Fundamental mechanisms of fuel and cladding performance

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Objectives:

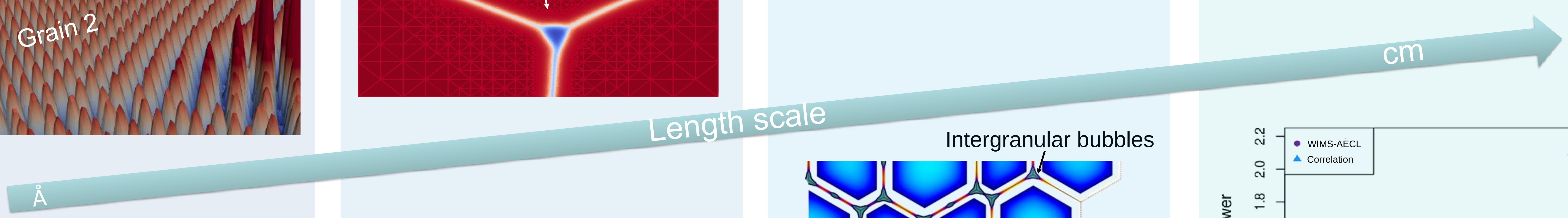
- Extend and exploit developed expertise in a range of modelling techniques for advanced fuel and cladding designs
- Demonstrate advances through publications and presentations
- Support participation in conferences and OECD NEA initiatives
- Develop capability to respond to stakeholders needs

Stakeholder: CNSC

Leveraging / supports:

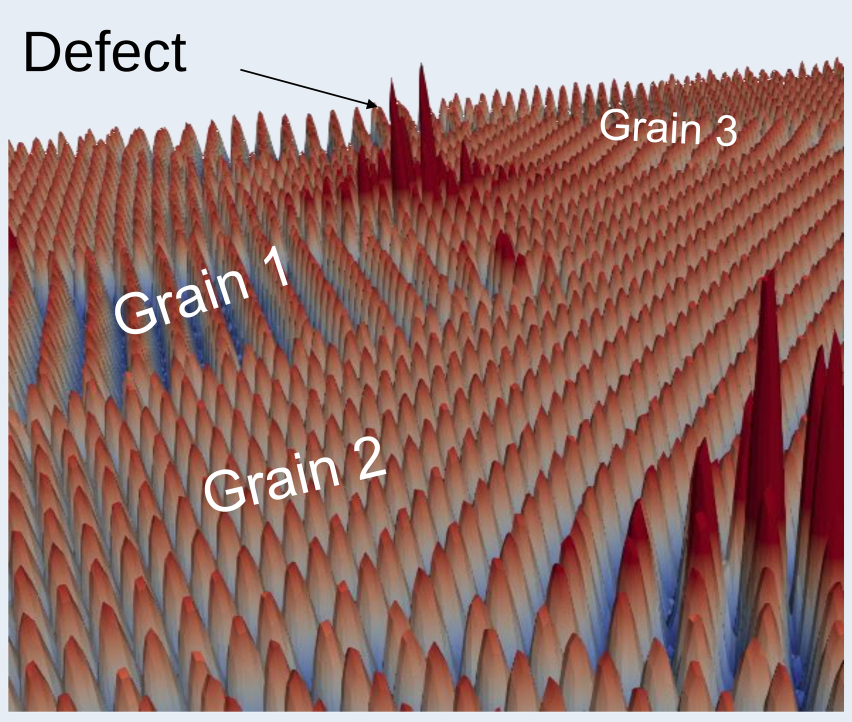
- OECD Nuclear Energy Agency projects:
  - Thermodynamics of Advanced Fuels International Database
  - Working Party on Multiscale Modelling
  - Working Party on Scientific Issues of Reactor Systems
- Cooperative Action Plan between the US DOE and NRCan
- CANDU Owners Group
- Canadian Universities: RMC, UOIT

