

Dancing with Defects: *Micromechanics under Extreme Environments*

Computational Design of Structural Materials | UTwente

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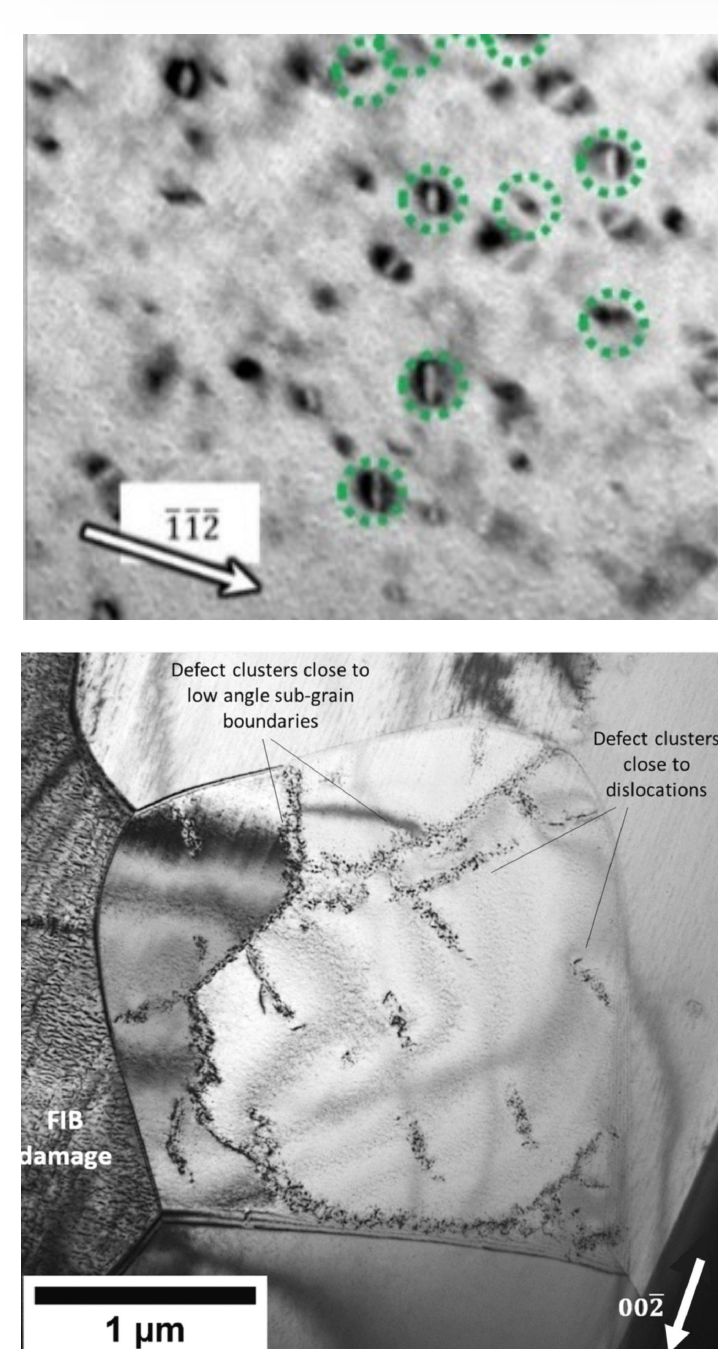
“Defects may seem like imperfections, but in the world of materials science, they are the key to unlocking extraordinary properties and pushing the boundaries of what's possible!”

