REPORT DOCUMENTATION PAGE

Form Approved OMB NO. 0704-0188

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
04-02-2015	Final Report	16-Sep-2013 - 15-Sep-2014

4. TITLE AND SUBTITLE
Final Report: Mathematical and Computational Aspects of Multiscale Materials Modeling, Mathematics-Numerical analysis, Section II.A.a.3.4, Conference and symposia organization II.A.2.a

5a. CONTRACT NUMBER
W911NF-13-1-0203

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
611102

6. AUTHORS
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5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES
Rensselaer Polytechnic Institute
110 8th Street

Troy, NY 12180 -3522

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES)
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSOR/MONITOR'S ACRONYM(S)
ARO

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
64443-MA-CF.1

12. DISTRIBUTION AVAILIBILITY STATEMENT
Approved for Public Release; Distribution Unlimited

13. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT
This grant was used to support the organization of the international conference "Multiscale Materials Modeling: Mathematical and Computational Aspects" at Rensselaer Polytechnic Institute, during the period June 10-12, 2014. The conference was organized under the auspices of the International Center for Applied Computational Mechanics (ICACM) and is the 8th meeting organized in this series. The conference brought together researchers from US, France and Canada working on various aspects of physics-based multiscale modeling of the mechanical behavior of

15. SUBJECT TERMS
mathematical modeling; physica modeling; computational methods; conference organization

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Catalin Picu
UU	UU	UU	UU		19b. TELEPHONE NUMBER
					518-276-2195

Standard Form 298 (Rev 8/98)
Prescribed by ANSI Std. Z39.18

Report Title

Final Report: Mathematical and Computational Aspects of Multiscale Materials Modeling, Mathematics-Numerical analysis, Section II.A.a.3.4, Conference and symposia organization II.A.2.a

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Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

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Total Number:	

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Names of other research staff

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Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

The description of the activity is provided in the attached file.

Technology Transfer

Report Type:	Final Report
Proposal Number:	64443MACF
Agreement Number:	W911NF1310203
Proposal Title:	Mathematical and Computational Aspects of Multiscale Materials Modeling, Mathematics-Numerical analysis, Section II.A.a.3.4, Conference and symposia organization II.A.2.a
Report Period Begin Date:	09/16/2013
Report Period End Date:	09/15/2014

Abstract

This grant was used to support the organization of the international conference "Multiscale Materials Modeling: Mathematical and Computational Aspects" at Rensselaer Polytechnic Institute, during the period June 10-12, 2014. The conference was organized under the auspices of the International Center for Applied Computational Mechanics (ICACM) and is the 8th meeting organized in this series. The conference brought together researchers from US, France and Canada working on various aspects of physics-based multiscale modeling of the mechanical behavior of materials. The details of the organization are presented in this report along with outcomes of the meeting relevant for the future directions in this field.

Report

Introduction

The International Center for Applied Computational Mechanics was established 7 years ago by a group of researchers from France and US working in the field of Mathematics and Mechanics. The Center has organized meetings every year over the past 7 years.

The subjects covered in the past included, but were not limited to, geomaterials, energetic materials, plastic deformation in metals and alloys, granular materials etc. In all these meetings the focus was on mathematics, physics and computational aspects. Mathematical aspects included constitutive equations development, stability, stochasticity, uncertainty quantification, etc.

The conference has a simple format, with one common session. The talks are given only by invited speakers, while non-invited participants may present posters.

The meeting organized in 2014 (supported in part by this grant) continued along this path. The focus was on multiscale aspects of material behavior. This was the first meeting of the series having the mathematical, physical and computational integration of phenomena taking place on multiple scales as the central subject. Most previous meetings were focused on specific scales, phenomena or material systems. Mathematical issues related to modeling, uncertainty quantification and error control were the central theme of the meeting.

