

Multi-scale nuclear fuel simulation: PLEIADES/VER software

M. Ibrahim

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M. Ibrahim. Multi-scale nuclear fuel simulation: PLEIADES/VER software. NuFuel-MMSNF 2019 Workshop, INSPYRE, Nov 2019, villigen, Switzerland. cea-02972775

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Submitted on 20 Oct 2020

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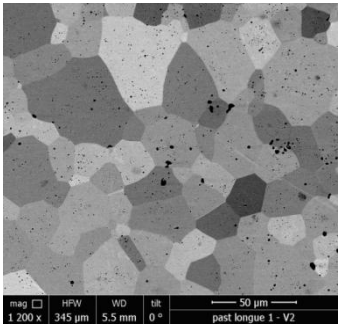
DE LA RECHERCHE À L'INDUSTRIE

Multi-scale nuclear fuel simulation: PLEIADES/VER software

M. Ibrahim

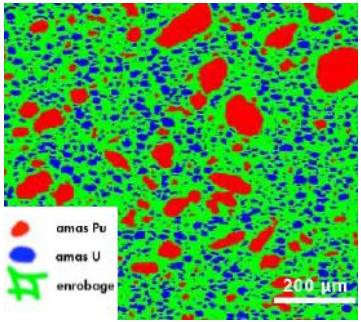
NUCLEAR FUEL HETEROGENEITY

Grains / Grains boundary



UO_2 fuel

Inclusions / matrix



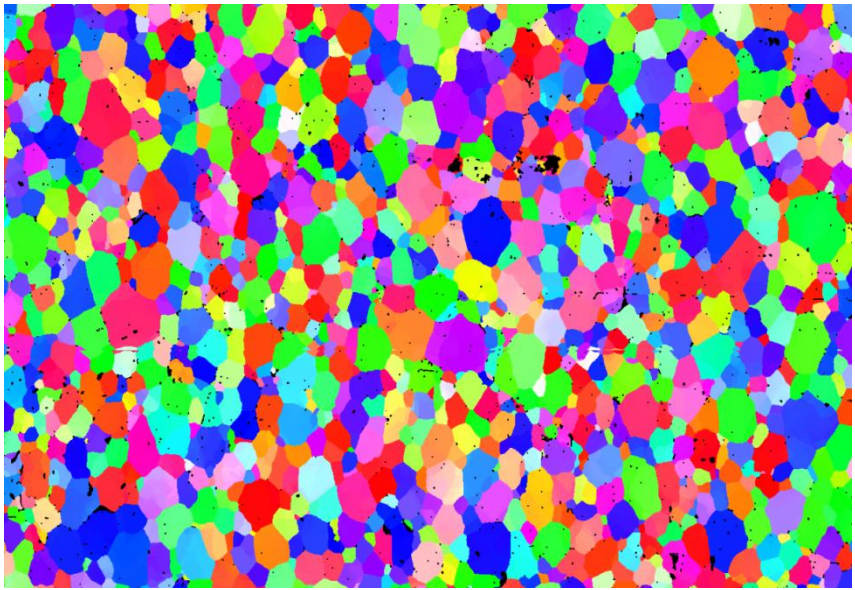
MOX fuel

Comprehension and simulation of the fuels thermo-mechanical behavior → comprehension of the microstructural phenomena

- Simulation at the micro-scale → behavior at the grains or inclusions scale
- Homogenization
  - Heterogeneous microstructures → effective behavior (macroscopic model) → implementation in fuel performance software

Impossible to simulate an entire pellet with its heterogeneities

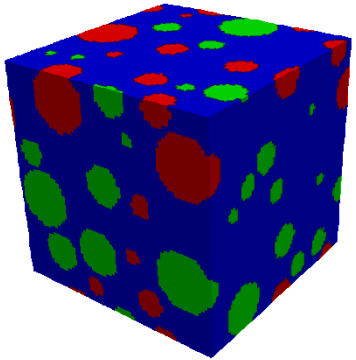
- In general, the heterogeneity's dimension is small compared to the pellet dimension:
  - High-cost numerical simulation
- Microstructural observations: the heterogeneities are reproduced in the whole pellet

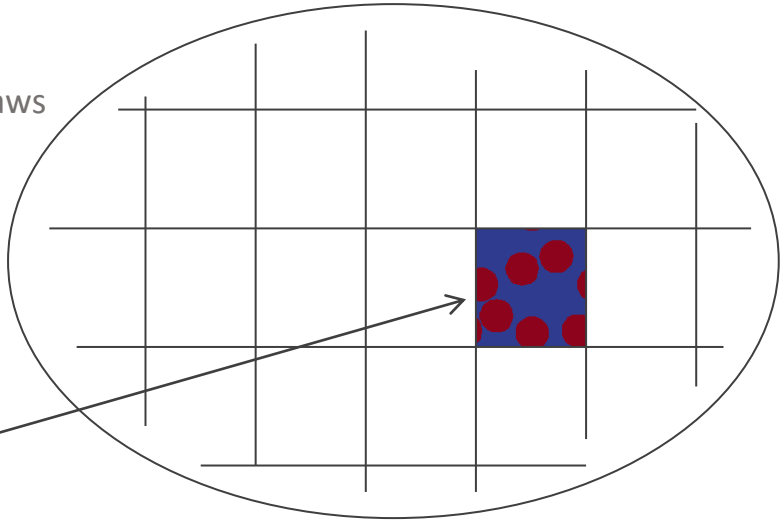


- Modeling using random medium with the following mathematical properties:
  - Stationary
  - Ergodic

