# Maria Emelianenko

Contact Voice: (703) 993-9688 Exploratory Hall, Room 4454 Information Department of Mathematical Sciences Fax: (703) 993-1491 George Mason University E-mail: memelian@gmu.edu Fairfax, VA 22030 USA WWW: math.gmu.edu/~memelian Research Numerical methods and applied PDE, modeling of nonlinear systems, multigrid methods, Interests optimization, stochastic processes, applications to materials science, physics and biology FULL-TIME George Mason University, Fairfax, VA Positions Dean's Fellow, College of Science 01/2017 - 05/2018Professor, Department of Mathematical Sciences 08/2017 - present Associate Professor, Department of Mathematical Sciences 08/2012 - 08/2017Assistant Professor, Department of Mathematical Sciences 08/2007 - 08/2012Affiliate Faculty, Computational Materials Science Center Carnegie Mellon University, Pittsburgh, PA CNA Postdoctoral Research Associate, Center for Nonlinear Analysis 08/2005 - 08/2007Pennsylvania State University, University Park, PA Research Assistant, Mathematics Department 2003 - 2005Teaching Assistant/Associate, Mathematics Department 1999 - 2003VISITING University of California Los Angeles, IPAM, Los Angeles, CA Positions Senior Fellow, Core Faculty Participant Program on Understanding Many-Particle Systems with Machine Learning 09/2016 - 12/2016Park City Mathematics Institute, Park City, UT Institute for Advanced Study, Princeton, NJ Principal Lecturer, Undergraduate Faculty Program "Mathematics and Materials" PCMI Summer Program July 2014 University of California Los Angeles, IPAM, Los Angeles, CA Senior Fellow, Core Faculty Participant Program on Materials Defects 09/2012 - 12/2012**EDUCATION** Pennsylvania State University, University Park, PA Department of Mathematics Ph.D. Mathematics, Minor in High Performance Computing 08/2005 Thesis: "Multilevel and Adaptive Methods for Some Nonlinear Optimization Problems" Advisor: Prof. Qiang Du 08/2002M.A. Mathematics Thesis: "Analysis of Constrained Multidimensional Birth-Death Processes" Advisor: Prof. N. Gautam Moscow State University, Moscow, Russia Department of Computational Mathematics and Cybernetics

M.S. Applied Mathematics, summa cum laude

06/2001

ferential equations" Advisor: Prof. A. Bratus **B.S.** Computer Science/Math, summa cum laude 06/1999Co-PI, "Experimental and Mathematical Discovery for HIV" MDR seed grant, \$40,000 2017 Co-PI, "Modeling Prospects of Malaria Elimination in Haiti" MDR seed grant, \$33,000 2017 co-PI, NIST "SURF: Experience for Mason Undergraduates" grant, NIST summer internships for Mason students (\$27,000, \$18,000) 2016, 2017 co-PI, GMU Provost seed grant for "Suppemental Funding of Mathematical Sciences PhD Program", to jump start Industry Immersion Program, \$447,816 2017 - 2019Senior Personnel (Lead Institution: CMU), NSF conference grant, Applied Mathematics, "Topics in Applied Nonlinear Analysis: Recent Advances and New Trends", \$31,500 PI, NSF QED-EXTREEMS grant, \$600,000 2014 - 2017Title: EXTREEMS-QED: Undergraduate Research in Computational and Data-Enabled Mathematics PI. NSF CAREER grant, Computational and Applied Mathematics, \$452,000 2011 - 2017Title: CAREER: Developing Mathematical Tools for Modeling Complex Materials Systems co-PI, NSF-MAA RUMC grant, \$2,600 2012 - 2013Title: Undergraduate Mathematics Conference in Washington Senior Personnel, DTRA Phase II grant, \$7,568,564 2012 - 2017Title: Translational Peptide Research for Personnel Protection co-PI, NSF REU grant, \$334,000 2012 - 2013Title: REU: Research, Education and Training in Computational Mathematics and Nonlinear Dynamics of Biological, Bio-inspired and Engineering Systems co-PI, AWM Sonia Kovalevsky Day awards, \$1795, \$1950 2011, 2012 PI, NSF grant, Computational Mathematics, \$267,000 2009 - 2012Title: Mesoscale Computational Modeling and Analysis of Materials Microstructure PI, ORAU's Ralph E. Powe Junior Faculty Enhancement Award, \$10,000 2009 - 2010Title: Mesoscale Computational Modeling and Analysis of Materials Microstructure co-PI, NSF grant for establishing an REU SITE at GMU, \$180,000 2009 - 2010Title: REU: Multidisciplinary REU in Computational Mathematics and Nonlinear Dynamics of Biological, Bio-inspired and Engineering Systems PI, Summer Research Award, GMU (university-wide competitive grant), \$5,200 2008 Title: Mathematics of Materials Research-related:

Invited talk, 8th Intl. Conference on Multiscale Materials Modeling, Dijon, France, 10/10/2016
 Plenary address, 9th European Conference on Elliptic & Parabolic Problems Gaeta, Italy 05/26/2016

Jan 2014 – Dec 2016

• Secretary (elected), SIAM Activity group on Mathematics of Materials

Thesis: "Numerical approach to solving Andronov-Hopf and Bogdanov-Takkens systems of dif-

Grants

Honors and Awards

o PSU Graduate School Alumni Society Early Career Award	2014
o Mason Emerging Researcher/Scholar/Creator Award	2013
o Invited tutorial, Materials Defects Program, IPAM, UCLA	eptember 2012
o Invited lecture, PIRE lecture series, Carnegie Mellon University, Pittsburgh, PA	March 2012
o ORAU Ralph E. Powe Junior Faculty Enhancement Award	2009
o First Place in Poster Competition, Gordon Research conference on Physical Metall	urgy 07/2006
o Travel Award, Gordon Research conference on Physical Metallurgy	07/2006
o SIAM Student Travel Award, SIAM Meeting, New Orleans	07/2005
o Honorable Mention in Student Paper Competition, Copper Mountain Conference	04/2005
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Teaching-related:	
o Invited presentation, minisymposium on "Implementing Transformational Undergraduate Model-	
ing Experiences" at SIAM Annual Meeting	July 2016
o Pearson's One Math Professor honoree	Fall 2015
• Project NExT Fellow (nation-wide competition)	2008 - 2009
o Dean's Recognition for Outstanding Teaching, CMU	2005
o Graduate Assistant Outstanding Teaching Award Nomination, PSU	2004
o Graduate School Teaching Certificate, PSU	2004
o Teaching with Technology Certificate, PSU	2004
$\circ$ Teaching Associate Certificate, Department of Mathematics, PSU	2003
Earlier fellowships and other certificates:	
o Davey Fellowship, Department of Mathematics, PSU	2003
o Applied Management Principles Certificate, Purdue University	2002
• Eberly College of Science Fellowship, PSU	1999
• Moscow City Mayor's stipend for Distinguished Students, Moscow State University	
• Dean's List, Moscow State University	1996 - 1999
o Dubna Foundation of Science and Education Scholarship	1995 - 1996