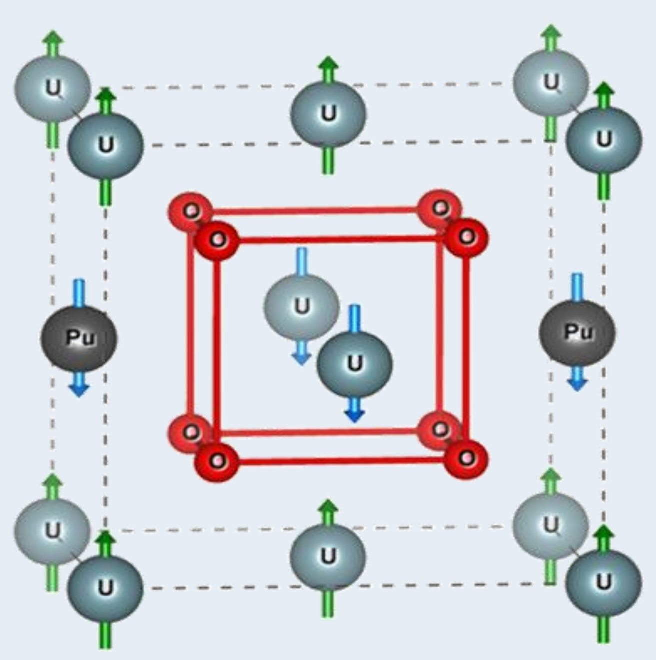
Tasks: Tasks are divided by length-scale following a multiscale paradigm and each feature two complementary modelling approaches.



Material properties

The Phase Field Crystal model captures energetics of atomic arrangements including grain boundary energies and defects.

