JACOBIAN-FREE MULTISCALE METHODS (JFMM): APPLICATION TO RADIATION DAMAGE

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Focus Material: Metals

Focus of the Presentation: *Physics-based multi-scale model development*

Abstract

The advantage of hierarchical multiscale methods is the ability to model arbitrary nonlinearities at the micro-scale without postulating any *a priori* constitutive assumption at the macro-scale. However, the major challenge is to efficiently compute the macroscopic tangent or Jacobian, if a Newton-type nonlinear solver is used, which is consistent with the evolution of the macroscopic stress at the macroscale material point. The Jacobian-free multiscale modeling technique circumvents explicit computation of the Jacobian at the macro-scale by using a Newton-Krylov process [1]. This has a major advantage in terms of storage requirements and computational cost over existing approaches based on homogenized material coefficients in which explicit Jacobian computation is required at every Newton step. A particularly interesting application of this method is being pursued in computing the mechanical response of polycrystalline aggregates of FCC metal subject to neutron irradiation with dislocation and defect density-based hardening rules that is shown to capture the experimentally observed grain-level phenomena [2].

References

[1] Rahul, De, S., 2011. An efficient block preconditioner for Jacobian-free global-local multiscale methods. *Int. J. Numer. Methods Eng.* 87, 639-663.

[2] Rahul, De, S., 2014. Multiscale modeling of irradiated polycrystalline FCC metals. *Int. J. Solids Struct.* 51, 3919-3930.