# Publications

REFEREED PAPERS
AND PROCEEDINGS

33. D. Torrejon, M. Emelianenko, "Generalized master equations for random walks with time-dependent jump sizes", accepted to SIAM J. Appl. Math., 2018

1996

o Highest Distinction ("'Gold Medal"') on graduation from high school

- 32. K. Saleme Ruiz, M. Emelianenko, "The role of topology in microstructure-property relations: a 2D DEM-based study", Modelling Simul. Mater. Sci. Eng., 26 (2018) 014001
- 31. R. Otis, M. Emelianenko, Z-K. Liu, "Efficient sampling strategies for global energy minimization of multi-component phases with internal degrees of freedom", Comp. Mat. Sci., **130** (2017), p. 282-291
- 30. D. Torrejon, M. Emelianenko, D. Golovaty, "Continuous time random walk based theory for a one-dimensional coarsening model", J. Ellip. Parab. Eq., 2 (2016), p. 183–199
- 29. I. Yegorov, M. Emelianenko, "A kinetic approach to modeling general-texture evolution in two-dimensional polycrystalline grain growth", Comp. Mat. Sci., 125 (2016), p.224–242
- 28. I. Yegorov, C. Torres, M. Emelianenko, "A Boltzmann-type kinetic model for misorientation distribution functions in two-dimensional fiber-texture polycrystalline grain growth", Acta Materialia, 109 (2016) p. 230–247
- 27. K. Barmak, E. Eggeling, M. Emelianenko, Y. Epshteyn, D. Kinderlehrer, R. Sharp, S. Ta'asan, "Recent Developments in Material Microstructure: a Theory of Coarsening", Mater. Res. Soc.

- Symp. Proc., Cambridge Journals, 1753 (2015)
- 26. C.Torres, M. Emelianenko, D. Golovaty, D. Kinderlehrer, S.Ta'asan, "Numerical analysis of the vertex models for simulating grain boundary networks", SIAM J. Appl. Math., **75(2)** (2015), p. 762–786
- 25. J. Snider, I. Griva, X. Sun, M. Emelianenko "Set-based framework for Gibbs energy minimization", CALPHAD, 48 (2015), p. 18–26
- 24. M. Emelianenko, D. Torrejon, M. DeNardo, A. Socolofsky, A. Ryabov, T. Collins, "Estimation of Rate Constants in Nonlinear Reactions Involving Chemical Inactivation of Oxidation Catalysts", J. Math. Chem., **52**, Issue 5 (2014), p. 1460–1476
- 23. K. Barmak, E. Eggeling, M. Emelianenko, Y. Epshteyn, D. Kinderlehrer, R.Sharp, and S.Ta'asan "Materials microstructures: entropy and curvature driven coarsening", RIMS Proceedings, U. Kyoto, 1881, p. 71-91 (2014)
- 22. Refereed book chapter: K. Barmak, E. Eggeling, M. Emelianenko, Y. Epshteyn, D. Kinderlehrer, R. Sharp and S. Ta'asan, "A Theory and Challenges for Coarsening in Microstructure", Springer INdAM Series, "Analysis and Numerics of Partial Differential Equations", in memory of Enrico Magenes, 2013
- 21. J. Zhang, M. Emelianenko, Q. Du, "Periodic centroidal Voronoi tessellations", Intern. J. Num. Anal. Modeling, 9, p.950-969 (2012)
- 20. K. Barmak, E. Eggeling, M. Emelianenko, Y. Epshteyn, D. Kinderlehrer, R.Sharp, and S.Ta'asan, "Predictive theory for the grain boundary character distribution", Materials Science Forum, 715-716, 2012, p.279–285 (Special Issue on ReX and GG IV)
- 19. Z. Di, M. Emelianenko, S. Nash, "Truncated Newton-based multigrid algorithm for centroidal Voronoi calculation", Numer. Math. Theor. Meth. Appl., 5, No. 1, (2012) pp. 242–259
- 18. A. Baranova, J. Bode, G. Manyam, M. Emelianenko, "An efficient algorithm for systematic analysis of nucleotide strings suitable for siRNA design", BMC Res. Notes, 4(1):168 (2011)
- 17. K. Barmak, E. Eggeling, M. Emelianenko, Y. Epshteyn, D. Kinderlehrer, R. Sharp, S. Ta'asan "Critical events, entropy, and the grain boundary character distribution", Physical Review B, 83, 134117 (2011)
- Editor's suggestion, with accompanying Viewpoint
- 16. K. Barmak, E. Eggeling, M. Emelianenko, Y. Epshteyn, D. Kinderlehrer, R. Sharp, S. Ta'asan, "An entropy based theory of the grain boundary character distribution", DCDS-A, **30**, no. 2 (2011), p.427–454
- 15. M. Atkins (mentors: D. Anderson, M. Emelianenko, Y.Mishin), "A Method of Calculating the Thickness of a Solid-Liquid Interface", SIAM Undergraduate Research Online, 3, 2010
- 14. M. Emelianenko, "Fast Multilevel CVT-based Adaptive Data Visualization Algorithm", Numer. Math. Theor. Meth. Appl., 3, No. 2 (2010), p.195-211
- 13. K. Barmak, E. Eggeling, M. Emelianenko, Y. Epshteyn, D. Kinderlehrer, S. Ta'asan, "Geometric growth and character development in large metastable systems", Rendiconti di Matematica, Serie VII, 29, Roma (2009), 1-13

