

Symposium 1: Mathematical issues in multiscale materials modeling

Organizes: Weinan E, Max Gunzburger, Mitchell Luskin, Rich Lehoucq

Oral Presentations

Blue: Invited talk (30 minutes)

Black: Contributed talk (20 minutes)

Green: Posters presentation

Monday Morning

Russel Caflisch, Multiscale methods for fluid and plasma dynamics

Endre Suli, Kinetic models for dilute polymers: analysis, approximation and computation

Petr Plechac, Coarse-graining of macro-molecular systems: mathematical and numerical methods

John H. Maddocks, Rob Manning and Ludovica Cotta-Ramusino, A path-integral formulation of DNA looping probabilities

Monday Afternoon

Gero Friesecke and Oliver Junge, Mean field approximation of transfer operators in high-dimensional conformation dynamics

Claude Le Bris, Some recent progress in elliptic homogenization

Qiang Du, Micro-macro FENE models for polymeric materials and their closure approximations

Leonid Berlyand, Homogenization with nonseparated scales

Monday Afternoon (2)

Eric Cancès, Toward multiscale modelling and simulation of fuel cells

Carlos Garcia-Cervera, Weinan E and Jianfeng Lu, Sub-linear scaling algorithms for the study of the electronic structure of materials

Michael Griebel, Jan Hamaekers and **Frederik Heber**, BOSSANOVA: A bond order dissection approach for efficient electronic structure calculations

Tuesday Morning

J. Tinsley Oden, Serge Prudhomme, Paul T. Bauman and Ludovic Chamoin, Adaptive control of modeling error for multiscale simulations

Max Gunzburger, Title TBD

Vikram Gavini, Electronic structure calculations at macroscopic scales

Denis Aubry, A numerical bridge between quantum and molecular dynamics based on the Ehrenfest theorem

Serge Prudhomme, Ludovic Chamoin, J. Tinsley Oden and Paul T. Bauman, On a stochastic approach for atomic-to-continuum coupling methods

Tuesday Afternoon

Mitchell Luskin, Marcel Arndt and Matthew Dobson, Mathematical validation and algorithms for the quasicontinuum method

Ronald Miller, Ellad Tadmor and Mitchell Luskin, Comparing the accuracy and efficiency of multiscale methods

Jill Reese and Max Gunzburger, Optimization-based atomistic-to-continuum coupling

Yanzhi Zhang, A Quadrature-rule type approximation for the quasi-continuum method

Wednesday Morning

Pingbing Ming, Analysis of quasicontinuum method

Rolf Krause and Konstantin Fackeldey, Weak coupling and high performance algorithms in multiscale methods

Richard Lehoucq and Stewart Silling, Peridynamics, molecular dynamics, and classical (nonlinear) elasticity

Michael Parks, Molecular dynamics at larger scales: Peridynamics as an upscaling of molecular dynamics

Xavier Blanc, Claude Le Bris, **Frederic Legoll** and Carsten Patz, Coarse-graining the free energy of atomistic systems: a simple case

Thursday Morning

Hamid Garmestani, Inverse microstructure design based on statistical correlation functions

Vernet Lasrado, Devendra Alhat and **Yan Wang**, A Review of recent transition state search methods in phase transition simulation

Valdemar Melicher, Jan Busa, Finite element heterogeneous multiscale method and micromagnetism

Catalin Picu and Monica Soare, Homogenization of stochastic fractal microstructures

Poster Presentations

Wednesday Afternoon

1. **Xi Chen** and Max Gunzburger, Finite element methods for a peridynamic model of mechanics
2. **Pablo Seleson** and Max Gunzburger, Bridging methods and boundary treatment for AtC coupling problems
3. **Abdmanam Elmaryami**, Effect of thermal cycling on hardness of plain carbon steel
4. **Onyekwelu U. Okeke** Electronic structure calculations of novel spinel oxynitrides
5. **Liping Liu**, Hashin-Shtrikman bounds for multiphase composites and their attainability
6. **Nicolas Castin** and Lorenzo Malerba, New approach to model point defects migration using a Monte-Carlo paradigm coupled with artificial intelligence
7. **Zoltan Dudas**, Regression possibilities of isothermal transformation (IT) and continuous cooling (CC) transformation diagrams using T-t elements
8. **Steve Fitzgerald** and Duc Nguyen-Manh, Analytic solution of the discrete double sine-Gordon model: application to crowdion migration in the bcc transition metals
9. **Alexander Barashev**, Stanislav Golubov, Yury Osetskiy and Roger Stoller, Generalisation of the diffusion-reaction theory for inclusion of complexes with long-range interaction range