-solver**
- Heat conduction
- Fixed source
- TUBRNP

**Mechanics sub-solver**
- Small strain
- Elasticity
- Zr pastic creep

**Heat Source**
- Mechanical laws

**Gap/Plena gas model**
- Boundary conditions
  - Gap conductance
  - Frictionless contact
  - Frictional Contact

**Behavioral models**
- Densification
- Swelling
- Growth
- Relocation
Straightforward extension:
- Swapping existing with similar classes.
- Reusing open-source codes.
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Previous works under linear-elastic framework

- Asymmetric heat exchange under dryout conditions\(^1\).
- Preliminary validation of fuel centerline for 8 rods low burnup rods of the IFPE database\(^2\).
- Fuel modeled as linear-elastic axisymmetric fuel rods

\(^1\) I.Clifford et al., *Studies on the effects of local power peaking on heat transfer under dryout conditions in BWRs*, 2019

\(^2\) A.Scolaro et al., *The OFFBEAT multi-dimensional fuel behavior solver*, (soon available on NED)
Preliminary FCT Validation – Results (1)

0-2 MWd/kg

2-15 MWd/kg
Preliminary FCT Validation – Results (2)

15-25 MWd/kg

25-40 MWd/kg
Renovated industrial and research interest.
Optimal testing ground for many important features.

Necessary ingredients for PCMI scenario analysis:

• Pellet-Cladding contact model

• Zircaloy rate-independent plasticity model;

• Zircaloy thermal and irradiation creep;

• Fuel isotropic cracking and creep.

• Frictional contact force

Starting Nov 2019
Contact Model

- Penalty method contact model with **conservative surface mapping (AMI)**:
  \[ p = \alpha \cdot g \cdot E \]
  \[ \alpha = \text{penalty factor}, \ g = \text{penetration}, \ E = \text{stiffness} \]

- Low penalty factor: helps convergence but might change the physics.

- High penalty factor: more accurate but needs stronger under-relaxation.

- Alternative approaches?
Contact Model Benchmark

- Punch test from the NAFEMS. Hard problem (almost point contact)!

Interfacial pressure on the cylinder outer surface

Normal Stress

- Analytic
- MSC.MARC quadratic
- OF – Level1
- OF – Level2
- OF – Level3
- OF – Level4

07/11/2019
Zircaloy Plasticity and Creep Models

- Rate independent von Mises plasticity model with linear strain hardening\(^1\).

- Limbäck-Anderson creep model based on implementation in Peregrine \(^2\).

- Prandtl-Reuss flow-rule for multi-axial stress states
  \[ \Delta \varepsilon_{c,i} = \frac{3\sigma_{\text{dev}}}{2\sigma_{\text{eff}}} \Delta \varepsilon_{c,\text{eff}} \]

- \[ \Delta \varepsilon_{c} = f(\sigma) \quad \text{but} \quad \sigma = 2\mu \varepsilon + \lambda \text{tr}(\varepsilon) - 2\mu \varepsilon_{\text{c}} - 2\mu \Delta \varepsilon_{c} \]

\(^1\) Simo, J.C. and Hughes, T.J.R., *Computational Inelasticity*, 1998
Plasticity Model Implementation

Assume elastic increment:
$$\Delta \varepsilon_n = \Delta \varepsilon_{el,n} + \Delta \varepsilon_{p,n-1}$$

Calculate trial stress:
$$\sigma_{tr,n}(\Delta \varepsilon_{el,n})$$

Yield criterion:
$$f(\sigma_{tr,n}, \varepsilon_p) \geq 0 ?$$

Calculate plastic strain increment:
$$\Delta \varepsilon_{p,n} = \Delta \lambda^n n^n$$

Update stress tensor:
$$\sigma_n = 2\mu \varepsilon_n + \lambda tr(\varepsilon \varepsilon) - 2\mu \varepsilon_{p}^t - 2\mu \Delta \varepsilon_{p,n}$$
Assume elastic increment:
\[ \Delta \varepsilon_n = \Delta \varepsilon_{el,n} \]

