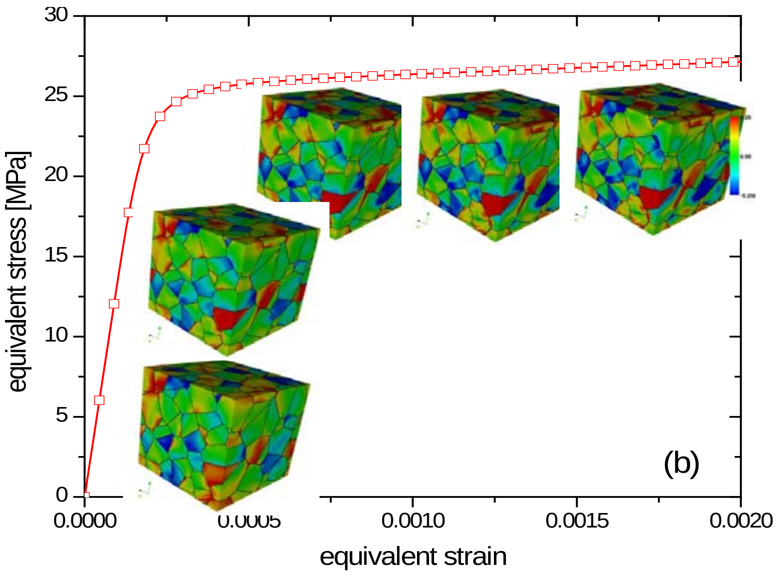
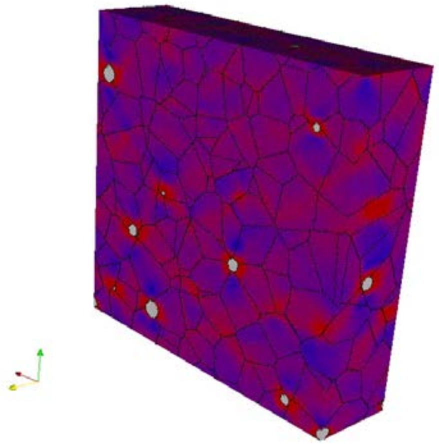
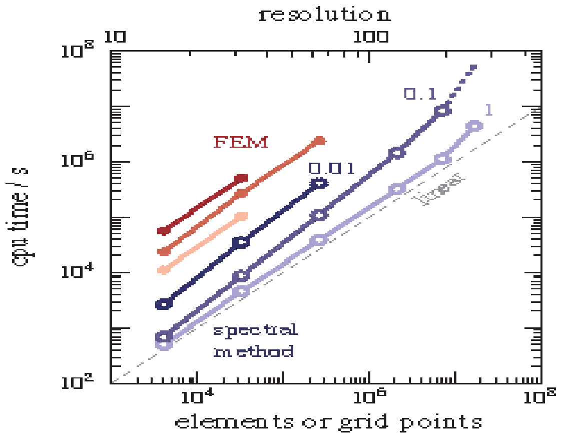
Full-Field polycrystal models: FFT suite

The suite of Full Field polycrystals models (V-PFFT, E-FFT, EVP-FFT) simulates the mechanical response and microstructure evolution of polycrystalline media under simple and complex loading as a function of temperature and strain rates. All codes are applicable to all existing crystal structures. Typical outputs include the average mechanical response of the aggregate, diffraction peaks position and width resulting from deformation, texture, internal stress distribution etc. Further, several advanced pacakges have been introduced to account for size effects in the materials microstructure (strain gradient package) as well as to treat incipient materials damage (dilatational package)





