Application for a TSM-DTC funded PhD studentship

Please complete this form electronically
and submit to Lilian Wanjohi (l.wanjohi@imperial.ac.uk)
by Friday January 8, 2010

1st supervisor
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3rd supervisor (optional)
Name:
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Please complete the following:

1. Project title **Functional Integral Formulation of the Quasicontinuum Method**

2. Project abstract (≤ 200 words please and please add 1 or 2 key references)

The quasicontinuum method is based on standard finite elements and constitutive equations derived from atomistic interactions. There are two main ingredients: (1) Finite elements on a mesh refined to the atomistic level near a defect, but coarsened in regions where the variation of atomic displacements is small; (2) The selection of "representative atoms," in terms of which the displacements of all atoms and the total energy of the system can be expressed. In the atomistic region, all of the atoms are representative atoms, while, in the coarse-grained region, the density of these atoms is substantially reduced.

The basic form of the quasicontinuum method is confined to zero-temperature static equilibrium, wherein lattice vibrations are neglected and dynamical and inertial effects during deformation are deemed unimportant. Attempts at extending the method to incorporate such effects have included zero-temperature dynamics based on classical equations of motion and coarse-graining based on the partition function. We propose to extend the quasicontinuum method by systematically coarse-graining the functional integral

representation of the atomistic system with a combination of analytic and numerical methods. The goal of this work is to obtain a systematic description of deformation behavior that incorporates controlled spatial coarse graining at finite temperatures.

References

E. B. Tadmor, M. Ortiz, R. and Phillips, Quasicontinuum analysis of defects in Solids, *Phil. Mag A* **73**, 1529–1563 (1996).

R. E. Miller and E. B. Tadmor, The quasicontinuum method: Overview, applications and current directions, *J. Comput-Aided Mater*. **9**, 203–239 (2002).

http://www.qcmethod.com

3. What is the multi-scale nature of the project? (≤ 100 words please)

The spatially-dependent coarse-graining of an atomistic system.

4. How do the expertises of the supervisors complement each other? (≤ 100 words please)

Foulkes: considerable experience in the evaluation of functional integrals with many degrees of freedom in his development of the quantum Monte Carlo method.

Vvedensky: considerable experience in developing methods for systematically coarse-graining lattice models and expressing their evolution as continuum equations.

5. Is there a self-contained 12-week MSc project that would usefully initiate this PhD project? (If the answer is no the project will not be offered as an MSc project)

Possibly a one- or two-dimensional version of the method for, say, harmonic springs with a single defect.