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Title:

A Multi-physics Mechanical Response of Fuel Pin Swelling

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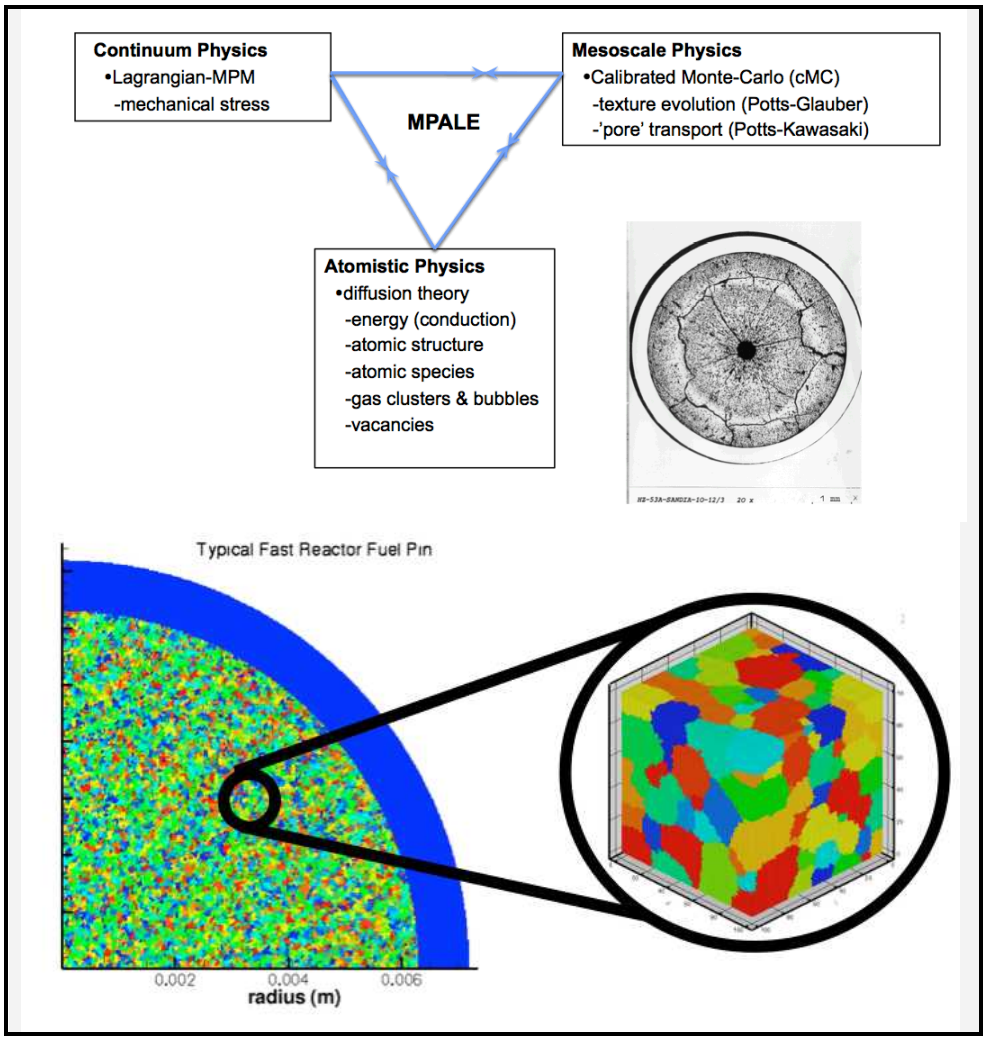
Meso-scale simulation of microstructural evolution in reactor fuels offers an intermediate perspective between atomistic simulation and macro-scale continuum models. The polycrystalline nature of materials is modelled explicitly with heat transfer, deformation, and fracture treated within the crystalline continuum framework. Grain boundaries are idealized as mobile, sharp dividing surfaces that move in response to thermo-mechanical driving forces. Vacancies, dislocations and gaseous fission gas products are modelled using evolving density fields. Modern large scale super computers enable the direct coupling of meso-scale information to the macro-scale; that is, the fuel pin. This simulation strategy permits the study of thermal transients on both the pin microstructure and the clad length scales.

To facilitate meso-scale fuels modelling, we have developed a hybrid paradigm which couples a Monte Carlo (MC) strategy for modelling grain boundary motion and pore transport with a deterministic continuum methodology for all other aspects of the simulation (e.g. mechanical stresses, heat transfer, and gaseous fission products). A time calibrated Potts model is used for the MC simulation; that is, a physical time step has been determined for the MC step to allow time accurate results. A particle-and-cell algorithm, the material point method (MPM), is used to compute the continuum level thermo-mechanical state. The implicit time integration, 3-D hybrid code, MPALE, uses a time splitting algorithm to couple the two methods; the entire spatial domain is acted on by both the MC and continuum models. The figure illustrates this coupling and also an example fuel pin computational domain. DFT is used to include strain effects into the diffusivities for the continuum-level transport.

We will describe MPALE with an emphasis on the volumetric swelling of a UO2 polycrystalline domain wherein fission gas moves in response to inhomogeneities in thermal, deformation and defect fields in addition to the solid state thermal expansion. We will present our status for obtaining a coupled meso-scale simulation capability for the simulation of nuclear fuel pin and clad interaction.



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