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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2nd supervisor
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3rd supervisor (optional)
Name:
CID (IC only):
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Please complete the following:

1. Project title **Coarse-Grained Classical and Quantum Molecular Dynamics**

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

The idea behind coarse-graining of classical molecular dynamics is to derive a reduced set of equations of motion on a finite-element mesh from an atomistic molecular dynamics Hamiltonian. When the mesh nodes and the atomic sites are identical, the coarse-grained equations of motion are exact. As the mesh size increases, shorter wavelength modes are eliminated, and their effect on the remaining modes is included through thermodynamic averaging.

The proposed research aims to examine coarse-graining approaches based on the functional integral representation of the dynamics of a system, rather than focusing on the equilibrium properties through the partition function. This could shed light on the relationship between molecular dynamics and the quasicontinuum method, as well as providing new avenues of investigation for the structural dynamics of nanostructures.

In regions of nearly ideal crystal, it may be possible to apply similar coarse-graining ideas to

the quantum mechanical density matrix, by writing it as a smoothly varying "envelope" transform of the density matrix of the perfect crystal and deriving equations of motion for the envelope. If this proves practical, it will allow the embedding of time-consuming quantum simulations of, for example, point defects, into effectively infinite solids at reasonable cost.

References

R. E. Rudd and J. Q. Broughton, Coarse-grained molecular dynamics and the atomic limit of finite elements, *Phys. Rev. B* **58**, R5893–R5896 (1998).

R. E. Rudd and J. Q. Broughton, Concurrent coupling of length scales in solid state systems, *Phys. Stat. Sol.* **217**, 251–291 (2000).

R. E. Rudd and J. Q. Broughton, Coarse-grained molecular dynamics: Nonlinear finite elements and finite temperature, *Phys. Rev. B* **72**, 144104 (2005).

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

The systematic elimination of atomistic degrees of freedom to obtain equations of motion for coarse-grained variables.

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

Foulkes: numerical evaluation of partition functions for complex many-particle systems; density-matrix methods

Vvedensky: formulation and coarse-graining of discrete models and expressing results as effective continuum equations of motion

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)

Working through the original formulation of classical coarse-grained molecular dynamics, with an application to a one-dimensional system.