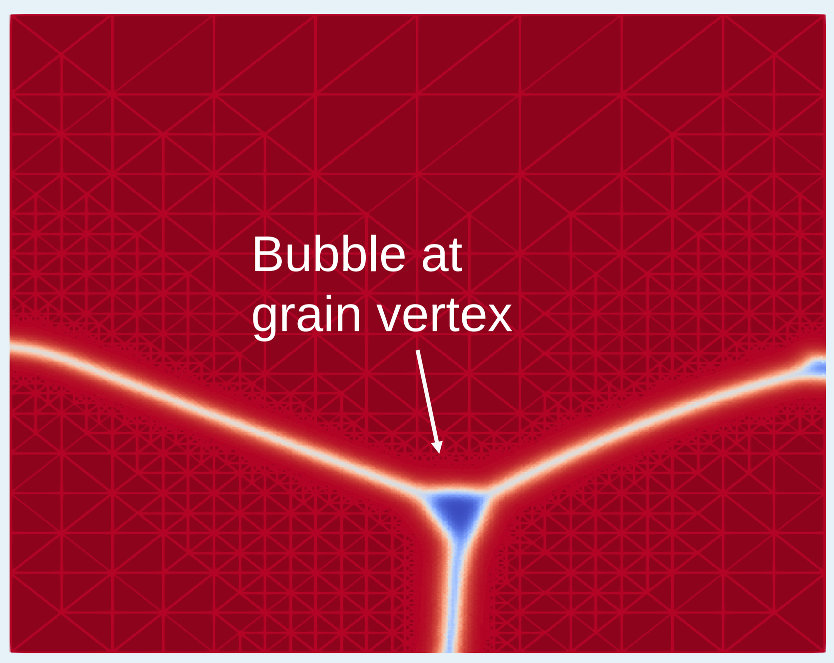


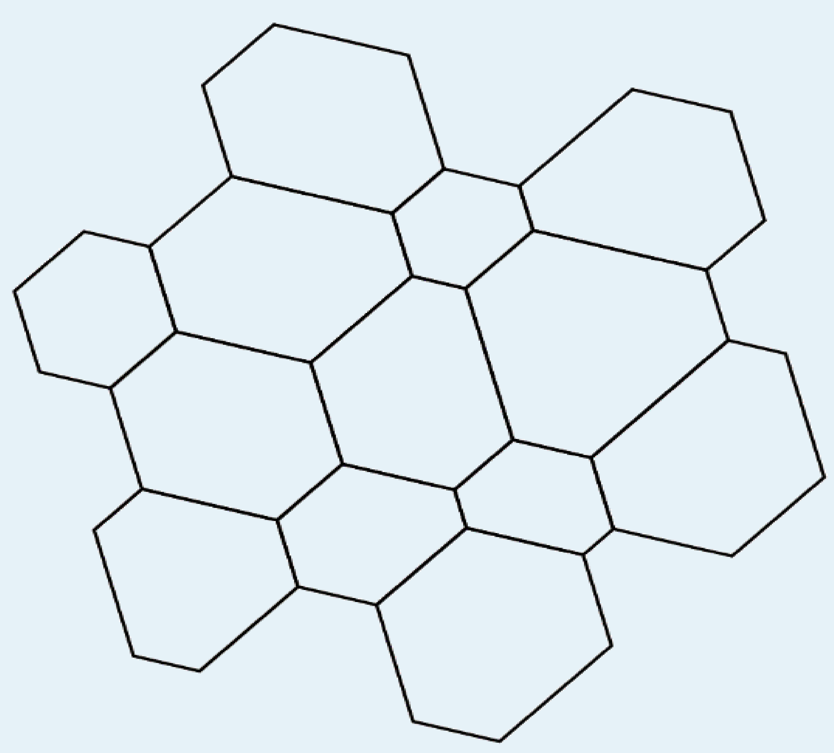


Density Functional Theory calculates thermophysical properties via electronic structure first principles and the Boltzmann Transport Equation.

Microstructure

An orientation-dependant phase-field model predicts grain growth and intergranular bubbles with adaptive mesh refinement

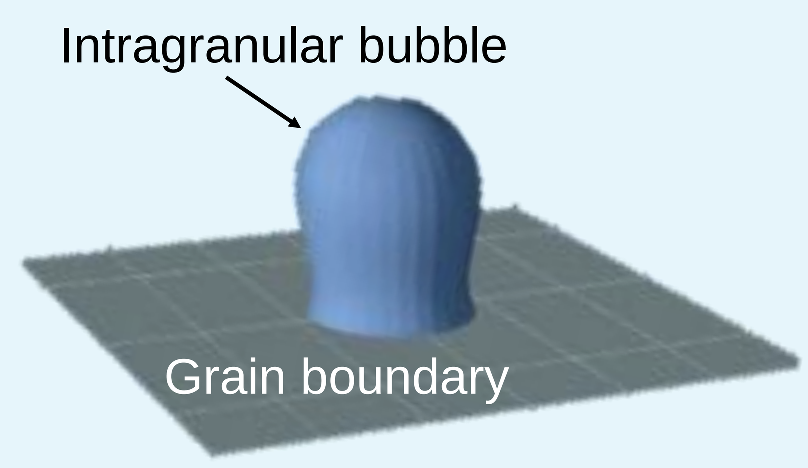


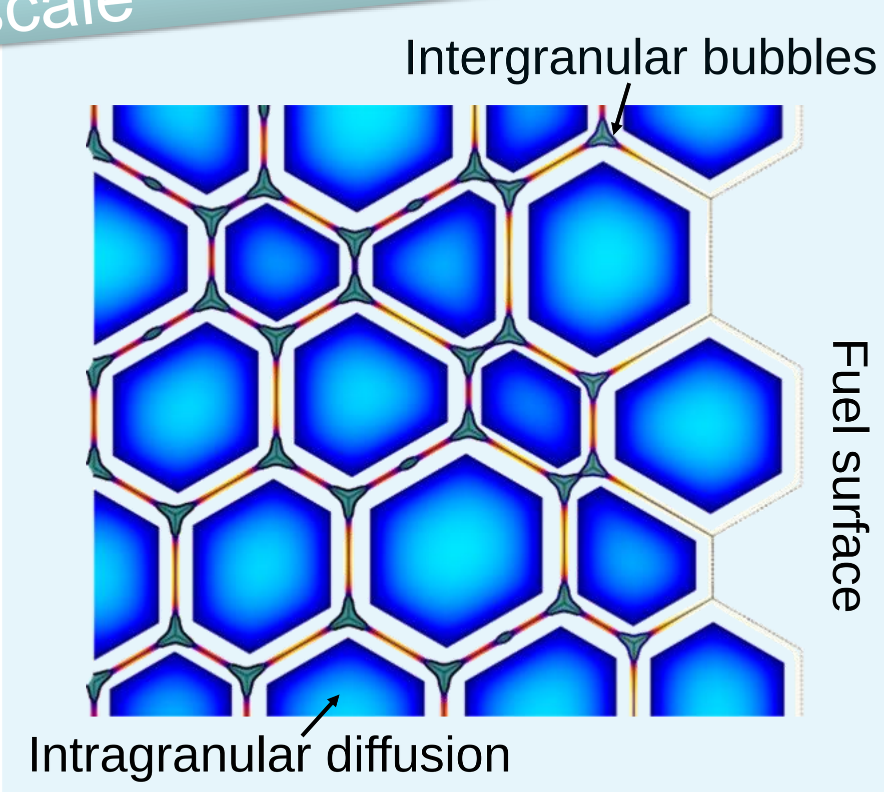


Lightweight tool for generating representative irregular-hexagonal microstructures with realistic characteristics

Fission gas behaviour

A phase-field model incorporating equilibrium thermodynamics is being developed to capture intragranular bubble behaviour.