Calculate trial stress:
\[ \sigma_{tr,eff,n}(\Delta \varepsilon_{el,n}) \]

Calculate effective stress:
\[ \sigma_{eff,n} = \sigma_{tr,eff,n} - 3 \mu \Delta \varepsilon_{c,n-1} \]

Calculate creep strain increment:
\[ \Delta \varepsilon_{c,n} = f(\sigma_{eff,n}) \Delta t \]

Update stress tensor:
\[ \sigma_n = 2\mu \varepsilon_n + 2\mu \varepsilon^1_{c} - 2\mu \Delta \varepsilon_{c,n} \]
Plasticity and Creep Models Benchmarks

- Plasticity → 3D NAFEMS benchmark
- Creep → benchmark from Liu et al.

- Code predictions match analytical results.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Analytical Solution</th>
<th>OFFBEAT</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\dot{\varepsilon}_i$ [s$^{-1}$]</td>
<td>3.08 E-10</td>
<td>3.08 E-10</td>
</tr>
<tr>
<td>$\dot{\varepsilon}_{\text{th}}$ [s$^{-1}$]</td>
<td>77.82 E-10</td>
<td>77.86 E-10</td>
</tr>
<tr>
<td>$\varepsilon_p$</td>
<td>3.527 E-3</td>
<td>3.529 E-3</td>
</tr>
<tr>
<td>$\varepsilon_{\text{c,eff}}$</td>
<td>4.336 E-3</td>
<td>4.339 E-3</td>
</tr>
<tr>
<td>$\varepsilon_{\text{c,radial}}$</td>
<td>1.987 E-3</td>
<td>1.990 E-3</td>
</tr>
<tr>
<td>$\varepsilon_{\text{c,azimuth}}$</td>
<td>4.331 E-3</td>
<td>4.334 E-3</td>
</tr>
<tr>
<td>$\varepsilon_{\text{c,axial}}$</td>
<td>2.344 E-3</td>
<td>2.344 E-3</td>
</tr>
</tbody>
</table>
Plasticity Model – Test Case

- 6 pellets, MPS in the middle.
- RIA-like scenario: 500 kJ/kg pulse of 40ms, total transient time of 50s.
- Perfectly plastic cladding.
- Stress concentration in front of defect.
Creep Model – Test Case

- Axi-symmetric model with 10 pellets.
- Dish and chamfers included.
- Pellets attached through land.
Creep Model – Test Case

- Two simulations: elastic and creep/plastic cladding.
- Penalty factor = 1
- Mesh: 26000 cells.
- 5 hours on one core (Intel® Xeon® CPU E5-1660 v4 with 8 3.2 GHz cores)
Creep Model – Results

- Power
- Burnup

Detail for section of the cladding. Geometry warped with displacement 50x

Model Scaled 2x in radial direction
Creep Model – Test Case

End of phase at constant power, $t = 5000$ hrs

End of simulation, $t = 5000$ hrs + 160 s
Test-cases show feasibility for PCMI scenarios. **Need for mechanical behavior validation:**
- elongation and cladding deformation.
- PCMI benchmark from NEA.
- 3D validation?

Near future development efforts related to PCMI:
- Fuel isotropic cracking and creep model.
- Frictional contact force.

PCI scenarios:
- Coupling with thermochemistry (and CFD?)
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OFFBEAT – Multi-physics and Coupling Possibilities

OpenFOAM CFD solvers or GeN-FOAM

\[ T_{c,o} \quad q'' \]

Gap-gas conditions, gaseous swelling

2D/3D information

Fission rate

Initial conditions

SCIENTIX

OFFBEAT

TRANSURANUS

Serpent

\[ T = \text{temperature} \]

\[ Q(r) = \text{power distribution} \]

\[ q'' = \text{heat flux} \]

\[ T_{c,o} = \text{clad outer temperature} \]
OFFBEAT – Serpent Coupling

OpenFOAM CFD solvers
or GeN-FOAM

$T_{c,o}$

$q''$

Gap-gas conditions,
gaseous swelling

2D/3D
information

SCIANTIX

OFFBEAT

TRANSURANUS

Fission rate

Initial conditions

$T$ = temperature
$Q(r)$ = power distribution
$q''$ = heat flux
$T_{c,o}$ = clad outer temperature