Computational
Design and
Structural
Materials



BACKGROUND

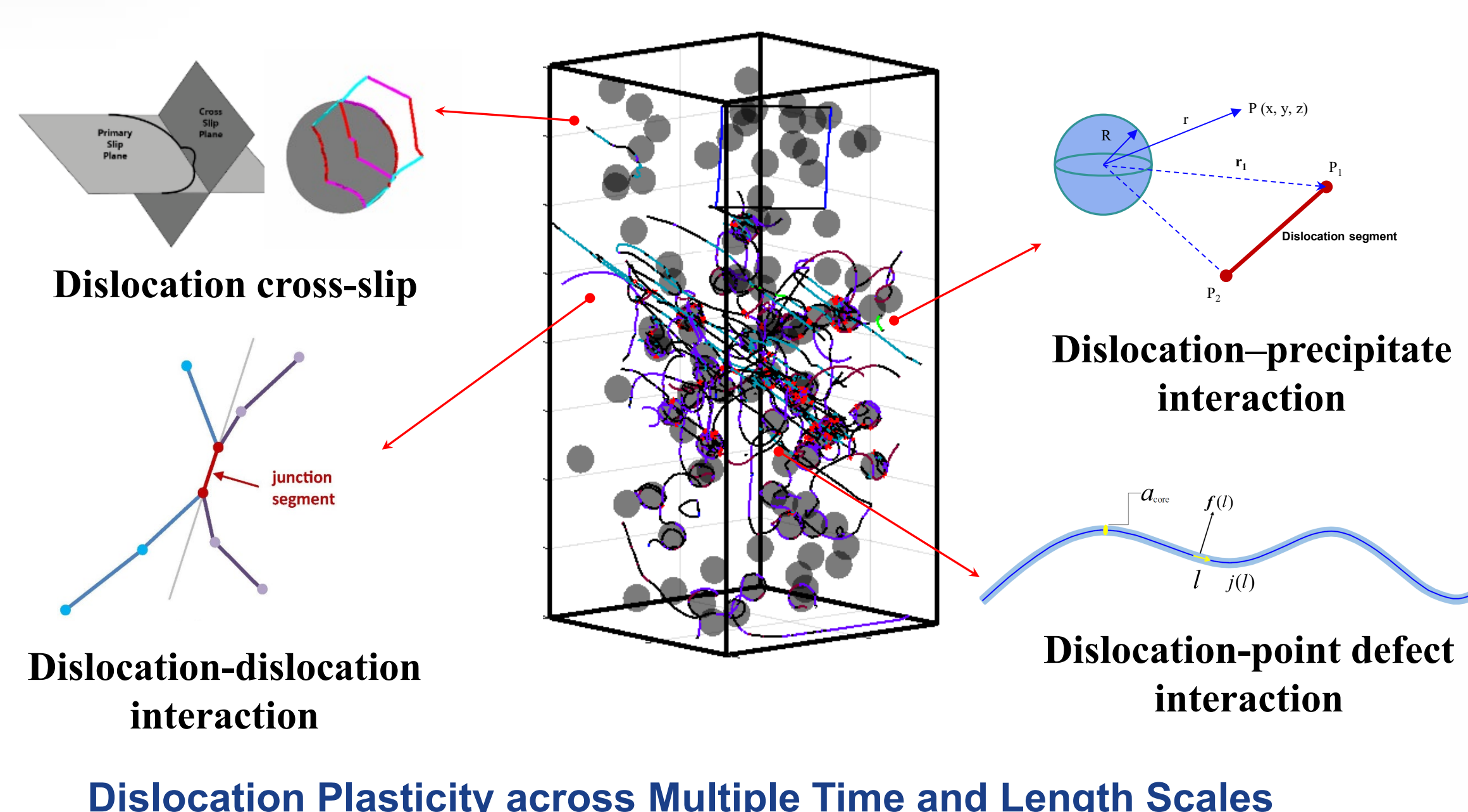
Defects under Extreme Environments



From the power generating industry to the Microelectromechanical system, materials are facing extreme conditions as they encounter ever more demanding environments, such as **high temperatures** and **radiation damage**. In which, microstructural defects occur over different scales, ranging from atomic-level imperfections like vacancies and interstitials, to larger-scale defects such as dislocations, grain boundaries, and cracks.

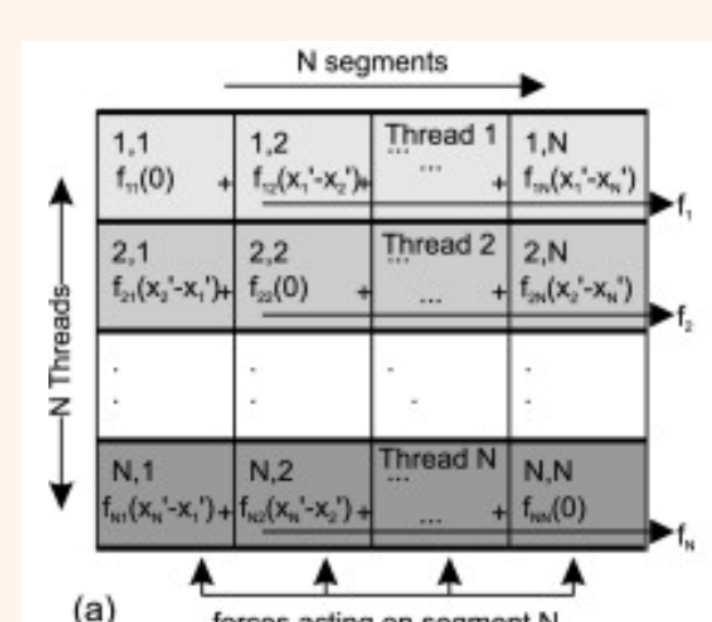
OBJECTIVES

Incorporates the intricate interactions of various defects - point defect, precipitates, etc - into dislocation dynamics model to examine mechanical behaviors under extreme conditions.