- 12. K. Barmak, M. Emelianenko, D. Golovaty, D. Kinderlehrer, and S. Ta'asan., "A new perspective on texture evolution", Intl. J. of Num. Anal. and Modeling, 5, Supp (Special Issue on Modeling, Analysis and Simulations of Multiscale Nonlinear Systems), 2008, p.93–108
- 11. K. Barmak, M. Emelianenko, D. Golovaty, D. Kinderlehrer, S. Ta'asan, "Towards a statistical theory of texture evolution in polycrystals", SIAM J. Sci. Comput., **30** No. 6 (2008), p. 3150–3169
- 10. M. Emelianenko, L. Ju, A. Rand, "Nondegeneracy and weak global convergence of the Lloyd algorithm in  $\mathbb{R}^d$ ", SIAM J. Numer. Anal., **46** Issue 3 (2008), p.1423–1441
- 9. Q. Du, M. Emelianenko "Uniform convergence of a nonlinear energy-based multilevel quantization scheme via centroidal Voronoi tessellations", SIAM J. Numer. Anal., **46**, Issue 3 (2008), p. 1483–1502
- 8. K. Barmak, M. Emelianenko, D. Golovaty, D. Kinderlehrer, and S. Ta'asan., "On a statistical theory of critical events in microstructural evolution", Proc. of the 11th International Symposium on Continuum Models and Discrete Systems (CMDS11), Paris, France, 2007
- 7. Q. Du, M. Emelianenko and L. Ju "Convergence properties of the Lloyd algorithm for computing the centroidal Voronoi tessellations", SIAM J. Numer. Anal., 44, Issue 1 (2006), p. 102–119
- 6. M. Emelianenko, Z.-K. Liu, Q. Du "A New Algorithm for the Automation of Phase Diagram Calculation", Comp. Mater. Sci., **35**, Issue 1 (2006), 61-74 [In ScienceDirect Top 25 Hottest Articles]
- 5. Q. Du, M. Emelianenko "Acceleration schemes for computing the centroidal Voronoi tessellations", Numer. Linear Algebra Appl., 13, Issue 2-3 (Special Issue on Multigrid Methods) (2006), p. 173–192
- 4. Q. Du, M. Emelianenko, H.-C. Lee and X. Wang "Ideal point distributions, best mode selections and optimal spatial partitions via centroidal Voronoi tessellations", Proc. 2nd Intl. Symp. on Voronoi Diagrams in Sci. and Engr., Seoul, Korea, Oct 2005 (VD2005), pp. 325-333, 2005
- 3. Q. Du, M. Emelianenko "A multilevel energy-based quantization scheme", Lecture Notes in Comp. Sci. Eng., 55, Widlund, Olof B.; Keyes, David E. (Eds.), Springer, Berlin (2007), p.533–541
- 2. M. Yacoubi, M. Emelianenko and N. Gautam "Pricing in next generation network queuing model to guarantee QoS", Perform. Evaluation, 5, issue 1 (2003), 59-84 [In Top 10 downloads from Performance Evaluation website in 2003]
- 1. E.B. Dushanov, M.G. Emelianenko and G.Yu. Konovalova, "On formats of the representation of real numbers and algorithm for automatic declaration of constants of the computer real arithmetic", J. Comput. Meth. Sci. Eng., 2, issue 1-2 (2002), p.57–62

# Publications on Education

1. M. Emelianenko, "Helping Undergraduates See Mathematics in Material World", SIAM News, 43, Number 6, 2010

Books

- 2. M. Emelianenko, J. Gemmer, D. Kinderlehrer, P. Shipman, "A primer on Mathematical Methods in Materials Science", under contract with SIAM, 2017
- $1.\ M.$  Emelianenko, "Multilevel and adaptive methods for nonlinear optimization problems", VDM-Verlag, 116 pages (2010) ISBN: 978-3-639-22436-8

PREPRINTS, UNREFEREED CONFERENCE PROCEEDINGS 8. K. Barmak, E. Eggeling, M. Emelianenko, Y. Epshteyn, D. Kinderlehrer, R. Sharp, S. Ta'asan,

- "An Entropy Based Theory of the Grain Boundary Character Distribution", Center for Nonlinear Analysis, No. 11-CNA-001, 2011
- 7. K. Barmak, E. Eggeling, M. Emelianenko, Y. Epshteyn, D. Kinderlehrer, R. Sharp, "Critical Events, Entropy, and the Grain Boundary Character Distribution", Center for Nonlinear Analysis, No. 10-CNA-014, 2010
- 6. K. Barmak, E. Eggeling, M. Emelianenko, Y. Epshteyn, D. Kinderlehrer, R. Sharp, S. Ta'asan, "Predictive Theory for the Grain Boundary Character Distribution", Center for Nonlinear Analysis, No. 10-CNA-013, 2010
- 5. K. Barmak, M. Emelianenko, D. Golovaty, D. Kinderlehrer, S. Ta'asan, "On a statistical theory of critical events in microstructure evolution", Center for Nonlinear Analysis, No. 07-CNA-005, 2007
- 4. M. Emelianenko, D. Golovaty, D. Kinderlehrer, S. Ta'asan, "Texture evolution via continuous time random walk theory", Center for Nonlinear Analysis, No. 06-CNA-011, 2006
- 3. M. Emelianenko, D. Golovaty, D. Kinderlehrer, S. Ta'asan, "Grain boundary evolution: new perspectives", Center for Nonlinear Analysis, No. 06-CNA-010, 2006
- 2. G.A. Emel'yanenko, M. Emelianenko, T.T. Rakhmonov, E.B. Dushanov, G.Yu. Konovalova, "On efficiency of critical-component method for solving singular and ill-posed systems of linear algebraic equations", preprint JINR, Dubna, Russia, arXiv:math/0108074, 2001
- 1. G.A. Emel'yanenko, V.N. Samoilov and M.G. Emelianenko "The uncertainty principle in numerical linear algebra", in Proc. Intl. Conf. on Comp. Math. Part I-II, (2002), 104–106, ICMMG, Novosibirsk