Previous meeting is this series were held at:

2007: University of Florida, Shalimar
2008: DGA, Rocamadour
2009: University of Florida, Shalimar
2010: University of Paris XIII, Institut Henri Poincaré
2011: IUTAM Symposium, Florida
2012: Rutgers University, New Jersey
2013: University of Grenoble, France

The goals of the meeting were:

- Review the current state of modeling and understanding plastic deformation
  - Mathematical models
  - Computational techniques currently used
  - Multiscale modeling and multiscale experiments
  - Scale coupling
  - Role of instabilities
- Outline the outstanding challenges in both plasticity and multiscale modeling in general
- Promote interactions between participants

Organization details:

Speakers: 24

Registered participants, including invited speakers: 33

Actual number of participants, including local faculty, students and postdocs as well as visitors from General Electric, Research and Development: 45 to 50

Duration: 2 days

Length of talks: 30 or 40 minutes, 12 speakers per day

Program:

ICACM 2014: Multiscale Materials Modeling: Mathematical and Computational Aspects

AGENDA, Tuesday, June 10, 2014

Room: Center for Industrial Innovation, CII 4050

8 :00	**Registration**
8 :20	**Welcome**
Session 1.1 Chair: Catalin Picu	
8 :30 – 9 :10	**Benoit Devincre**, CNRS-ONERA, The Discrete-Continuum Model: An Important Breakthrough to Simulate the Mechanical Properties of Dislocated Crystals with Complex Boundary Conditions
9 :10 – 9 :50	**Anter El-Azab**, Purdue University, Mathematical and Computational Modeling of Dislocation Patterns and Strain Hardening in Crystals
9 :50 – 10 :20	**Michael Demkowicz**, Massachusetts Institute of Technology, Interface Design Using Reduced Order Mesoscale Models
10 :20 – 10 :40	**Break**
Session 1.2 Chair: Anter El-Azab	
10 :40 – 11 :20	**James Sethna**, Cornell University, Bending Crystals: The Evolution of Cell Boundary Dislocation Structure
11 :20 – 11 :50	**Jianfeng Lu**, Duke University, Numerical Analysis of Atomistic-to-Continuum Hybrid Methods
11 :50 – 12 :20 :	**Djimedo Kondo,** Universite Pierre et Marie Curie Paris, Strength Properties of Ductile Nanoporous Materials: Theoretical Models and Assessment by Atomistic Simulations
12 :20 – 14 :00	**Lunch** – on site
Session 1.3 Chair: Antoinette Maniatty	
14 :00 – 14 :30	**Arash Yavari**, Georgia Institute of Technology, Non-Riemannian Geometries and the Nonlinear Mechanics of Distributed Defects
14 :30 – 15 :10	**David Srolovitz**, University of Pennsylvania, Atomistic Simulations of the Deformation of Nanocrystalline Metals: Applications to Dislocation Dynamics in Polycrystals
15 :10 – 15 :40	**Min Zhou**, Georgia Institute of Technology, Prediction of Macroscopic Fracture Toughness from Microstructure
15 :40 – 16 :00	**Break**
Session 1.4 Chair: Min Zhou	
16 :00 – 16 :30	**Nathan Barton**, Lawrence Livermore National Laboratory, Direct Multiscale Embedding of Polycrystal Plasticity Enabled by Adaptive Sampling
16 :30 – 17 :00	**Antoinette Maniatty,** Rensselaer Polytechnic Institute, Stabilized Finite Element Method for Multiscale Polycrystal Plasticity
17 :00 – 17 :30	**Regis Cottereau**, Ecole Centrale Paris, A Coupling Method for Stochastic Polycrystalline Models at Different Scales
19:00	**Dinner** (Russell Sage Dinning Hall, in campus)

AGENDA, Wednesday, June 11, 2014

Room: Center for Industrial Innovation, CII 4050

Session 2.1 Chair: Ronald Miller

8 :30 – 9 :10 : **David McDowell,** Georgia Institute of Technology, Modeling Interface-Mediated Metal Plasticity at Small Scales

9 :10 – 9 :40 : **Ghiath Monnet,** RED R&D, MMC, Multiscale Simulations of Temperature and Strain Rate Sensitivity of Strengthening Induced by Coherent Precipitates: from Atomic to Continuum Scale

9 :40 – 10 :10 : **David Rodney,** Universite de Lyon, Overcoming Old Barriers in Thermally-Activated Plasticity

10 :10 – 10 :30 : **Break**

Session 2.2 Chair: David Rodney

10 :30 – 11 :00 : **Ronald Miller,** Carleton University, Finite Temperature and Finite Deformation: New Tools for More Efficient and Accurate Atomistic Simulation

11 :00 – 11 :40 : **Armand Beaudoin,** University of Illinois at Urbana-Champaign, Study of Microplasticity Through 3D X-ray Diffraction

