European collaboration on nuclear fuel behavioural analyses under EU-OperaHPC

1/11/2022 SYP - OperaHPC - Janne Heikinheimo

Do we need better fuel performance codes?

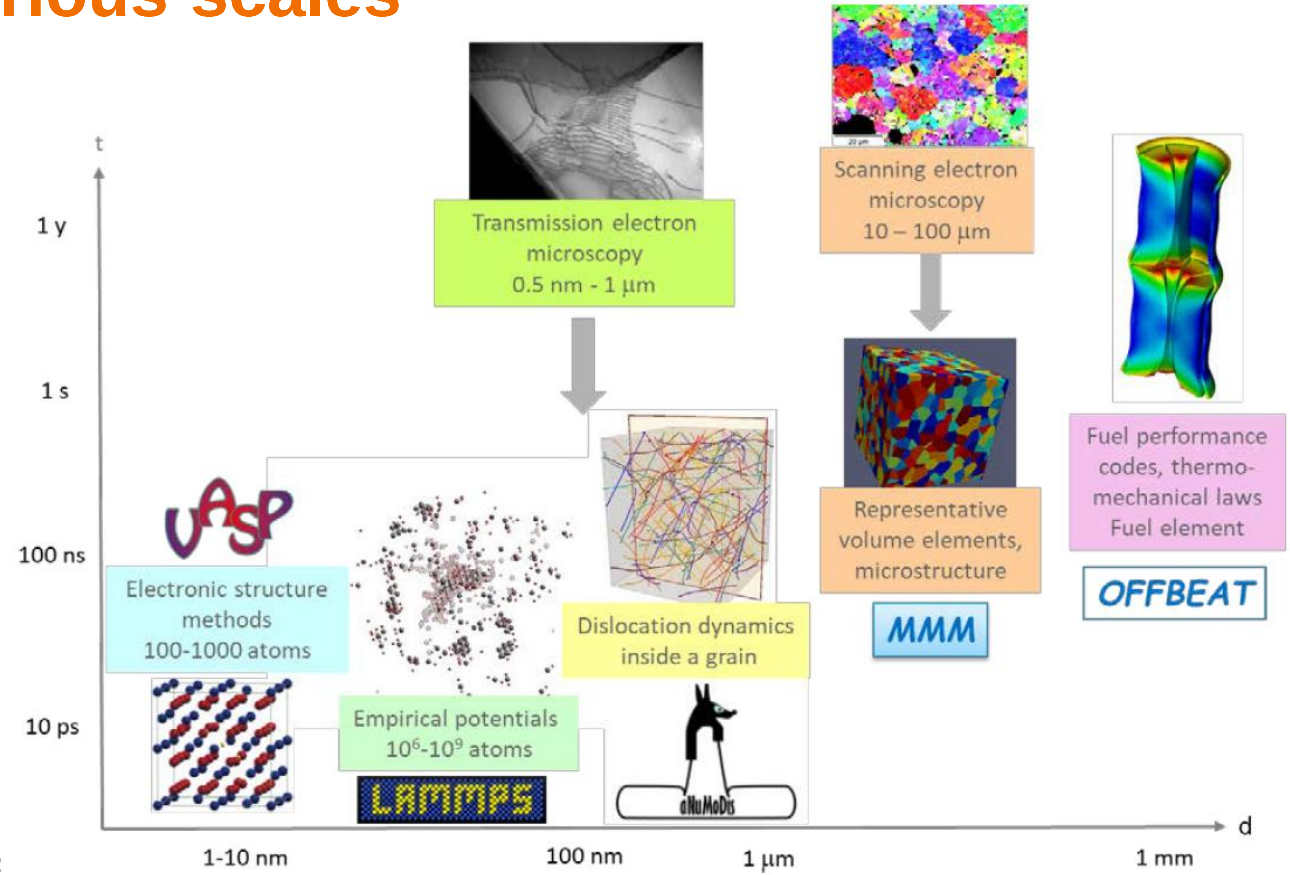
- Validated codes and long experience of normal operational conditions
- Accident scenarios?
- New fuels with little validation data?
- Facilities for fuel irradiation experiments?
- Utilization of lower scale computational tools and coupling to fuel performance models?