# Papers in Preparation

- 2. J. Snider, I. Griva, M. Emelianenko, "Vacancies and molar Gibbs energy", in preparation
- 1. Z. Di, M. Emelianenko, M. Vazquez, P. Houser, V. Maggioni, "CVT-based method for optimal placement of water gauges", in preparation

# GMU SERVICE SUMMARY

- 1. GMU COS Dean's Fellow, 2017-2018
- 2. Member, Office of Research Computing Advisory Board, 2017 present
- 3. Member, University Graduate Scholarship committee, 2017 present
- 4. GMU COS Executive Council, at-large member, 2016 2018
- 5. GMU COS Nominations Committee, 2009 2013
- 6. GMU Math Graduate Committee, 2015 present
- 7. GMU Math Policy & Hiring Committee, 2010 2012
- 8. Coordinator, Provost-sponsored Industrial Immersion Program (IIP) for Math graduate students, 2016 present
- 9. PI and Coordinator, NIST-GMU undergraduate internship program (joint grant with Volgenau School of Engineering), 2016 present
- 10. PI, GMU EXTREEMS undergraduate research program (involves 27 undergraduate students including 3 Puerto Rico students), 2014 2017
- 11. Organizer, Mason Chapter of Mathematics of Planet Earth SIAM Activity Group (includes members from Math, GGS and Civil Engineering departments)
- 12. Association for Women in Mathematics club faculty mentor, coordinating Women in Math activities and outreach events between GMU and local schools

- 13. Research Panel for Pakistan Scholars participant, GMU, April 20, 2016
- 14. Participant, Bootstrapping Research at Mason Panel, August 2012
- 15. Participant, GMU COS CAREER panel, April 2012, April 2014
- Co-organized 3 undergraduate research conferences (UMC2012, UMC2013, UMC2016)
- 17. Organized 1st GMU Industrial Modeling workshop (MMD2015)
- 18. Co-organized 4 research conferences (SIAM MS10, NIST UQ 2016, DelMar 2016, CMU 2016)
- 19. Co-organized 2 STEM outreach events (Sonia Kovalevsky GMU Middle and High School Mathematics Days)
- 20. Co-organizer, Applied & Comp. Math seminar, Dept. of Mathematical Sciences, 2007 2010
- 21. Chair, Committee on Departmental Website Redesign, Fall 2009
- 22. GMU Math Prelim grading and preparation ODE and Numerical Analysis, 2007 present
- 23. GMU Math and SPACS qualifying exam grading and preparation ODE, PDE, Numerical Analysis, 2007 present

## Professional activities & Service

# $\circ\,$ National scientific conference/workshop organization:

- (7) member of the Organizing committee, SIAM Conference on Mathematical Aspects of Materials Science (MS18), Portland, OR July 9-13, 2018
- (6) Chair of the Organizing committee, Mason Modeling Days workshop (2nd GMU Modeling workshop), George Mason University, Arlington VA June 28-July 1, 2017 ~60 nationwide academic participants from various disciplines https://sites.google.com/site/masonmodelingdays
- (5) co-chair of the Organizing committee (with I. Fonseca, A. Tudorascu, Y. Epshteyn, D. Slepcev) "Topics in Applied Nonlinear Analysis: Recent Advances and New Trends" conference, July 18-20, 2016 at Carnegie Mellon University, Pittsburgh, PA  $\sim$ 50 participants, poster sessions https://www.math.cmu.edu/CNA/kinderlehrer75
- (4) co-chair of the Organizing committee (with H. Antil and P. Seshaiyer), "DelMar Numerics Day" conference, GMU, May 14, 2016  $\sim\!80$  participants http://delmar.math.umd.edu
- (3) co-chair of the Organizing committee (with Igor Levin), "Uncertainty Quantification in Materials Science" workshop, NIST, January 14-15, 2016  $\sim 30$  participants

http://www.nist.gov/mml/mmsd/workshop-on-quantification-of-uncertainties-in-material-science.cfm

- (2) chair of the Organizing committee, Mason Modeling Days workshop (1st GMU Modeling workshop), George Mason University, Fairfax VA June 9-14, 2014  $\sim\!\!40$  nationwide academic and industrial participants https://sites.google.com/site/masonmodelingdays2014
- (1) member of the Organizing committee, SIAM Conference on Mathematical Aspects of Materials Science (MS10), Philadelphia on May 23−26, 2010 ~400 participants http://www.siam.org/meetings/ms10

#### • Professional development workshop organization:

- (5) chair of the Organizing committee, AWM Career workshop, SIAM Annual Meeting, Boston MA, July 2016 (~40 participants, a 2-day event including 2 research minisymposia, career panel and poster session)
- (4) chair of the Organizing committee, SIAM Professional Development Evening, SIAM CSE15, Salt Lake City, UT March 2015 ( $\sim$ 100 participants, a 3-hour event with 2 panel discussions and a networking session)
- (3) co-organizer, SIAM Professional Development Evening, SIAM Annual Meetings 2013, 2014 (~100 participants, a 3-hour event with 2 panel discussions and a networking session)
- (2) co-organizer, AWM workshop, SIAM Annual Meeting, San Diego CA July 2013 (~40 participants, 2-day event including 2 research minisymposia, career panel and poster session)
- (1) co-organizer, "AWM Workshop: Opportunities Beyond Academia", ICIAM, Vancouver, Canada, July 2011 (~40 participants, a 2-day event including 2 research minisymposia, career panel and poster session)

## • Undergraduate research conference organization:

- (4) co-organizer, Undergraduate Mathematics Conference in Washington (UMC), College of William & Mary, Williamsburg, VA, April 8, 2017 (~20 participants)
- (3) co-organizer, Undergraduate Mathematics Conference in Washington (UMC), George Washington University, Washington, DC, April 2, 2016 (~30 participants)
- (2) chair of the Organizing committee, Undergraduate Mathematics Conference in Washington (UMC), George Mason University, Fairfax VA, April 6, 2013 (~30 participants)
- (1) co-organizer, Undergraduate Mathematics Conference in Washington (UMC), George Washington University, Washington, DC April 21-22, 2012 (~30 participants)