Change of scale

- Scale separation:
  - Numerical simulation of the microstructure (REV)
  - Construction of homogenized laws and properties
  - Numerical simulation of the homogeneous macroscopic structure





REV's dimension calculated using statistical tools

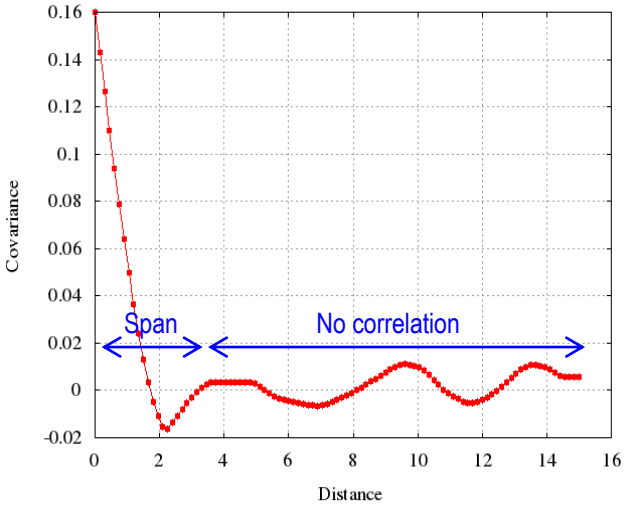
- Geometry's spatial covariance:
  - Phase indicator

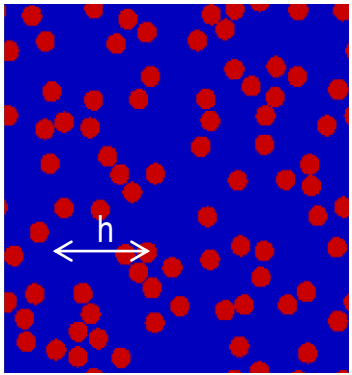
    $F(x) = 1 \; si \; x \in Inclusion$

    $F(x) = 0 \; si \; x \in Matrix$
  - Covariance function

    $C(h) = cov(F(x), F(x+h))$
    $= E[F(x) \times F(x+h)] - E[F(x)]^2$

- REV's dimension:
  - Theory of the integral span
  - Depend on the desired precision
  - Example: MOX fuels
    - Precision 10% → 100µm
    - Precision 1% → 500µm

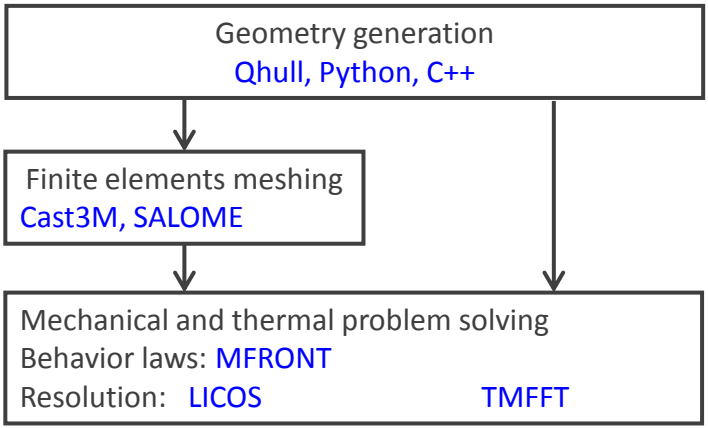




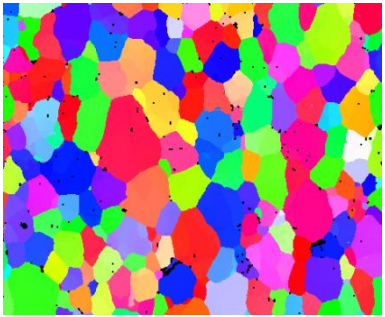
Purely geometrical criteria

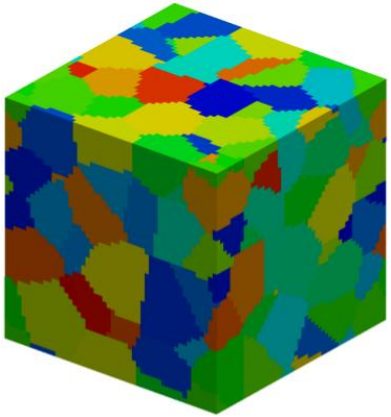
Attention: mechanics → covariance function of the stress field