11 :40 – 12 :20 : **Michel Potier-Ferry,** Universite de Lorraine, Multi-scale Instabilities

12 :20 – 14 :00 : **Lunch** – on site

Session 2.3 Chair: Ioan Ionescu

14 :00 – 14 :30 : **Jerome Weiss,** Universite Joseph Fourier Grenoble, From Continuous to Crackling Plasticity

14 :30 – 15 :00 : **Hamed Hatami-Marbini,** Oklahoma State University, An Experimental and Computational Framework for Investigating the Mechanical Behavior of Corneal Stroma

15 :00 – 15 :40 : **Jacob Fish,** Columbia University, Practical Multiscaling

15 :40 – 16 :00 : **Break**

Session 2.4 Chair: Jerome Weiss

16 :00 – 16 :40 : **Jia Li,** Universite de Paris Nord, Interaction Between Anisotropic Damage and Dynamic Wave Propagation in Brittle Materials

16 :40 – 17 :10 : **Vivek Shenoy,** University of Pennsylvania, Multiscale Modeling of Compositional Stresses in Nonstoichiometric Oxides

17 :10 – 17 :40 : **Assad Oberai,** Rensselaer Polytechnic Institute, Subgrid Models for Multi-Parameter Problems

18:00 **Departure to Saratoga Springs for dinner**

Outcomes of the meeting: Outstanding research issues identified by the participants

● The representations of dislocations on various scales are entirely different (explicit atomistic models, discrete dislocation dynamics models (DDD), continuum representations). Coupling of these models is difficult. Coupling of atomistics and DDD models has been explored to some extent, but the coupling between DDD and continuum models of the evolution of large populations of dislocations is essentially unexplored.

None of these models account for additional complexities introduced for example by the presence of solute, precipitates and twins.

● In particle models, coarse grained representations have been developed using rather formal methods (e.g. Mori-Zwanzig). This formulation allows writing the evolution equation for the coarse system (or the associated Liouvillian). From this, it is possible to go further to larger scales to develop DPD (dissipative particle dynamics) or even fluid mechanics models. In the case of plastic deformation and associated fracture and damage accumulation, no such coarse graining methodology has been developed so far. This is one of the important missing links in multiscale modeling of material behavior.

● Concurrent coupling of models of the Quasicontinuum type are still to be developed, especially at non-zero temperatures. There are big computational challenges in 3D and simply using larger computers is not a solution.

● An emergent view of plastic deformation is that of a non-monotonic process, which takes place by large jumps forward separated by periods when there seems to be little activity. These have been termed "avalanches" and are different from larger scale instabilities. Avalanches have been observed on the small scales in many material systems, mainly by acoustic emission experiments. Although the deformation is unsteady on the small scales (microns and below), it appears steady on larger scales. The "smoothing" out of this process is not properly represented in any current models of deformation.

The relationship between plastic deformation and critical phenomena is currently being explored.

● The use of non-Riemanian geometry to represented bodies with defects is still being explored. The concept here is that one can map the real space in which materials carry residual stresses to a curved space in which the equivalent configuration is stress-free. This presents the advantage that as one applies deformation, the initial state is well-defined and a real reference configuration. In addition, the deformation itself can be defined as an evolution of the mapping bringing the system from real space to the fictitious described above. This method has is similar to that used in relativity to account for space curvature, but its application to mechanics of classical continua has not been explored extensively in the recent years.

● In many situations one needs to compute energetic barriers for various processes. This is usually done using transition state methods, such as the Nudged elastic band method. These methods provide the path taken by the system in phase space as it evolves between two equilibrium configurations. The point of highest energy on this path is the energetic barrier of interest. Many methods that address this problem exit. However, none of these is perfect. Improvements in this area are very much needed.

● The validity of interatomic potentials used in atomistic models of matter is an important, recognized issue. Potentials provide only approximations of the real interactions and are bound to fail in regions where large strains and strain gradients exist (e.g. at defect cores). Efforts are continuously made to improve potentials. This problem is conceptually identical to the error introduced in larger scale models due to coarse graining steps taken on sub-scales. There is no simple, thereotical answer for this issue.

● Uncertainty propagation. The mathematical issue of how uncertainty propagates across scales and from one model to another is of great importance. A related issue is to ask: how variability (moments larger than one of the distribution function) of fields influences the mean (first moment of the distribution function) of the system scale response.