### • Minisymposium organization:

- (12) co-organizer, "Advances in CALPHAD Methods" minisymposium, SIAM MS18, Portland, OR. July 2018
- (11) co-organizer, "Coarsening in microstructure" minisymposium, SIAM MS18, Portland, OR, July 2018
- (10) co-organizer, "Mathematical advances in hydrology: non-stationarity and data assimilation" minisymposium, SIAM Mathematics of Planet Earth conference, Philadelphia, Sept 2016
- (9) co-organizer, "Recent developments in analytical and numerical modeling of recrystallization, grain growth and related phenomena" minisymposium, SIAM MS16, Philadelphia, May 2016
- (8) co-organizer, "Mathematical challenges in phase diagram calculation" minisymposium, SIAM MS16, Philadelphia, May 2016
- (7) co-organizer, "Advances in multigrid methods and their applications", minisymposium, SIAM CSE15, Salt Lake City, UT March 2015
- (6) co-organizer, "Recent Advances in Studies and Applications of Centroidal Voronoi Tessellations" minisymposium for ICIAM, Vancouver, Canada, July 2011
- (5) member of the Organizing committee, organizer of a minisymposium on Undergraduate Research, co-organizer of a minisymposium on interface kinetics, SIAM Conference on Mathematical Aspects of Materials Science (MS10), Philadelphia, PA, May 23 26, 2010

- (4) co-organizer, "Kinetic Approaches in Materials Science" minisymposium for 2009 SIAM Conference on Analysis of PDEs, Miami, FL, Dec. 7-10, 2009
- (3) co-organizer, "Recent Advances in Algorithms and Applications of Centroidal Voronoi Tessellation and Optimal Quantization" minisymposium for 2008 SIAM Annual Meeting, San Diego, CA,July 7-11, 2008
- (2) co-organizer, "Grain Boundary Evolution" minisymposium for SIAM Conference on Mathematical Aspects of Materials Science(MS08), Philadelphia on May 11–14, 2008
- (1) co-organizer, "Centroidal Voronoi Tessellations: Theory, Algorithms and Applications" minisymposium for SIAM Workshop on Combinatorial Scientific Computing (CSC07), Costa Mesa, CA, Feb 17–19, 2007

#### Editorial board service

Associate Editor, SIAM Undergraduate Research Online (SIURO), 2013 - present

#### • Regular referee for:

Model. and Simulation in Mater. Sci. and Engr., CALPHAD, Intl. J. Num. Methods in Fluids, Mathematical Reviews, Pattern Recognition, Trans. Visualization and Comp. Graphics, SIAM Multiscale Modeling and Simulation, J. of Computational Physics, J. Engr. Mathematics, SIGGRAPH Proceedings, Computer Aided Design, Applied Mathematical Modeling, SIAM J. Applied Math, SIAM J. Num. An., SIAM J. Cont. Optim.

## o Panel participation: COS Research Forum panel, GMU, Feb 2017

Research Panel for Pakistan Fellows, GMU, April 2016

Panel on education, invited member, IMA Materials Genome workshop, Sept 2012

SIAM Forward Looking Session, invited panel member, SIAM Mathematics of Materials Meeting, May 2010

 $\operatorname{NSF}$ panels: May 2009, March 2010, March 2011, March 2012, October 2014, June 2015, June 2016, April 2017

NSF Committee of Visitors: February 2013

### Undergraduate research activities:

PI, GMU QED-EXTREEMS program, 2014 - 2018

Associate Editor, SIAM Undergraduate Research Online (SIURO), 2013 - present

Co-PI, GMU REU: Research, Education and Training in Computational Mathematics and Nonlinear Dynamics of Biological, Bio-inspired and Engineering Systems, 2012-2013

Co-PI, GMU Multidisciplinary REU Program in Computational Mathematics and Nonlinear Dynamics of Biological, Bio-inspired and Engineering Systems, 2009-2010

Computational Science Training for Undergraduates in the Mathematical Sciences (CSUMS) student mentor, GMU, 2008-2013

Summer Undergraduate Applied Math Institute student mentor, CMU, May 30 – July 17, 2007

## Scientific community service

#### Long-term engagements:

Secretary (elected), SIAM Activity group on Mathematics of Materials, Jan 2014 – Dec 2016 Member, SIAM Education Committee working group on Professional Development, 2012-2015

Lecturer, Undergraduate Faculty Program, Park City Mathematical Institute/Institute for Advanced Study, Park City, UT

June - July 2014

#### One-time commitments:

co-Organizer, SIAM Professional Development Evening, SIAM Annual Meeting July 2013, July 2014, March 2015 (CSE15)

Panelist, "Building the Materials Data Infrastructure" workshop, Arlington VA, Jan 21, 2015 "Helping undergraduates see mathematics in the material world", invited paper for SIAM News, Volume 43, Number 6 2010

#### o Outreach activities

### Long-term engagements:

Chair, AWM SIAM Workshop sub-committee, 2015–2017

Member, AWM Meetings Committee, 2015 - 2018

co-PI, Sonia Kovalevsky GMU Middle and High School Mathematics Day, May 20, 2011 and May  $4,\,2012$ 

Member, AWM SIAM Workshop Committee, 2010 – 2013

Mason representative, Centreville High School Women in Mathematics club (panel participation: March 2013, April 2014, March 2016; Mason field trip co-organizer: March 2015)

Faculty advisor, GMU AWM Chapter, 2011 - present

Faculty member, Women in Scientific DOMains, GMU 2007 – 2012

Member, Women of Mathematics group, PSU 2000-2005

#### One-time commitments:

Speaker, AWM Career workshop, SIAM CSE15, Salt Lake City, UT March 2015

Panelist, GWU AWM Networking event, April 2014

Faculty panel participant, GMU Graduate student career workshop, Nov 2011

Speaker, GWU Summer Program for Women in Mathematics, June 2011

Panelist, Women in Science group, CMU 2006

Sponsored participant, "Career Options for Women in Mathematics" workshop, IMA, Minneapolis, Feb 4-5, 2005

### • Teaching innovation:

Participant, GMU SIMPLE Teaching Development Project, 2015 – present

Developed 1 new undergraduate and 1 new graduate topics courses

Primary author of an undergraduate textbook on Mathematical Methods in Materials Science, under contract with SIAM Book Acquisitions

## $\circ$ Professional memberships:

Affiliate faculty, Center for Computational Materials Science (CMaSC)

Associate, Computational Materials Science Network (CMSN)

Societies: SIAM, AMS, MAA, AWM. Member of SIAG on Materials Science, Uncertainty Quantification, Mathematics of Planet Earth.