VER software offers tools for multi-scale calculations

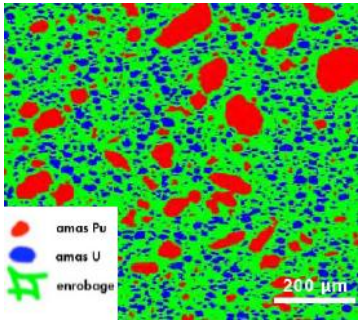


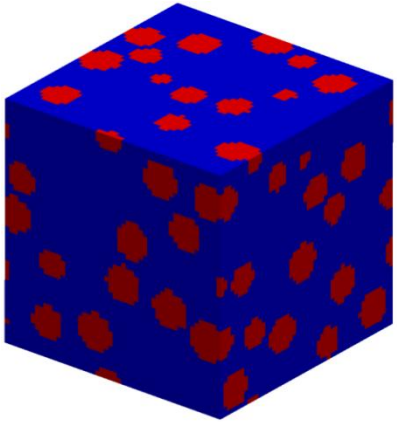
- Different types of microstructures
- Two methods for thermo-mechanical resolution:
  - Finite Elements Method with Licos software
  - Fast Fourrier Transfom with TMFFT software





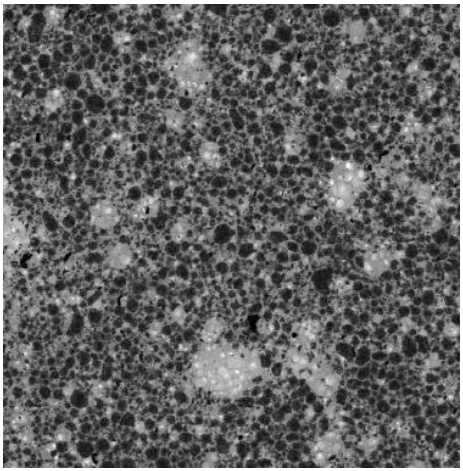
- Polycrystal

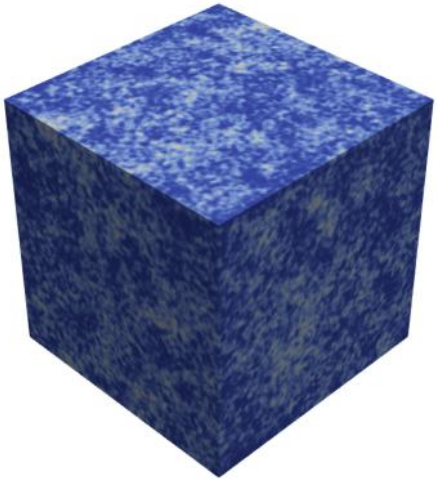




- Matrix/inclusion (spherical inclusions representing U and Pu clusters)

