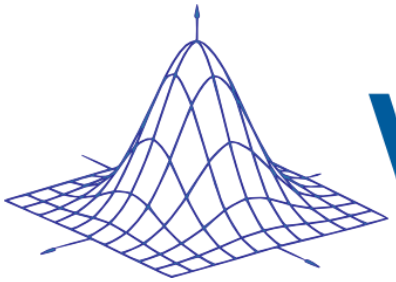

WCPM

Warwick Centre for Predictive Modelling Seminar Series

Modelling crystal nucleation and growth

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Thursday, 30th April, 4 p.m.
LIB1, Lower Level, Main Library

Abstract: Nucleation of a crystal from within a supercooled melt, or supersaturated solution, is first stage in forming many materials, from pharmaceuticals to undesirable deposits of scale or harmful biological crystals such as kidney stones. As a genuinely nanoscale process, the process would seem ideally suited to study via atomistic simulation methods. Recent accelerated simulation methods have allowed calculation of nucleation rates in some simple systems, a quantity directly comparable to experiment. However, the disagreement between simulations and experiment is typically measured in tens of orders of magnitude – far from predictive.
In this talk I'll discuss some of the difficulties in obtaining quantitative information on nucleation via simulation, illustrated with a number of examples from the literature and research within our group. Particular emphasis will be placed on nucleation of ice, the prototypical crystallisation problem.

More info: http://www2.warwick.ac.uk/fac/sci/wcpm/seminars