## Presentations for Broader audience

- · "Modeling initiatives for upper-level math majors: looking back, forward and across time scales", invited talk at the minisymposium entitled "Implementing transformational undergraduate modeling experiences", SIAM Annual Meeting, Boston, July 11-14, 2016
- · "New age of mathematics: more than meets the eye", Honors college seminar talks, 2015, 2017
- · "The road less traveled: an interdisciplinary mathematician's journey", AWM workshop talk, SIAM CSE15, Salt Lake City, UT, March 2015
- · "Modeling materials and beyond", SIAM Faculty Symposium, GMU, October 2014

- $\cdot$  "Mathematics under the Microscope", GWU Summer Program for Women in Mathematics, June 2011
- $\cdot$  "Mathematics under the Microscope", GMU Undergraduate Research in Computational Mathematics program, June 2011
- · "A mathematician's journey: what matters and why", PSU SIAM chapter presentation, University Park, PA, May 2011
- · Keynote speaker, annual PSU Graduate Open House/Alumni Conference, March 29, 2008
- · "Crossing boundaries and shaping the world: interdisciplinary math approach", Women In Scientific DOMains meeting, GMU, Dec. 4, 2007

# INVITED RESEARCH PRESENTATIONS

- · "Kinetic Modeling of Materials Coarsening", Applied Math seminar, UCSD, December 1, 2016
- $\cdot$  "Kinetic Modeling of Materials Coarsening", invited keynote talk, IPAM workshop, UCLA, October 25, 2016
- "Kinetic Modeling of Materials Coarsening: from individual grains to network statistics", keynote talk, 8th International Conference on Multiscale Materials Modeling taking place in Dijon, France, on October 9-14, 2016
- · "Using SVD and CVT to Study Precipitation Patterns in U.S.", minisymposium talk, SIAM MPE16, Philadelphia, Oct 1, 2016
- · "PDE-based Modeling of Coarsening in Polycrystals", plenary talk, 9th European Conference on Elliptic and Parabolic Problems, Gaeta, Italy, May 23-27, 2016
- · "Kinetic Modeling of Crystalline Misorientation Distribution Functions During Coarsening", workshop presentation, Fields Institute Toronto, ON April 28, 2016
- "Kinetic Modeling of Coarsening in Polycrystals", Applied Math seminar, WVU, March 4, 2016
- · "Simulating and predicting statistical features of crystal growth in polycrystalline materials", US Naval Academy, Annapolis, MD, Oct. 13, 2015
- · "The role of statistics in mesoscale mathematical modeling of coarsening in polycrystals", Statistics seminar, Sept. 11, 2015
- · "PDE-based modeling of coarsening in polycrystalline materials", minisymposium talk, AWM Research Symposium, U. of Maryland, March 2015
- $\cdot$  "Optimization challenges in phase diagram calculation", minisymposium talk, AMS Sectional Meeting, Georgetown University, March 2015
- $\cdot$  "Advances in multiscale mathematical modeling of materials: from phase diagrams to interface dynamics", minisymposium talk, AVS-61 Symposium, Baltimore MD, November 2014
- · "Computational modeling of polycrystals: accuracy and sensitivity analysis", minisymposium talk, JMM, Baltimore MD, January 2014
- · "Centroidal Voronoi Tessellations: from Lloyd method to multigrid and beyond", Numerical Analysis seminar, University of Maryland, College Park, September 2013
- $\cdot$  "Modeling rare events in microstructure evolution", Mesoscale and Continuum Scale Modeling of Materials Defects workshop, IPAM, UCLA November 2012
- · "Mathematical modeling of polycrystals", IMA Special Workshop, Mathematics and the Materials Genome Initiative, Minneapolis, September 2012
- · "Mathematical modeling of interfacial dynamics in polycrystals", Materials Defects Tutorial, IPAM, UCLA September 2012

- $\cdot$  "Mesoscopic modeling of grain growth", minisymposium talk, SES meeting, Atlanta GA October 2012
- · "Computational modeling of coarsening in polycrystalline materials, poster presentation, OCI CAREER Workshop, Arlington, VA June 2012
- · "Coarsening in materials: new takes on an old problem", invited talk, PSU, State College, PA April 2012
- · "Modeling rare events in microstructure evolution", invited lecture, PIRE lecture series, Carnegie Mellon University, Pittsburgh, PA March 2012
- · "Advances in multiscale modeling of coarsening in materials", invited talk, PDE seminar, University of Maryland, College Park, March 2012
- · "Constrained optimization approach to multicomponent phase diagram calculation", invited seminar, Beijing International Center for Mathematical Research (BICMR) at Peking University thematic program on "Mathematical Theory and Simulation of Phase Transitions", November 2011
- · "Advances in Multiscale Kinetic Modeling of Grain Growth in Polycrystals", minisymposium talk, AMS Sectional Meeting, Salt Lake City, Utah, October 2011
- · "Advances in Multiscale Kinetic Modeling of Grain Growth in Polycrystals", minisymposium talk, SES Annual Meeting, Northwestern University, Chicago, IL October 2011
- · "Advances in Kinetic Modeling of Grain Growth in Polycrystalline Materials", minisymposium talk, ICIAM, Vancouver, Canada, July 2011
- "Advances in Multiscale Kinetic Modeling of Grain Growth in Polycrystals", Workshop on Macroscopic Modeling of Materials with Fine Structure, Carnegie Mellon University, Pittsburgh PA May 2011
- · "Towards a Unified Statistical Theory of Texture Evolution in Polycrystals", minisymposium talk, SIAM MS10, Philadelphia, PA, May 23-26, 2010
- · "Fast Multilevel CVT-based Adaptive Data Visualization Algorithm", invited talk, CS department, GMU, April 13, 2010
- · "Kinetic Approaches in Mesoscale Modeling of Polycrystals", minisymposium talk, SIAM PD09, Miami, FL, Dec 8, 2009
- · "Mesoscale theory of texture evolution in polycrystals", invited talk, Applied Math colloquium, UMBC, Dec. 4, 2009
- · "Mesoscale modeling of materials microstructure", invited talk, Applied Math seminar, University of Delaware, Oct. 27, 2009
- · "Kinetic Theories in Multiscale Modeling of Polycrystals", invited talk, Multiscale Modeling and Simulation of Materials minisymposium, SIAM-SEAS Annual Meeting, U. South Carolina, April 4, 2009
- · "Kinetic Theories in Multiscale Modeling of Polycrystals", invited talk, FRG workshop on Kinetic Description of Multiscale Phenomena: Modeling, Theory and Computation, U. of Maryland, College Park, March 4, 2009
- · "Nonlinear dynamical phenomena in mesoscale modeling of polycrystals", special session presentation, AMS Annual meeting, Washington, DC, Jan 8, 2009
- · "Voronoi diagrams, quantization and clustering: theory and applications", invited colloquium talk, George Mason University, Fairfax, VA, Oct 17, 2008
- · "Understanding stochastic events in microstructure evolution", invited colloquium talk, Georgetown University, Washington, DC, Oct 3, 2008
- · "Understanding stochastic events in microstructure evolution", invited talk, PDE seminar, U. Maryland, College Park, Oct 2, 2008