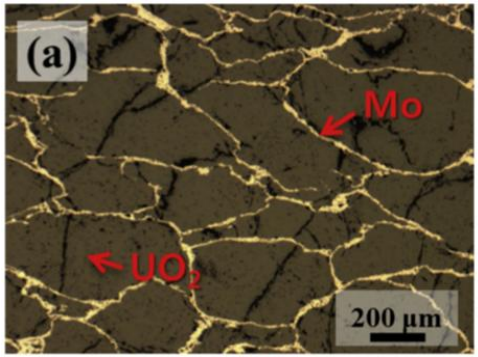
MICROSTRUCTURES

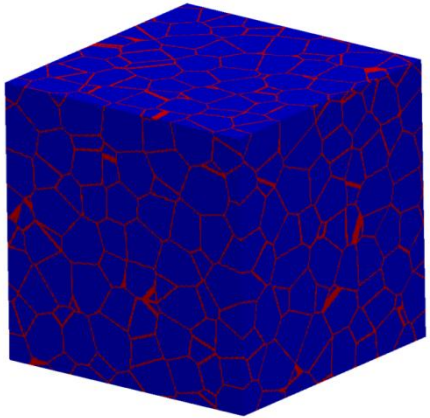




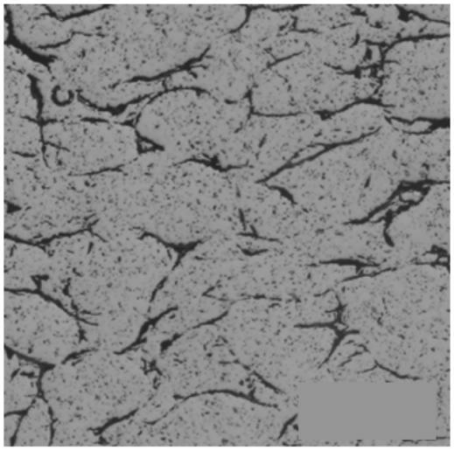
- MOX fuel with continuous Pu phase

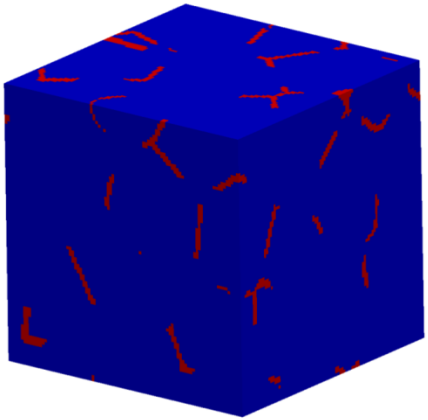
MICROSTRUCTURES





- Polycrystal with “grain boundary” phase

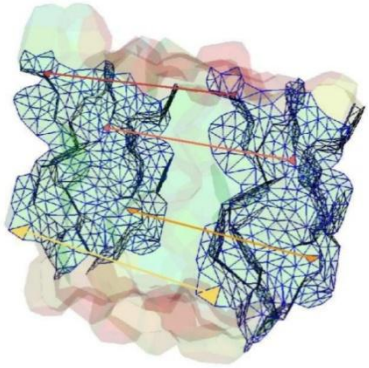




- Polycrystal with flat porosity

Periodic medium

- Simplifying hypothesis
- Good properties: no edge effect



Thermic example

$$\mathrm{div}(\lambda\,\mathrm{grad}(T)) + q = 0$$

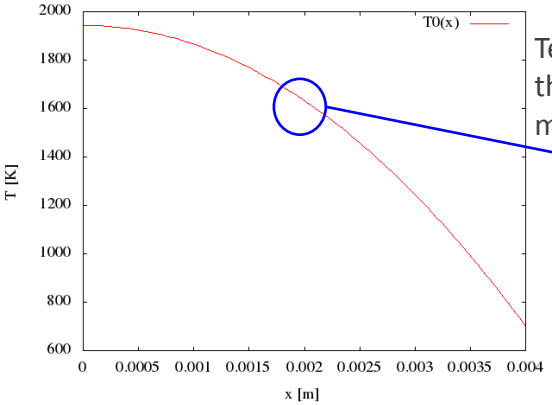
- Periodical thermal conductivity λ(x)
- Periodical heat source q(x)

- Development of the solution

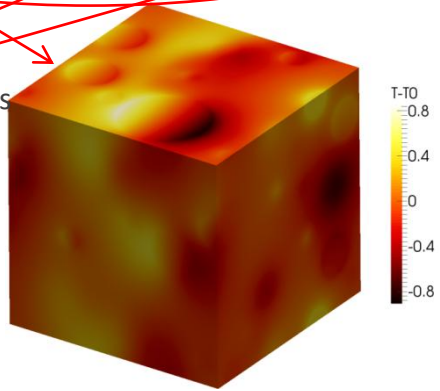
$$T(x) = T_0(x) + \tau_q(x) + \frac{\partial T_0}{\partial x}(x)\tau_1(x) + \frac{\partial^2 T_0}{\partial x^2}(x)\tau_2(x) + \mathrm{K}$$

Temperature of the homogeneous medium

Periodic corrections



Periodic REV simulation



Homogenization for thermal problems

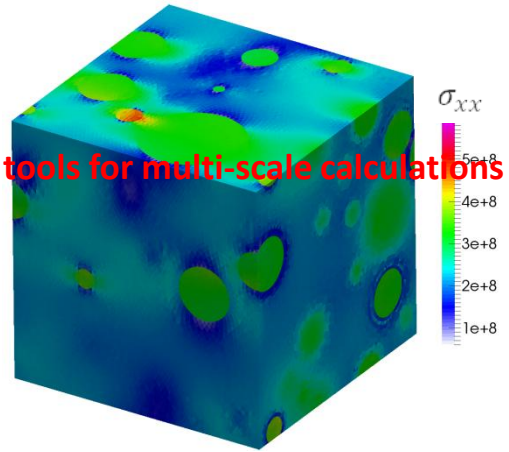
- Variable of interest: temperature
  - Low variations
- Goal: identification of the equivalent material properties

Homogenization for mechanical problems

- Variable of interest: displacement derivatives (ε) and stress (σ)
  - High variations
- Goal: identification of the equivalent material properties, and the stress field at the micro-scale

VER software offers tools for multi-scale calculations and regroups the research studies done in this domain

$E_{xx} = 0{,}1\% \longrightarrow$



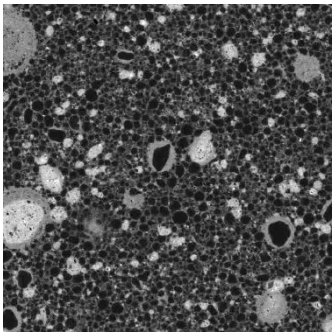
$\longrightarrow \max(\sigma_{xx}) = 600MPa$

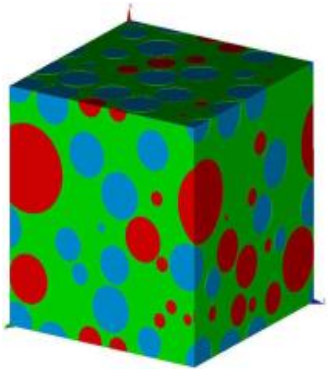
$\Sigma_{xx} = <\sigma_{xx}> = 233MPa$

Better representation of MOX microstructure*

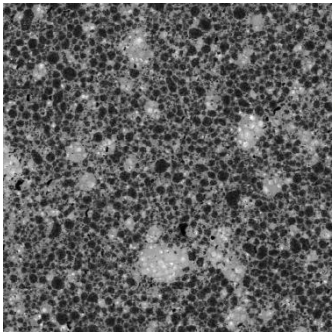
*A. El Abdi, Génération de milieux aléatoires continus périodiques et calculs mécaniques par FFT, CFM2019

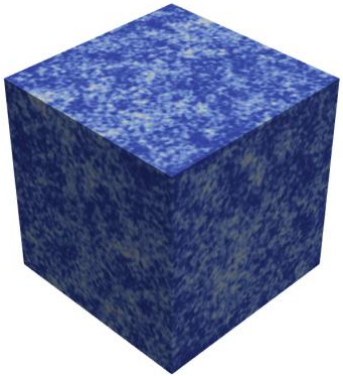
- Standard MOX: random elements
- New MOX fabrication: random functions
- Transition between microprobe images to numerical REV
  - Statistical tools
- Local mechanical behavior: elasto-viscoplasticity
- Homogenization using Non uniform Transformation Field Analysis (NTFA)