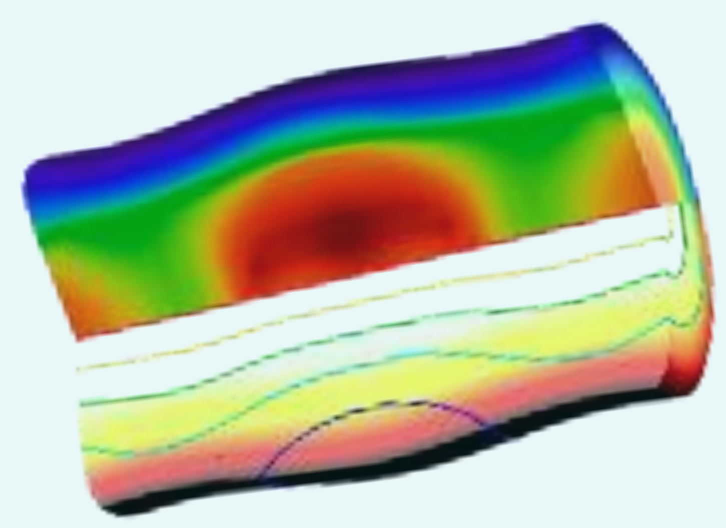


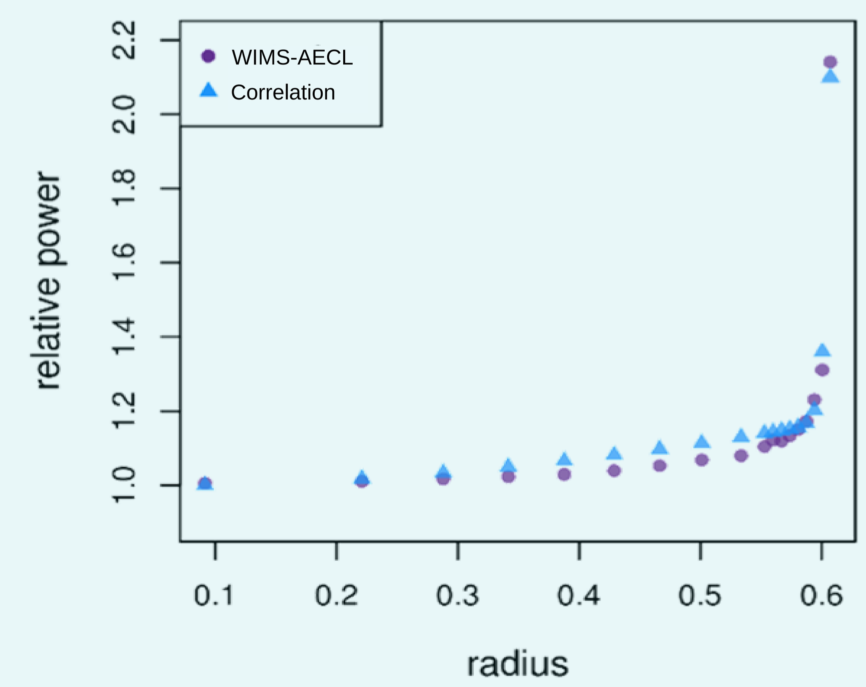


The Included Phase Model efficiently simulates mesoscale intergranular bubble growth, percolation, and venting on realistic, heterogeneous microstructures.

Integral fuel performance

Fuel Performance codes, such as BISON and FAST, incorporate and couples lower length-scale results into an integral performance model.





Machine Learning was applied to develop a correlation of the fission heat source in fuel from WIMS-AECL, for use in fuel performance codes.

This work leverages with the following internal projects:

- Modelling In-reactor Applications of MOX Fuel (ended)
- Computational methods and modelling tools for advanced nuclear fuels development