OperaHPC - OPEn HPC theRmomechanical tools for the development of eAtf fuels

Approach and tools used by nuclear industry

Basic research	Code development	Industrial application	E&T, dissemination
Missing data Elementary mechanisms Physics-based models ↑ Study of non-linear mechanical behaviour of fuel under irradiation Multiscale modelling Separate effect experiments	Open source 3D HPC simulation tools with parallel computing capabilities Mesoscale: MMM Engineering scale: OFFBEAT Meshless prototype tool ↑ Numerical developments Multiphysics coupling Parallelization Unceirtainty quantification Quality assurance	Improved insdustrial models Thermo-mechanical behaviour of accident tolerant fuel elements in normal and DBA conditions (PCMI, RIA, LOCA) ↑ Time reduction methods Application of codes developed to innovative fuel concepts and DBA conditions	Transfer of approach, tools and results Training of new generation of researchers and engineering ↑ Open data Open source Exchange scheme MOOC, Schools Workshops End-user group

Techniques, methods and codes used at various scales



Project structure

Basic research

WP1 Multiscale modelling and characterization of the nonlinear mechanical behaviour of irradiated fuel

WP2 Development of multiscale mechanical models for fuel elements

WP3 Calculation of input data and boundary conditions using state-of-the-art fuel performance codes

Code development

WP4 Development of 3D HPC simulation tools for the thermo-mechanical behaviour under irradiation

WP5 Validation, Uncertainties and Sensitivity Analyses

Industrial application

WP6 Knowledge transfer to simplified models for industrial fuel performance codes

WP7 Simulation of innovative fuel elements in new operating conditions

WP8 E&T, dissemination and communication

WP9 Project Management

- WP1 Multiscale modelling and characterization of nonlinear mechanical behaviour of (irradiated) fuel
  - Understand and measure creep and/or rupture behaviour of irradiated UO_2 fuel (follow-up of INSPYRE)
    - ✓ Thermal and irradiation induced creep
    - ✓ Rupture properties at low scales

- WP2 Development of multiscale mechanical models for fuel elements
  - Improved mechanical models including data yielded by WP1
    - ✓ Homogenized models for heterogeneous microstructure
    - ✓ Analysis of needs concerning cladding?
    - ✓ Microscopic & macroscopic physics based laws for fuel element

- WP3 Calculation of input data and boundary conditions using state-of-the-art fuel performance codes (lead: VTT)
  - Multiphysics calculation of data for HPC codes developed in WP4: Power density, Coolant temperature, BU, isotopic evolution…
  - Development of transfer (one-way coupling) procedure to HPC codes

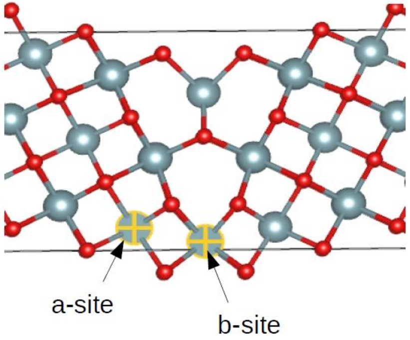
- WP4 Development of 3D HPC simulation tools for the thermo-mechanical behaviour under irradiation (open source, physics-based)
  - Fuel Element Scale: OFFBEAT
    - ✓ 3D effects not addressed by a 1D or 2D cylindrical assumption
    - ✓ HPC to avoid modelling simplification
  - Microstructure Scale: MFEM/MFront
    - ✓ HPC for a Representative Volume Element (statistics of heterogeneities)
  - Implementation of results from WP1 to WP3 in tools

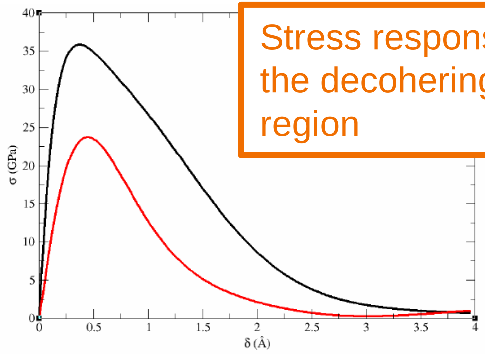
- WP5 (Verification &) Validation, Uncertainties and Sensitivity Analyses
  - Validation of tools at fuel element and microstructure scales developed in WP4 in transient conditions: PCMI, LOCA, RIA… using available experimental data
  - Uncertainty / sensitivity analyses on specific aspect: Impact of BU?
- WP6 Knowledge transfer to simplified models for industrial fuel performance codes
  - Tools & methods for computation time reduction
  - Application: improvement of industrial model(s) to be identified
  - Selection among phenomena simulated in WP4, must be relevant to WP7 activities: fuel fragmentation and/or gap closure?
- WP7 Simulation of innovative fuel elements in new operating conditions
  - ATF, other innovative design?
  - Operation in varied energy mix (Flexibility)
  - Transfer of approach and knowledge to users