Standard MOX





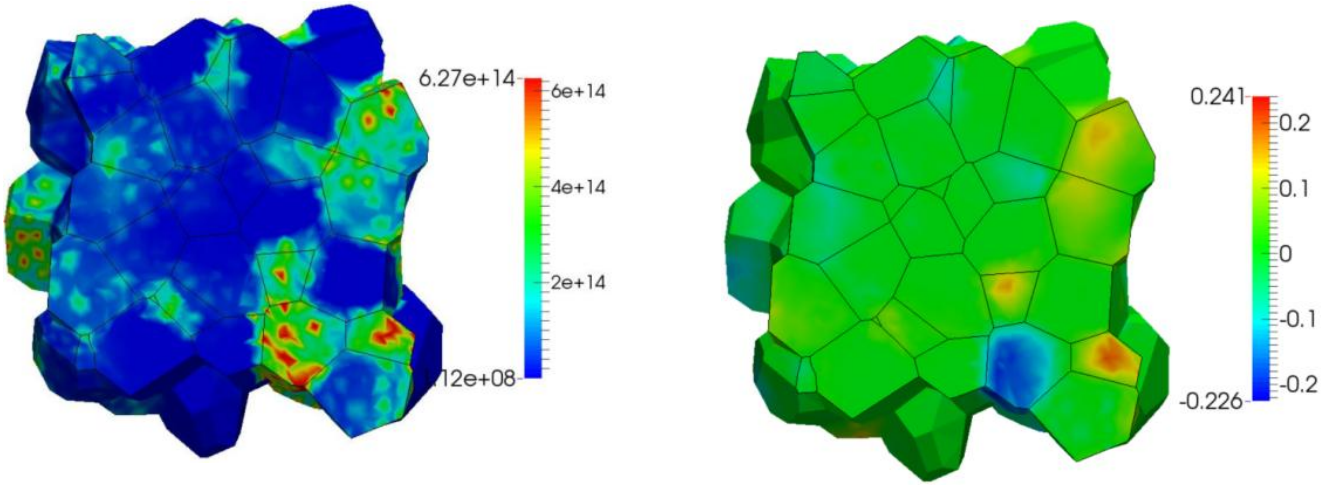
New MOX fabrication

Cristal viscoplastic modeling of UO_2 fuel*

- Micro-mechanical behavior law based on dislocation glide

*L. Portelette, Analyse des mécanismes de glissement des dislocations dans l'UO2 à l'aide de la modélisation multi-échelles comparée à l'expérience, PhD thesis 2018

Dislocation density → Shear field



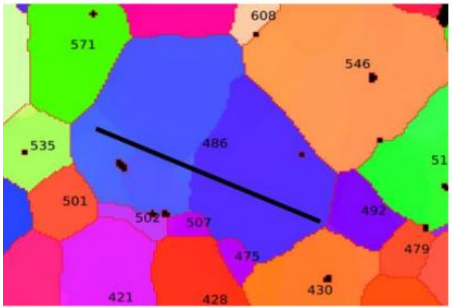
Cristal viscoplastic modeling of UO_2 fuel*

- Micro-mechanical behavior law based on dislocation glide
- Comparison between experimental and simulated stress fields

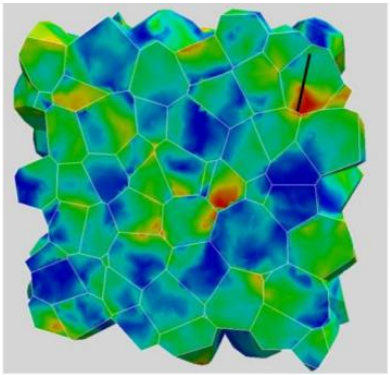
*L. Portelette, Analyse des mécanismes de glissement des dislocations dans l'UO2 à l'aide de la modélisation multi-échelles comparée à l'expérience, PhD thesis 2018

Rotation of the crystalline network:

