Workshop IV: Computational Methods for Multiscale Modeling of Materials Defects

Monday December 3, 2012

8:00–8:55 *Check-In/Light Breakfast (Hosted by IPAM)*

8:55–9:00 *Welcome and Opening Remarks*

9:00–9:50 **Wing Liu** (Northwestern University)
Mathematics, Mechanics and Physics of Materials, Uncertainty, and the Archetype-Genome Exemplar

10:00–10:15 *Break*

10:15–11:05 **Claude Le Bris** (École Nationale des Ponts-et-Chaussées)
Two topics related to nonperiodic multiscale problems

11:15–11:30 *Break*

11:30–12:20 **Assyr Abdulle** (École Polytechnique Fédérale de Lausanne (EPFL))
Adaptive reduced basis numerical homogenization methods

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Frederic Legoll** (Ecole Nationale Des Ponts et Chaussees (LAMI))
Variance reduction approaches in stochastic homogenization

3:30–4:00 *Break*

4:00–4:50 **Houman Owhadi** (California Institute of Technology)
Homogenization with arbitrary rough coefficients and super-localization

5:00–6:30 *Poster Session & Reception (Hosted by IPAM)*

Tuesday December 4, 2012

8:00–9:00 *Continental Breakfast*

9:00–9:50 **Jacob Fish** (Columbia University)
Multiscale Design System - Theory, Applications and Software Demonstrations

10:00–10:15 *Break*

10:15–11:05 **Adriana Garroni** (Università di Roma “La Sapienza”)
Asymptotic analysis of a system of edge dislocations

11:15–11:30 *Break*

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11:30–12:20 **Chris Larsen** (Worcester Polytechnic Institute)
New variational problems for material defect evolution

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Qiang Du** (Pennsylvania State University)
Nonlocal peridynamic theory for materials modeling

3:30–4:00 *Break*

4:00–4:50 **Karsten Albe** (Technishche Universtitat Darmstadt)
Deformation behaviour of nanocrystalline alloys studied by hybrid MD/MC simulations

Wednesday December 5, 2012

8:00–9:00 *Continental Breakfast*

9:00–9:50 **Virginie Ehrlacher** (École Nationale des Ponts-et-Chaussées)
Greedy algorithms for linear eigenvalue problems: application to the buckling of cellular materials with defects

10:00–10:15 *Break*

10:15–11:05 **Florian Theil** (University of Warwick)
Periodic minimizers of atomistic energies in two and three dimensions

11:15–11:30 *Break*

11:30–12:20 **Harold Park** (Boston University)
Multi-Timescale Approaches to Investigate Plasticity in Amorphous Solids

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Mitchell Luskin** (University of Minnesota, Twin Cities)
Atomistic-to-Continuum Coupling Methods

3:30–4:00 *Break*

4:00–4:50 **Xingjie Li** (Brown University)
Positive-Definiteness of the Blended Force-Based Quasicontinuum Method

Thursday December 6, 2012

8:00–9:00 *Continental Breakfast*

9:00–9:50 **Dionisios Margetis** (University of Maryland)
A two-scale view of crystal facets

10:00–10:15 *Break*

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10:15–11:05 **Petr Plechac** (University of Delaware)
Parameterisation and multilevel approximations of coarse-grained dynamics in KMC simulations

11:15–11:30 *Break*

11:30–12:20 **Peter Smereka** (University of Michigan)
Kinetic Monte Carlo for Strained Epitaxial Growth

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Jiun-Shyan Chen** (University of California, Los Angeles (UCLA))
Meshfree Method for Multiscale Materials Modeling

3:30–4:00 *Break*

4:00–4:50 **Giovanni Samaey** (KULeuven)
A micro/macro parareal algorithm for singularly perturbed ODEs

Friday December 7, 2012

8:00–9:00 *Continental Breakfast*

9:00–9:50 **Kaushik Bhattacharya** (California Institute of Technology)
Towards density functional theory calculations of defects in crystals

10:00–10:15 *Break*

10:15–11:05 **Weizhu Bao** (National University of Singapore)
Phase Field Approach for Simulating Solid-State Dewetting Problems

11:15–11:30 *Break*

11:30–12:20 **Mikko Haataja** (Princeton University)
Multilayer Thin Film Growth on Crystalline and Quasi-crystalline Surfaces: A Phase-field Crystal Approach

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Axel Voigt** (Technishche Universtitat Dresden)
Grain growth - how atomistic effects might influence scaling laws and size distribution functions