From atomic scale to continuum damage model (WP2)

VTT

DFT





Stress response of the decohering region

Microscopic damage model

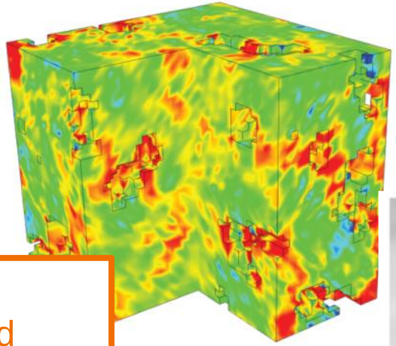
Cleavage resistance

Damage evolution

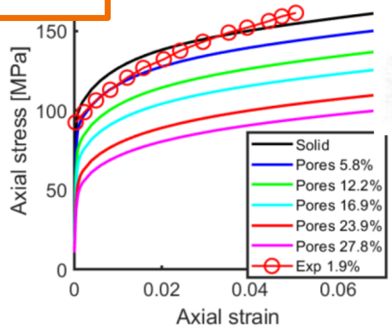
Rate of damage accumulation

Softening due to damage

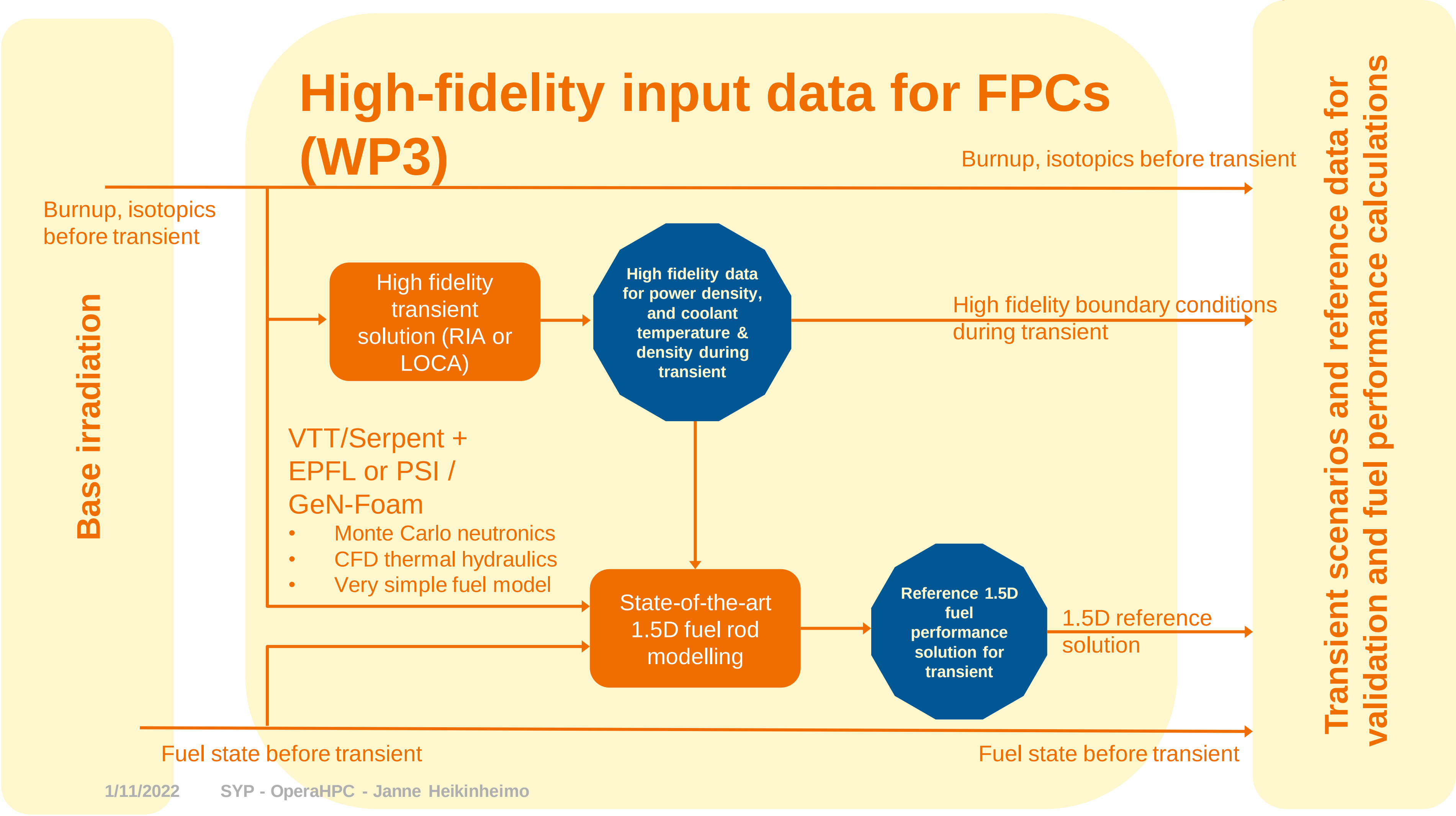
Mechanical behaviour and validation



Microstructural mechanical and damage behaviour

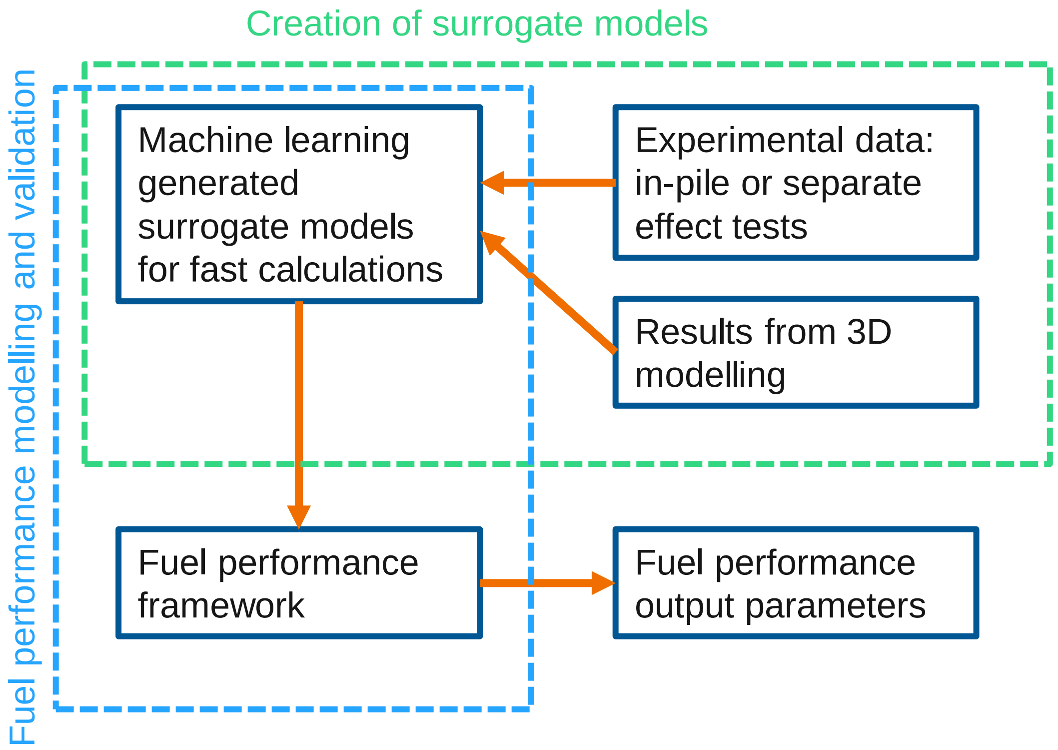


High-fidelity input data for FPCs (WP3)



Machine learning approach for reduced order calculations (WP6)

- Improved 1.5D models taking into account also 3D phenomena, such as hourglass shaping of the pellet
- Fast models will be trained based on available experimental data and 3D modelling tools



Summary of staff effort

Partner	WP1	WP2	WP3	WP4	WP5	WP6	WP7	WP8	WP9	Total
1. CEA	113	8		19	13	12	8	4	8	185
2. BANGOR	39									38
3. CIEMAT		46	3		8	4				61
4. EDF		7				3	5			15
5. ENEA				12	7	16	5	2		42
6. FRA							17			17
7. LEI			2			5	12			19
8. NINE					8	5				13
9. NNL				49.5[49]	3[49]					52.5
10.POLIMI			5	25	12	13		6		61
11. SINTEC								5	7	12
12. UJV		10					20	1.5		31.5
13. UNIPI					7	11				18
14. VTT	6	15	14		2	12	4			53
15. PSI			8	16	8					32
16. EPFL			11	15	12		6	3		47
17.KTH	7							1		8
Total	165	86	43	136.5	80	81	77	22.5	15	706

Current activity

- Consortium agreement
- Preparations for the kick-off meeting
- The project start on 1.11.2022 and will last for 4.5 years

beyond
the obvious

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