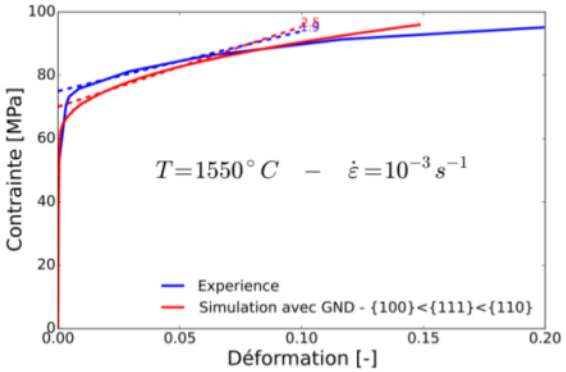
EBSD



FE simulations



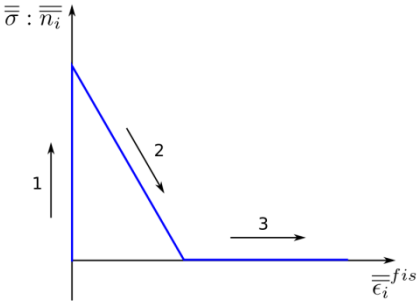
Mean stress

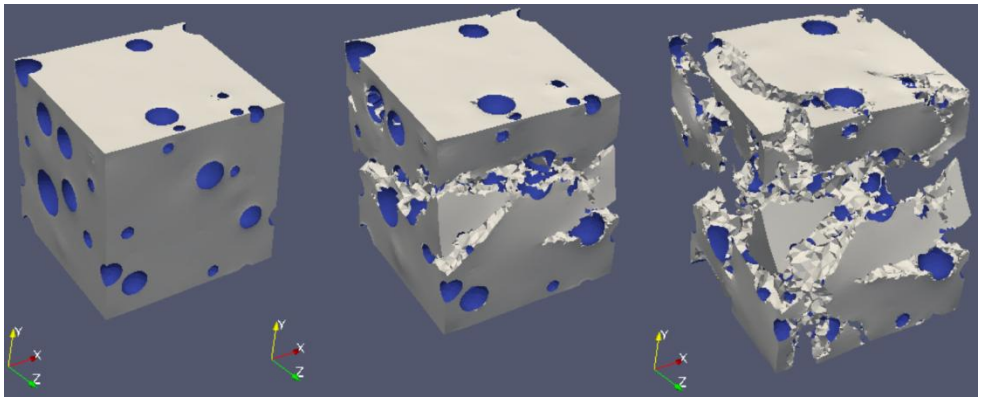


High Burn-up Structure (HBS) cracking*

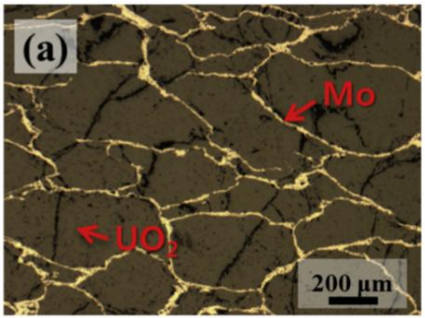
- Pressurized HBS bubbles
- Simulation under Loss of Coolant Accident(LOCA) transients conditions
- Predict the fragmentation of the HBS, to be compared to heat treatment tests

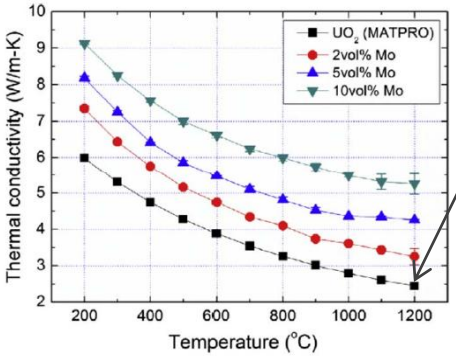
*C. Esnoul, Comportement à rupture du combustible des Réacteurs à Eau Pressurisée, par une approche micro-mécanique, en conditions accidentelles, PhD thesis 2018