$T = \text{temperature}$

$Q(r) = \text{power distribution}$

$q'' = \text{heat flux}$

$T_{c,o} = \text{clad outer temperature}$
Fuel power profile evolves with burnup!
- Complicated function of rod (and assembly) design parameters and enrichment.

Main effect: lower centerline temperature.

Traditionally in fuel performance codes either:
- impose radial profile or
- use simplified neutronics model
  → e.g. **TUBRNP module in TRANSURANUS**
Motivations for OFFBEAT/Serpent Coupling

- Traditional approach:
  + computational cost.
  + well validated with traditional UO2 fuel in PWRs.
  - fitting parameters for new fuel.
  - one-group diffusion with strong absorbers.
  - asymmetric cases?

- Coupling fuel performance and neutron transport codes:
  + no need for fitting parameters.
  + could be used with strong absorbers or in non conventional configurations.
  + could handle asymmetric cases.
  - computational cost.
- Using the **Serpent Multi-Physics Interface**.

- A Python wrapper code coordinates the two codes.

- Temperatures from OpenFOAM to calculate cross sections.

- Power profile from transport calculation.

- Burnup simulation: compositions handled within Serpent.
### PWR UO2 Rod

#### Model Details

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel Radius</td>
<td>4.65 mm</td>
</tr>
<tr>
<td>Material</td>
<td>UO2 (3.5 wt-% enriched)</td>
</tr>
<tr>
<td>Linear power</td>
<td>20 W/mm</td>
</tr>
<tr>
<td>Radial mesh</td>
<td>20 burnup zones</td>
</tr>
<tr>
<td>Gap width</td>
<td>190 µm</td>
</tr>
<tr>
<td>Cladding thickness</td>
<td>0.535 mm</td>
</tr>
<tr>
<td>Material</td>
<td>Zircaloy-4</td>
</tr>
<tr>
<td>Temperature</td>
<td>600 K</td>
</tr>
<tr>
<td>Boron concentration</td>
<td>420 ppm</td>
</tr>
<tr>
<td>Pitch</td>
<td>1.496 mm</td>
</tr>
</tbody>
</table>

#### Serpent Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neutrons per cycle</td>
<td>50,000</td>
</tr>
<tr>
<td>Inactive cycles</td>
<td>50</td>
</tr>
<tr>
<td>Active cycles</td>
<td>300</td>
</tr>
<tr>
<td>Burnup scheme</td>
<td>CE/LI</td>
</tr>
<tr>
<td>Burnup step</td>
<td>2 MWd/kg</td>
</tr>
<tr>
<td>Maximum burnup</td>
<td>102 MWd/kg</td>
</tr>
<tr>
<td>Substeps</td>
<td>10</td>
</tr>
</tbody>
</table>
PWR UO2 Rod – Adaptive Search Mesh

- Adaptive search mesh algorithm:
  - Check only limited number of OFFBEAT cells for each interaction point.
  - Adaptive algorithm saves memory → gradually refining mesh

- Attention must be paid to statistics of each cells.

- Higher number of cells → more neutrons needed for smooth results.

- Possible problem for asymmetric cases.
Adaptive search mesh algorithm:
- Check only limited number of OFFBEAT cells for each interaction point.
- Adaptive algorithm saves memory → gradually refining mesh

Attention must be paid to statistics of each cells.

Higher number of cells → more neutrons needed for smooth results.