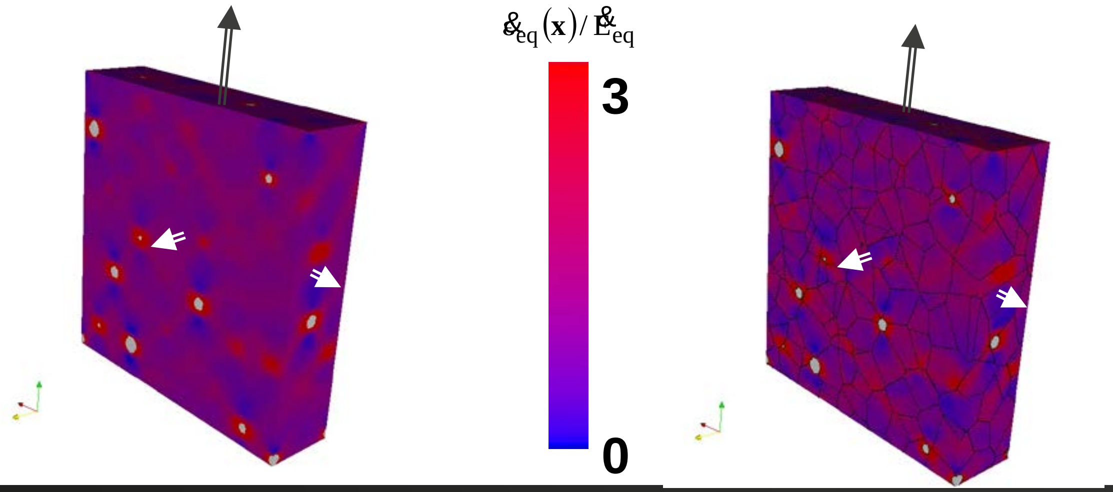


Principle: The approach relies on the use of Fast Fourier Transform methods to both equilibrium and compatibility requirements at point in the microstructure. The use of FFT based methods in comparison with FEM allows for significant speeddups rendering polycrystal simulations amenable to data analytics treatment.

Full-Field polycrystal models: example

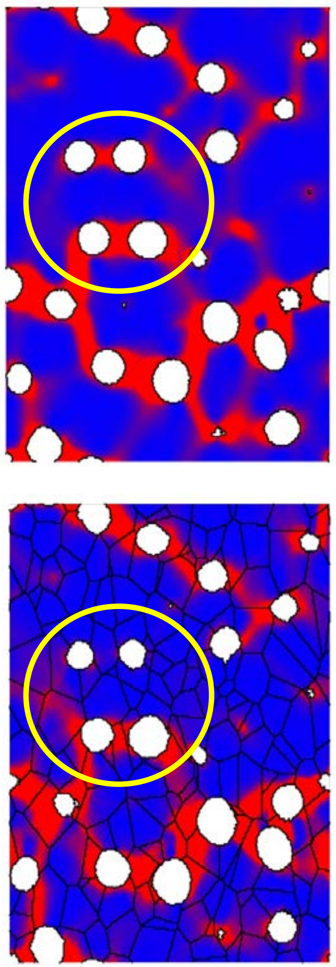
Problem: In polycrystalline materials, microstructure (e.g. grain orientation, grain boundaries, second phases, etc.) controls ductile damage: nucleation, growth and coalescence of cavities, both at quasi-static and dynamic strain-rates. No model is presently able to consider these effects.

Goal: predict damage development during shock loading of polycrystalline Cu



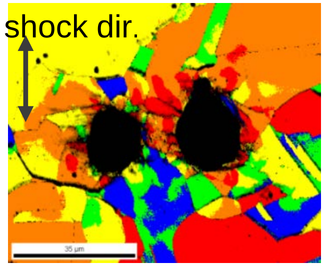
$\dot{\varepsilon}_{eq}(\mathbf{x}) / \dot{E}_{eq}$

$\phi = 11\%$



shocked Cu (**)

hard link → no



Taylor factor

	Min	Max
Blue	2.26886	2.54993
Green	2.54993	2.83101
Yellow	2.83101	3.11208
Orange	3.11208	3.39316
Red	3.39316	3.67423

soft link → coalescence