KAERI fabrication of micro-cell UO_2-Mo fuel



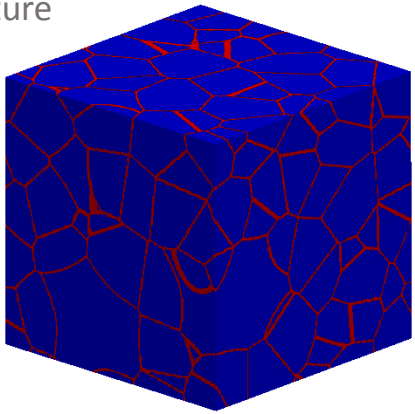


Simulations using VER software

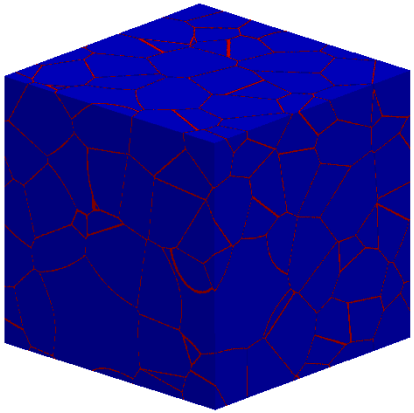
λ_{Mo} : from literature

λ_{UO2} : KAERI

ϕ_{Mo} = 10%



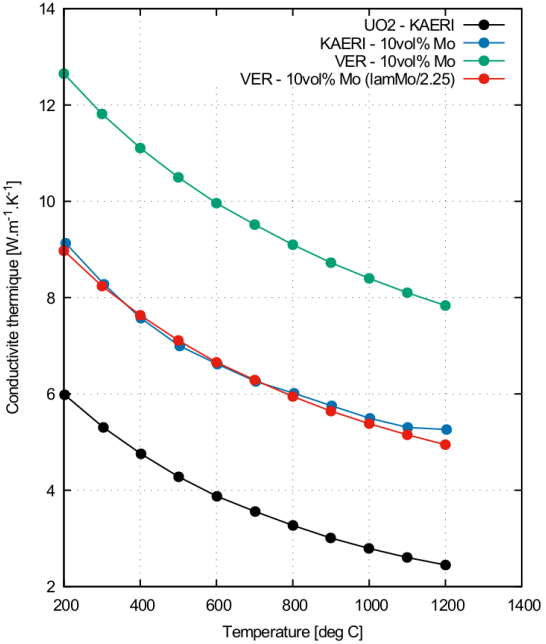
ϕ_{Mo} = 5%

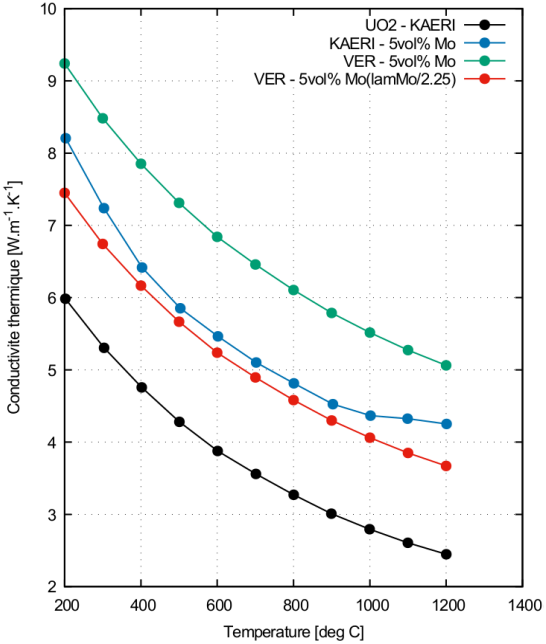


- D-J. KIM, JNM, 462(2015) 289-295

DETAILED EXAMPLE (THERMICS)

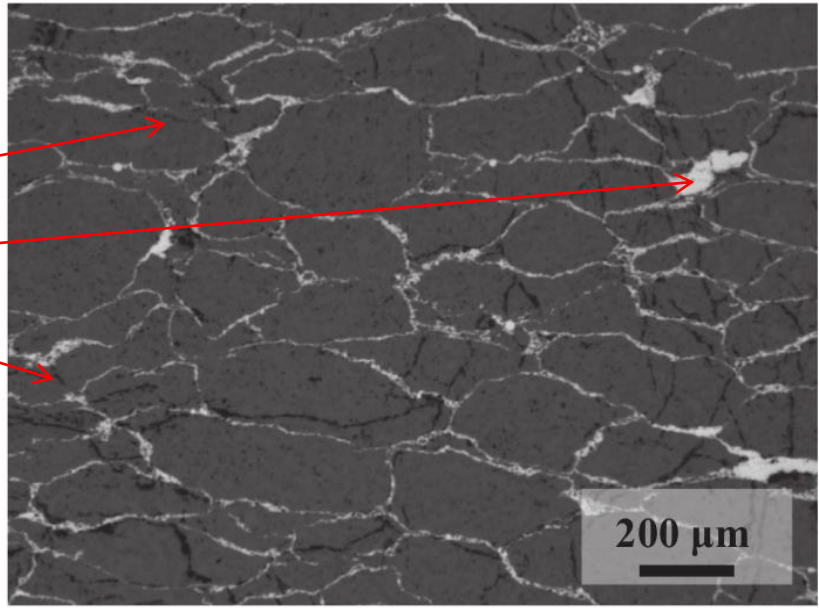
- λ_{eq} (VER) > λ_{eq} (KAERI)
- Reason : uncertainty on λ_{Mo} ? Impurities ?
- In order to obtain KAERI's results: $\lambda_{Mo} = \lambda_{Mo}/2.25$





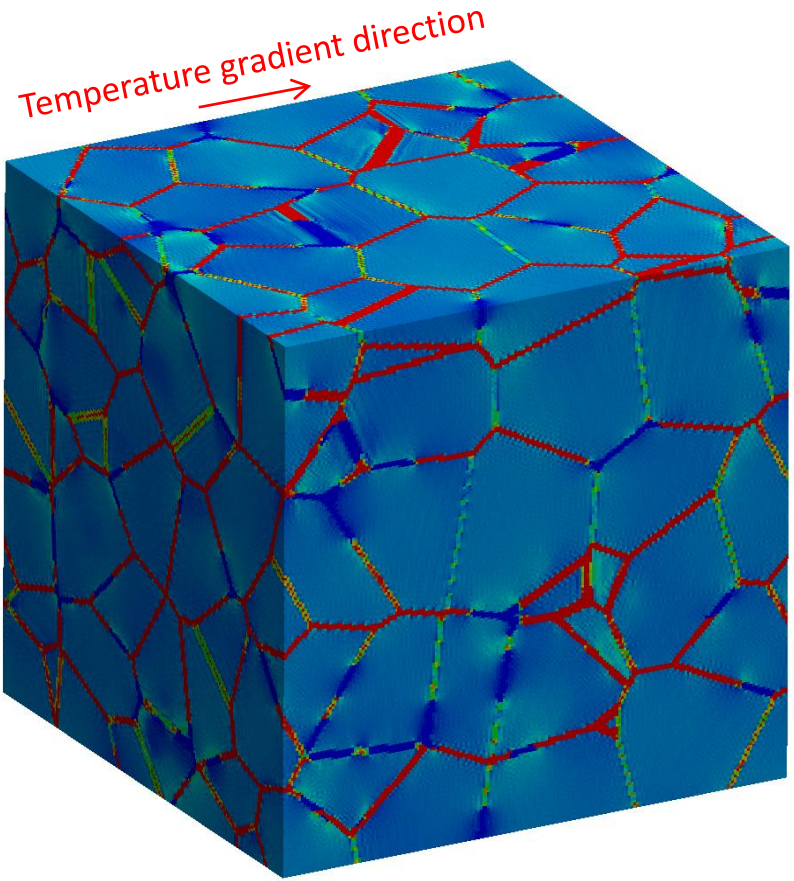
DETAILED EXAMPLE (THERMICS)