Possible problem for asymmetric cases.
PWR U02 Rod - Results

- Similar predictions at low/medium burnup.
- Different results at high burnup.
  - Saturation for TUBRNP
  - Buildup for coupling

Total Plutonium concentration evolution

![Graph showing Total Pu concentration evolution against burnup (MWd/kg)].
PWR UO2 Rod – Radial Profile

- No significant difference for the radial profiles

239Pu radial profiles

Power profiles comparison
**BWR UO2 Gd Rod**

**Model Details**
- **Radius**: 5 mm
- **Material**: UO2 (3 wt-% enriched)
- **Power density**: 20 W/g
- **Gd-pins content**: 3 wt-%
- **Temperature**: 873.15 K
- **Radial mesh**: 10 burnup zones (coupled)
- **Cladding thickness**: 0.5 mm
- **Material**: Zircaloy-2
- **Temperature**: 573.15 K

**Serpent Parameters**
- **Neutrons per cycle**: 50,000
- **Inactive cycles**: 50
- **Active cycles**: 300
- **Burnup scheme**: CE/LI
- **Burnup step (<10 MWd/kg)**: 0.25 MWd/kg
- **Burnup step (>10 MWd/kg)**: 5 MWd/kg
- **Maximum burnup**: 100 MWd/kg
- **Substeps**: 10

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- **BWR Serpent model**

  - **Gad OFFBEAT**
  - **Gad**
  - **No gad 1**
  - **No gad 2**
  - **No gad 3**
  - **No gad 4**
  - **No gad 5**
  - **Cladding**
  - **Water**

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- **07/11/2019**
• More pronounced differences.

• Differences start at the beginning of the irradiation.

Total Plutonium concentration evolution
BWR UO2 Gd Rod – Radial Profile

$^{239}\text{Pu}$, Burnup: 5 MWd/kg$_{HM}$

$^{239}\text{Pu}$, Burnup: 100 MWd/kg$_{HM}$

$^{239}\text{Pu}$ radial profiles
OFFBEAT/Serpent Coupling – Follow up

- Preliminary tests provide promising (and expected) results.

- **Computational cost is high** → no relevant gain for traditional fuel.

- **Interesting solution for:**
  - new fuel types → obtaining fitting parameters?
  - experiments with non-traditional features.
  - asymmetric scenarios.

- Y. Robert (now PhD student at Berkley) will continue to work on the project.

- Aim is to prove feasibility of OFFBEAT/Serpent coupling **for more realistic scenarios.**

- Examples:
  - 2D assembly with Gd-rods or void channel with angular binning of neutron flux.
  - 3D partial insertion of control rods in PWR.
OFFBEAT – SCIANTIX Coupling

OpenFOAM CFD solvers or GeN-FOAM

$T_{c,o}$

$q''$

Gap-gas conditions, gaseous swelling

2D/3D information

Initial conditions

SCIENTIX

OFFBEAT

TRANSURANUS

Fission rate

$T$

$Q(r)$

Serpent

$T = \text{temperature}$

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$T_{c,o} = \text{clad outer temperature}$
Collaboration with the JRC Karlsruhe

OpenFOAM CFD solvers or GeN-FOAM

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Offbeat

SCIANTIX

Gap-gas conditions, gaseous swelling

Fission rate

TRANSURANUS

Serpent

Initial conditions

$T_{c,o}$ = clad outer temperature
$T = temperature$
$Q(r) = power distribution$
$q'' = heat flux$

$07/11/2019$
Collaboration with the JRC Karlsruhe

- Visiting stay starting soon (thanks to ENEN+).

- Primary objective: analysis of fuel creep experimental results. → use advanced tools for designing and interpreting non-traditional experiments?

- Secondary objective: first strategy for OFFBEAT-TRANSURANUS coupling.
**Conclusions**

- OFFBEAT, a new open-source fuel behavior solver with focus on **multi-dimensional and multi-physics** aspects of fuel behavior.

- Efforts have focused on implementation, mainly for PCMI/PCI capabilities.

- **Need for more validation and applications!**

- OFFBEAT is open to various coupling possibilities:
  - OpenFOAM CFD (or GeN-Foam)
  - SCIANTIX
  - Serpent
Merci