WCPM/CSC joint seminar

Stochastic effects in mesoscale simulations

Steve Fitzgerald

Department of Applied Mathematics, University of Leeds

Monday, 14th November, 1 p.m.
D202 Seminar room, School of Engineering, 2nd Floor

Abstract: Many materials applications require high operating temperatures, where thermal fluctuations play a leading role. In this talk I will discuss how to correctly include these effects in computer simulations of materials at the mesoscale, focussing on the dynamics of point defects and dislocations. Mesoscale techniques, such as discrete dislocation dynamics (DDD), attempt to bridge the gap in length- and time-scales between atomistic approaches and engineering-component-scale continuum simulations. To do this they require phenomenological rules, many of which are speculative and over-idealized, such as the assumption that dislocation velocity is linearly proportional to the applied stress.

I will describe a new approach to deriving dislocation velocity rules, which fully captures the nonlinear and strongly temperature-dependent response of dislocations to applied stresses. I will also discuss a more direct stochastic simulation approach (Langevin dynamics), which explicitly treats thermal fluctuations in the degrees of freedom of interest (e.g. the coordinates of dislocations and point defects). This maintains individual defect resolution, without requiring transition rates to be known a priori (cf. kinetic Monte Carlo), but is only as reliable as the coarse-graining of the atomistic degrees of freedom.

A buffet lunch is available from 12:45 pm.

More info: http://warwick.ac.uk/wcpm/seminars
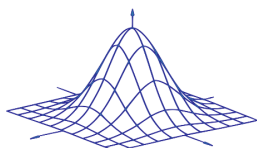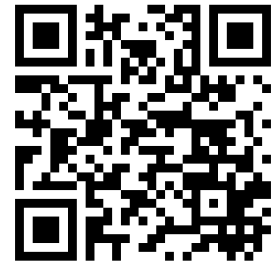
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