- Other possible reasons:
  - Interruption of the conductive heat path?
  - Lost Mo fractions in form of clusters?
  - Non conductive porosities?
- REV simulation with interruption of the heat path and porosities



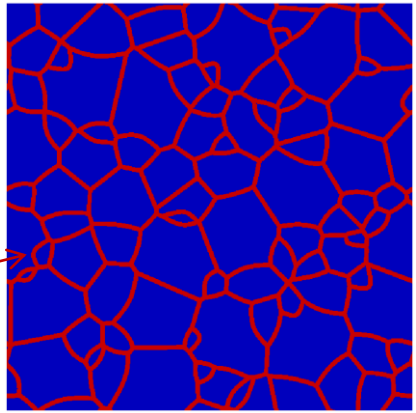
DETAILED EXAMPLE (THERMICS)

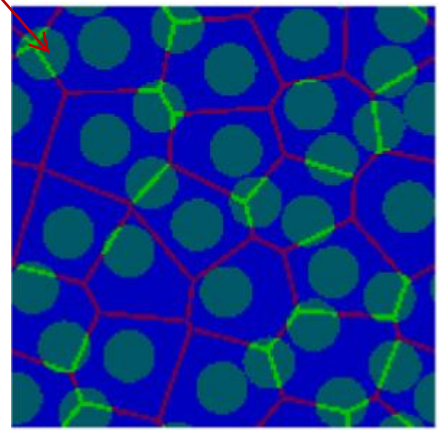
- REV simulation with interruption of the heat path and porosities
- No influence on λ_{eq}
- Despite the obstacles, the flux passes:
  - Through the connected metallic phase
  - By the UO_2/Mo exchange which is perfect
- Imperfect heat exchange between the phases? Contact resistance? Mo clusters? Anisotropic medium?

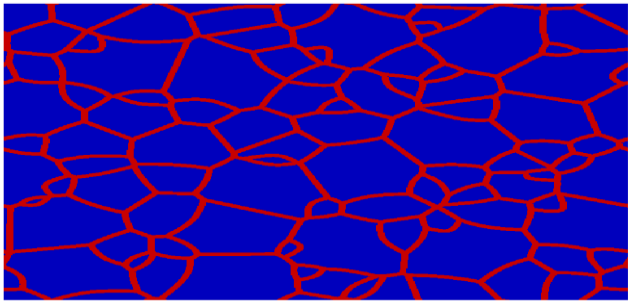


POSSIBLE VER DEVELOPMENTS

- Imperfect heat exchange between the phases? Contact resistance? Mo clusters? Anisotropic medium?
- To answer these questions → possible VER developments:
  - Adding a heat resistant phase between the metallic phase and the granulates
  - Adding spherical clusters to the microstructure
  - Stretching the geometry while keeping a constant width for the metallic phase

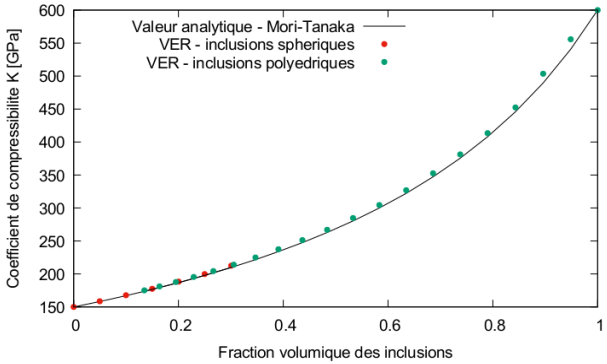


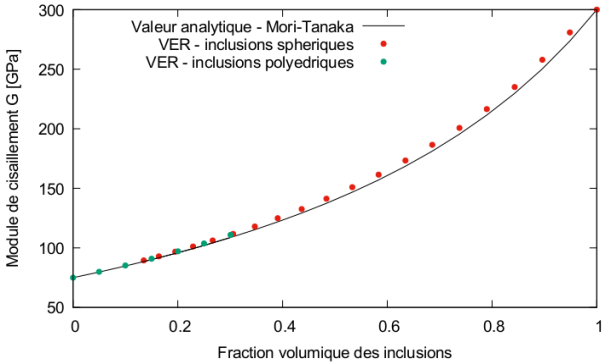




SUMMARY

- VER software: very good tool for multi-scale studies as shown if the verification test below (relative difference < 3,5%)





- Simulates different types of fuel:
  - UO_2
  - MOX
  - ATF
  - Fuel with flat porosities
- Thermal and mechanical simulations:
  - Elastic, viscoplastic, cracking, crystalline behavior, etc.

This work has been achieved in the framework of the PLEIADES project, financially supported by CEA, EDF and Framatome



THANK YOU FOR YOUR ATTENTION