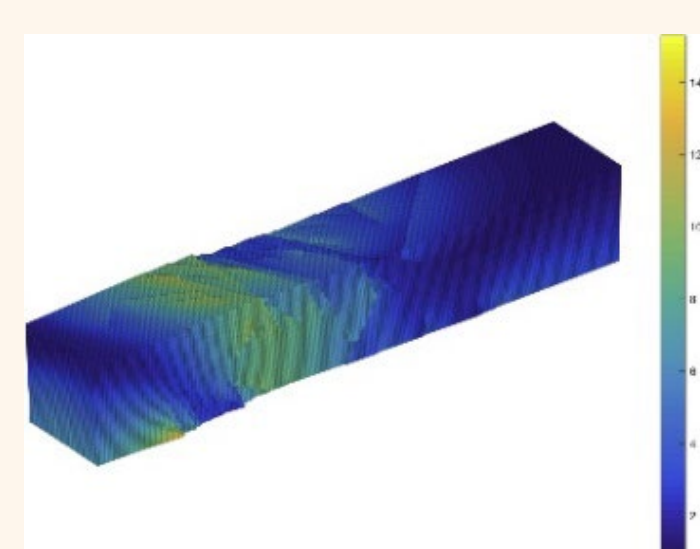


Dislocation Plasticity across Multiple Time and Length Scales

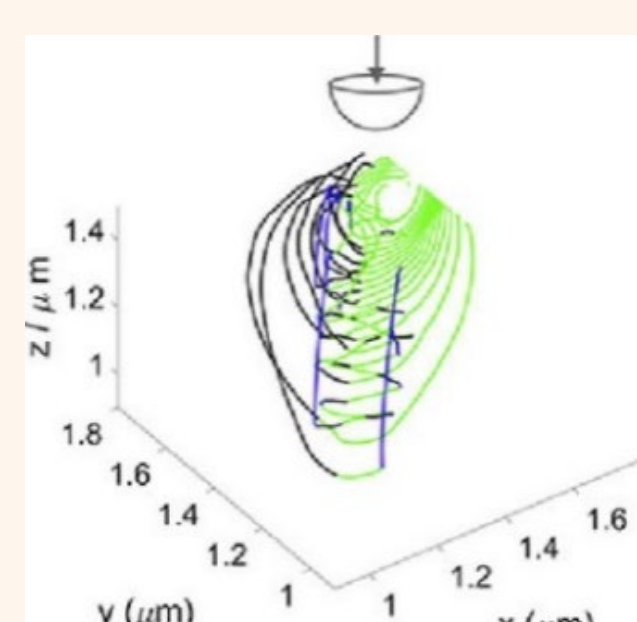
What's more...



GPU acceleration



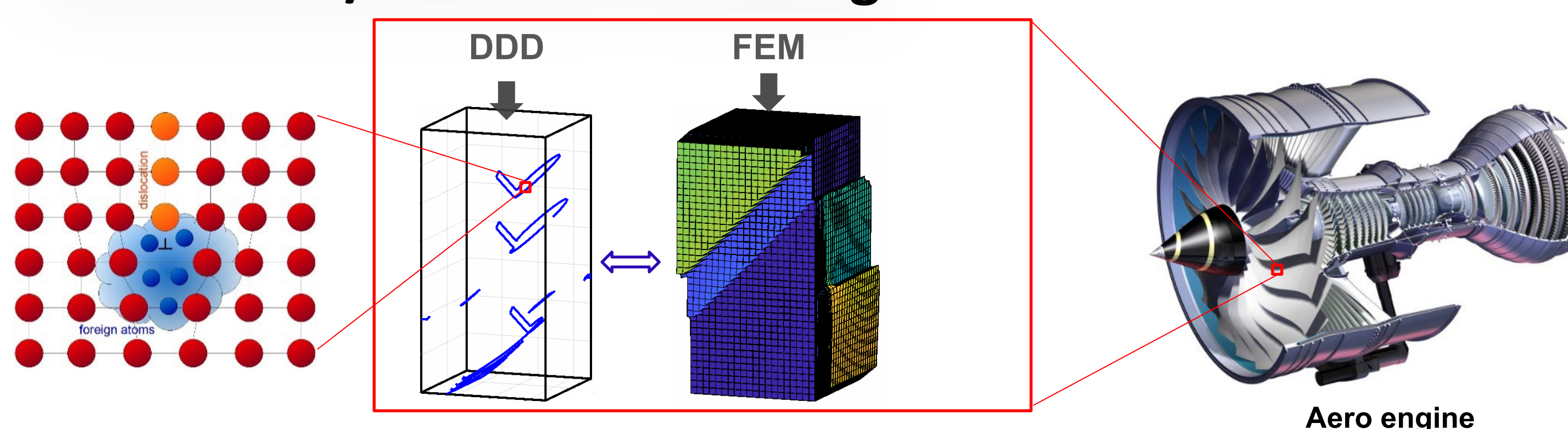
Cantilever bending



Nanoindentation

RESEARCH FIELD

- Material defect physics and science
- Multiscale materials modeling
- Dislocation Plasticity
- Mechanics/Diffusion modeling



