

**Predictive Modelling of Crack Growth:
Stochastic Coarse Graining from Atomic to Continuum Scale**
MSc/PhD Project Proposal for Mathematics for Real-World Systems CDT

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Background. Despite the potential for significant technological and economic impact, remarkably little is known about the fundamental fracture mechanisms that cause many materials to break. Accurate simulations of these kinds of processes at the atomic scale have only recently been made practical for the first time, using multiscale approaches which combine a quantum mechanical description of bond breaking processes with a classical description that captures long-range elastic effects [1]. The effect of individual defects [2] or chemical additives [3] on crack paths can now be studied to high precision. What is missing for an effective mean-field theory is a rigorous model reduction procedure that can capture the information lost during coarse graining, allowing defect nucleation and growth in random microstructures to be modelled. The overarching aim of this project is to develop such a procedure, incorporating uncertainty propagation across the scales.

Applications. The long-term goal of the project is to develop models which will not only improve our understanding of failure processes but also suggest strategies to control them. Real-world applications include developing sharper diamond cutting tools, suggesting strategies to reduce the unsustainably high energy cost of breaking up mineral ores to extract metals (~5% of total human energy consumption), and improving the resilience of submerged pipelines where the cost of inspection and/or repair is extremely high. The current generation of continuum models rely heavily on empirical crack growth criteria and constitutive equations. The lack of true predictive power in this area is a cause of great concern to industry. Adding reliable probabilistic “error bars” including the effects of model error, limited data, epistemic uncertainty and the coarse-graining procedure itself would be a huge step forward: the European Materials Modelling Council recently identified lack of uncertainty quantification as one of the major barriers holding back wider adoption of this kind of materials modelling in industry [4].

Overall Scope. The project supervisors have demonstrated for dislocations [5] and brittle cracks [6], respectively, that continuum elasticity remains accurate surprisingly close to defects, with non-linearity and discreteness localised to a nanoscale region. In fact the atomistic defect core is effectively decoupled from the far-fields, thus suggesting that it is possible to remove some of the empiricism in current continuum models by incorporating atomistic information that need not be computed on-the-fly. However, to move beyond perfect crystals, microstructural variation must be effectively included, making this a complex problem to attack. We propose to address this by averaging over a number of representative configurations at the microscale, then identifying and extracting the key information to a higher scale. Keeping track of information lost during the coarse graining process will enable uncertainty quantification. The application-domain knowledge of the project supervisors will be supplemented by expertise within Mathematics (e.g. Dr Tim Sullivan, Dr Florian Theil, Prof. Andrew Stuart), MathSys and WCPM (e.g. Prof. Nicholas

Zabaras). Ideas from variational inference, specifically in its Bayesian formulation, will be considered (e.g. relative entropy). A key advantage of these predictive modelling approaches is that data can be incorporated both from “above” (experiments) and “below” (atomic scale models), allowing the model errors arising from empirical constitutive equations to be estimated.

MSc Project. The MSc project will consider a simple material for which microstructural variation is an issue: amorphous silica glass. An indicative outline of the project is:

- Background reading on molecular simulation (e.g. from online *quippy* tutorials provided by the supervisor [7]) and continuum fracture mechanics (e.g., Lawn, 1993)
- Using an existing code developed by the project supervisor, generate crack path trajectories starting from representative glass structures (provided), using the computational resources available through the Centre for Scientific Computing.
- Learn how to analyse the output.
- Develop a deterministic continuum crack growth criterion (e.g. Griffith) fitting the data.
- Formulate a PhD project that incorporates:
 - A strategy to include microstructural uncertainty into the above procedure
 - Propagation of model, microstructural and epistemic uncertainty
 - Implementation within an end-user finite element code.
 - Application to industrially relevant problems, e.g., rocks (Rio Tinto), glass (Jaguar Land Rover) and/or metals (Thalys, Tata, AWE, RCNDE, BP). The latter may require two levels of coarse-graining: nano-scale to grain-scale to continuum.

In addition to expertise within MathSys and WCPM, relevant connections are being made with other researchers in Engineering (Dr Mohad Mousavi Nezhad), WMG (Dr Pantos Efthymiadis, Dr Lucasz Figiel) and with experimental work in the Ultrasonics (Dr Rachel Edwards) and Microscopy (Dr Neil Wilson) groups in Physics. There is strong potential for direct industrial collaboration during the project. Options for industrial co-funding and/or partners include:

- Rio Tinto Centre for Advanced Mineral Recovery
- JLR/Tata steel - CDT partners
- Thalys - CDT partners
- Other industrial links: AWE, Rolls Royce, SKF, BP, RCNDE

References

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