- · "Understanding stochastic events in microstructure evolution", Research Colloquium in Computational Materials Science, GMU, April 14, 2008
- · "Mesoscale modeling of polycrystals: understanding stochastic events in microstructure evolution", Applied Mathematics seminar, GWU, April 10, 2008
- · "On a statistical theory of critical events in miscrostructure evolution", Math Department Colloquium, Florida State University, Nov. 9, 2007
- · "Microstructure Evolution: Recent Progress and Open Questions", Applied Math seminar series, GMU, Sept. 21, 2007
- · "On a statistical theory of critical events in miscrostructure evolution", Computational & Data Sciences Colloquium, GMU, Sept. 20, 2007
- · "Centroidal Voronoi tessellations: concepts and applications", Undergraduate Colloquium series, CMU, Pittsburgh, PA, April 12, 2007
- · "Texture evolution: mathematical aspects", MIMP Seminar, MRSEC, CMU, Pittsburgh, PA, March 27, 2007
- · "Centroidal Voronoi tessellations: theory and applications", invited talk, CSUCI, Camarillo, CA, Feb 16, 2007
- · "Mathematical modeling and simulation of texture evolution", invited talk, US Naval Academy, Anapolis, MD, Feb 9, 2007
- · "Mathematical modeling and simulation of texture evolution", invited talk, Clarkson Univ., Potsdam, NY, Feb 5, 2007
- · "Mathematical modeling and simulation of texture evolution", invited talk, American Univ., Washington, DC, Feb 2, 2007
- · "Mathematical modeling and simulation of texture evolution", invited talk, Purdue Univ., West Lafayette, IN, Jan 31, 2007
- · "Mathematical modeling and simulation of texture evolution", invited talk, U. Tennessee, Knoxville, TN, Jan 29, 2007
- · "Mathematical modeling and simulation of texture evolution", invited talk, George Mason Univ., Fairfax, VA, Jan 26, 2007
- · "Mathematical modeling and simulation of texture evolution", invited talk, Illinois Inst. Tech., Chicago, IL, Jan 22, 2007
- · "Mathematical modeling and simulation of texture evolution", invited talk, U. Minnesota, Minneapolis, MN, Jan 19, 2007
- · "Mathematical modeling and simulation of texture evolution", contributed talk, Joint AMS Meetings, New Orleans, LA, Jan 4-8, 2007
- · "Mathematical modeling and simulation of texture evolution", invited talk, U. Akron, Akron, OH, Dec 13, 2006
- · "Mathematical modeling and simulation of texture evolution", invited talk, U. Pittsburgh, Pittsburgh, PA, Dec 5, 2006
- · "Mathematical Modeling and Simulation of Texture Evolution", invited presentation, A Conference on Applied Analysis on the Occasion of the 65th Birthday of David Kinderlehrer, CNA, CMU, Pittsburgh, PA, Oct 19 21, 2006
- "Mathematical modeling and simulation of the grain boundary character distribution", invited poster presentation, Gordon Research Conference on Physical Metallurgy, Plymouth, NH, July 23-28, 2006
- · "Uniform convergence of a nonlinear energy-based multilevel quantization scheme via centroidal Voronoi tesselations", minisymposium talk, Joint MAA-SIAM Meeting, Auburn, AL, March 31-April 2, 2006

- · "A nonlinear energy-based multilevel quantization scheme", invited talk, Frontiers in Nonlinear Analysis, CNA, CMU, Pittsburgh, Sept 8-10 ,2005
- · "Uniform convergence of a multilevel energy-based quantization scheme", invited talk, Minisymposium on centroidal Voronoi tessellations, New Orleans, July 11-15 ,2005
- · "A New Algorithm for the Automation of Phase Diagram Calculation", invited talk, MCSD Seminar Series, NIST, Gaithersburg, MD, March 22, 2005

# CONTRIBUTED PRESENTATIONS

- · "Novel multilevel CVT-based data binning algorithms", minisymposium talk, ICIAM, Vancouver, Canada, July 2011
- $\cdot$  "Mesoscale Modeling of Polycrystals", minisymposium talk, SIAM Annual Meeting, Pittsburgh, PA July 2010
- · "Texture evolution: new perspectives", poster presentation, 4th Intl. Multiscale Materials Modeling conference, Florida State University, Tallahassee, FL, Oct 27-31, 2008
- · "Voronoi-Based Binning Techniques: Acceleration Methods and Applications", minisymposium talk, SIAM Annual Meeting, San Diego, July 2008
- · "Mesoscale modeling of polycrystals: interplay of theory and simulation", minisymposium talk, SIAM MS08, Minisymposium on Grain Boundary Evolution, May 11, 2008
- · "Mathematical modeling and simulation of texture evolution", poster presentation, Barrett Lectures, U. Tennessee, Knoxville, TN, April 29-30, 2007
- · "Multidimensional Energy-based Multilevel Quantization Scheme and its Applications", minisymposium talk, SIAM CSE07, Costa Mesa, CA, February 19-23, 2007
- · "Toward a Statistical Theory of Texture Evolution", contributed talk, SIAM CSE07, Costa Mesa, CA, February 19-23, 2007
- · "A Nonlinear Energy-based Multilevel Quantization Scheme", contributed talk, XII Copper Mountain Conference on Multigrid Methods, Colorado, April 3-8, 2005
- · "Uniform convergence of a multigrid energy-based quantization scheme", poster presentation, IMA Workshop: Career Options for Women in Mathematics, Univ. of Minnesota, Minneapolis, MN, February 4-5, 2005
- · "Uniform Convergence of a Multigrid Energy-based Quantization Scheme", poster presentation, 16th International Conference on DDM, Courant Institute, January 12-15, 2005
- · "A New Algorithm for the Automation of Phase Diagram Calculation", poster presentation, NSF Division of Materials Research ITR Computational Workshop, UIUC, Urbana, IL, June 17-19, 2004