A multiscale Discrete-Continuum (DD-FEM) model that bridges the gap between the atomic and the continuum scales

METHODS

Coupling diffusion and dislocation motion

Under thermal activations, plastic strain is produced by dislocation glide at a rate controlled by climb - a diffusion-controlled dislocation motion.

Variational functional for multiple evolution processes of microstructures

$$\Pi = \Psi + \dot{G}$$

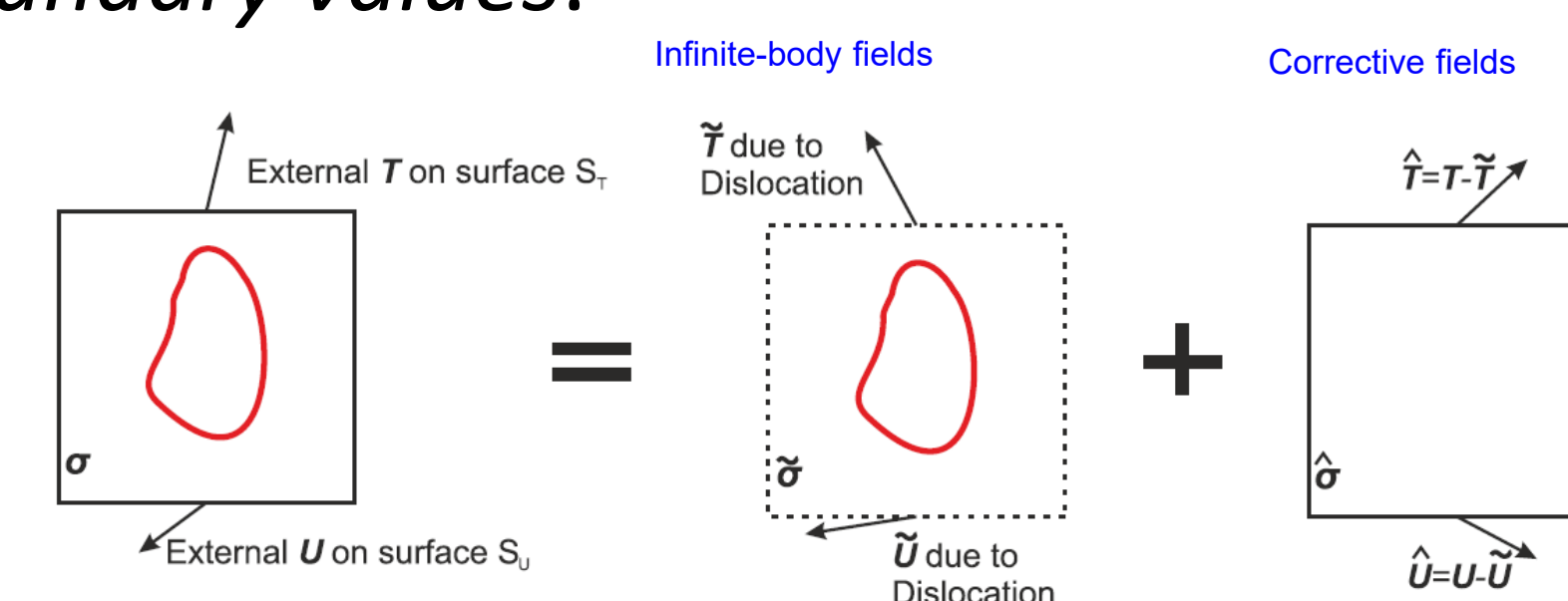
the rate of evolution of the system is given by the stationary value of Π

Ψ rate potential, contains contributions from all of the different kinetic and dissipative processes

$\dot{G}$ the rate of change of Gibbs free energy, the origin of the thermo-dynamic driving forces

Finite boundary conditions

Superposition principle is used to enforce the desired traction and displacement boundary values.



Superposition method

References

- [1] Liu F, Cocks A C F, Tarleton E. J Mech Phys Solids J MECH PHYS SOLIDS, 2023: 105300.
- [2] Liu F X, Cocks A C F, Tarleton E. Proc. R. Soc., 2021, 477(2250): 20210083.
- [3] Liu F, Cocks A C F, Tarleton E. J Mech Phys Solids J MECH PHYS SOLIDS, 2020, 135: 103783.