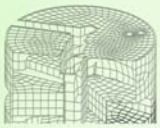
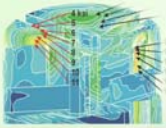
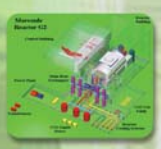
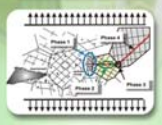



Modeling and Simulation Group

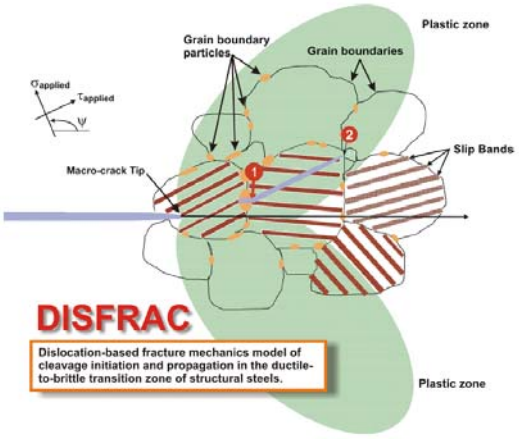



Dislocation-based Fracture – DISFRAC

Computational Structural Fracture Mechanics Team

The ORNL Modeling and Simulation Group (MSG) develops sophisticated numerical solutions for a wide range of scientific, engineering, and operational applications. MSG's core competency is computational physics and engineering, and within our Computational Structural Fracture Mechanics Team we have been developing a new computer code for research in the field of computational fracture mechanics. Funded by the U.S. Nuclear Regulatory Commission's Office of Nuclear Regulatory Research, the ***DISlocation-based FRACture*** (DISFRAC) computer program is an implementation in code of a recently-developed theoretical model of the near crack-tip fracture behavior of ferritic steels.

Main Characteristics



Currently, a significant focus of research is the development of fully predictive computer models of steel behavior under a variety of environmental conditions, including radiation embrittlement for prediction of nuclear reactor pressure vessel structural reliability. The theoretical model that is driving the development of DISFRAC is based on fundamental physical principles of deformation and fracture behavior. The theoretical model itself is a dislocation-mechanics based examination of the interaction between a macroscopic crack and a nearby accumulation of dislocations blocked by second phase particles. To provide closure to the model, it will be necessary to bridge a large range of length scales (from microns to cm) resulting in a significant computational challenge that can only be met by bringing to bear the capabilities of large scale parallel computers.

MSG is uniquely positioned to address this challenge in that it provides a confluence of theoretical modeling and high performance computing capabilities. We welcome the opportunity to discuss your potential applications and ways our computational resources can contribute to a solution.

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