## STUDENTS/POSTDOCS SUPERVISED AT GMU:

- o Postdocs:
  - 4. Katerine Salemeruiz (2016-2017)
  - 3. Ivan Yegorov (2015-2016)
  - 2. Claudio Torres (2012-2013)
  - 1. Boris Gafurov (2011-2012)
- o Graduate students:
  - 6. Jeff Snider (co-advisor, PhD thesis, current)
  - 5. Diego Torrejon (advisor, PhD thesis, defended Dec 2017)
  - 4. Zichao Di (co-advisor, PhD thesis, defended Aug 2013)
  - 3. Hasitha de Silva (advisor, research project 2010-2012)
  - 2. Jonathan Bode (research project co-advisor, 2010-2011)
  - 1. Thomas Stephens (advisor, research project, 2010-2011)

• Undergraduate students:

Robert Argus (advisor, EXTREEMS research project, 2015-2016)

Daniel Sun (co-advisor, summer research project, Summer 2012)

Matthew Farkas (advisor, REU research project, Summer 2012)

Matthew Villemarette (co-advisor, REU research project, Summer 2012)

Alex Price (co-advisor, REU research project, Summer 2012)

Diego Torrejon (co-advisor, CSUMS research project 2011-2012)

Michael Sharov(co-advisor, CSUMS research project 2011-2012)

Russell Mahoney (advisor, CSUMS research project 2010-2011)

Robert Hill (co-advisor, CSUMS research project 2010-2011)

Tom Stephens (co-advisor, CSUMS research project 2008-2009)

Mike Atkins (co-advisor, CSUMS research project, 2008-2009)

Joshua Snyder (advisor, CSUMS research project, 2009-2010)

Sandra Varela (co-advisor, REU research project, Summer 2010)

Ross Kistler (advisor, REU research project, Summer 2010)

Charles Cook, Alma College (advisor, REU research project, Summer 2009)

Angela Dapolite, Clarkson University (advisor, REU research project, Summer 2009; advisor, Honors thesis, 2010)

Member of dissertation committees: Manal Othman (Ph.D. thesis committee, Bioinformatics GMU, current), Jennifer Roames (M.S. thesis committee, Physics GMU, current), Yukiko Yarnall (M.S. thesis committee, Math, GMU, defended Spring 2016), Jessica O'Connor (Ph.D. thesis committee, Physics, GMU, defended Spring 2016), Michael Crone (Ph.D. thesis committee, Math GMU, defended Fall 2014), Veronica Bloom (Ph.D. thesis committee, CSI GMU, defended Spring 2014), Alexander Koufos (Ph.D. committee, CSI GMU, defended Spring 2015), Lei Wang (Ph.D. committee, Systems Biology GMU, current), Hypnos Hu (Ph.D. committee, CSI GMU, defended Spring 2015), Jieun Lee (Ph.D. thesis committee, George Washington University, Mathematics, defended May 2010), TJ Flynn (M.S. thesis committee, GMU Mathematics, defended Spring 2009), Mary Ann Graham (M.S. thesis committee, GMU Mathematics, defended Fall 2007), Ganga P. Purja Pun (Ph.D. thesis committee, GMU Physics, defended Fall 2011)

STUDENTS SUPERVISED AT CMU Tarek Elgindi (University of Wisconsin, REU student, CMU, Summer 2007), Morgan Shaffer (Mount Holoyoke College, REU student, CMU, Summer 2007), Michelle Baker (Shippensburg University, REU student, CMU, Summer 2007), Jian Wang (UT Knoxville, REU student, CMU, Summer 2007), Keith Rogers (Alabama State, REU student, CMU, Summer 2007), Alexander Chun (Northwestern University, REU student, CMU, Summer 2007)

## TEACHING EXPERIENCE

#### At George Mason University:

Math 689 (NEW grad topics course) Multiscale Methods - Spring 2016

Math 493/689 (NEW senior/grad topics course) Math. Methods in Materials Science - Spring 2015

Math 290 (sophomore) Intro to Advanced Math - Spring 2013

Math 114 (freshman) Calculus II - Spring 2013, Fall 2015

Math 678 (grad core) Partial Differential Equations - Fall 2011

Math 113 (freshman) Calculus I - Spring 2011, Fall 2011, Fall 2014

Math 214 (sophomore) Elementary Differential Equations - Fall 2008, Fall 2010, Spring 2011, Spring 2014, Spring 2016, Spring 2017

Math 413 (senior) Introduction to Applied Mathematics I - Fall 2010, Fall 2014, Fall 2017

Math 414 (senior) Introduction to Applied Mathematics II - Spring 2015, Spring 2018

Math 685/CSI 700 (grad) Numerical Methods - Spring 2008, Spring 2010

Math 677 (grad core) Ordinary Differential Equations - Fall 2009 Math 446/OR 481 (senior) Introduction to Numerical Analysis - Fall 2007

# At Carnegie Mellon University:

Math 21-369 (junior) Numerical Mathematics and Computing - Fall 2005, Fall 2006

## At Penn State University:

Math250 (sophomore) Ordinary Differential Equations - Spring 2004

Math251 (sophomore) Ordinary and Partial Differential Equations - Fall 2002, Spring 2002

Math231 (sophomore) Calculus of Several Variables - Fall 2001

Math220 (sophomore) Matrices - Spring 2001

Math22 (freshman) College Algebra II and Analytic Geometry - Fall 2000, Spring 2000

Math21 (freshman) College Algebra I - Summer 2000, Summer 2001