Ellad B. Tadmor

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Education

Technion – Israel Institute of Technology	Mechanical Engineering	B.Sc.	1987
Technion – Israel Institute of Technology	Mechanical Engineering	M.Sc.	1991
Brown University	Solid Mechanics	Ph.D.	1996

Professional Experience

2025–	Graduate Faculty, Chemical Engineering & Materials Science, University of Minnesota
2006–	Professor, Aerospace Engineering and Mechanics, University of Minnesota
2005–2006	Visiting Associate Professor, Aerospace Engineering and Mechanics, University of Minnesota
2004–2008	Associate Professor, Department of Mechanical Engineering, Technion – Israel Institute of Technology
1999–2004	Senior Lecturer, Department of Mechanical Engineering, Technion – Israel Institute of Technology
1998–1999	Lecturer, Department of Mechanical Engineering, Technion – Israel Institute of Technology
1996–1998	Postdoctoral Research Associate, Division of Engineering and Applied Sciences and Department of Physics, Harvard University
1996	Adjunct Professor and Research Associate, Division of Engineering, Brown University
1991–1996	Research Assistant, Division of Engineering, Brown University
1989–1991	Research Engineer, Structural Analysis Group, Weapon Systems Division, RAFAEL – Israel Armament Development Authority (Haifa, Israel)

Teaching Experience (UG=Undergraduate, G=Graduate, S=Spring, F=Fall)

EN130	Structural Analysis	G	Brown	S1996
(Unofficial)	Fracture Mechanics	G	Harvard	F1997, S1998
034028	Solid Mechanics 1	UG	Technion	S1999, F2000, S2000, F2001, S2001, F2003, F2004, S2005
035041	Mechanics of Microsystems	UG	Technion	S2002, S2003, S2004, S2005
036004	Fracture Mechanics	G	Technion	F1999, F2000, F2001, F2002, F2003, F2004
036060	Multiscale Modeling of Materials	G	Technion	F2005

AEM8595	Atomistic and Multiscale Modeling of Materials	G	UMN	F2005, S2006
AEM2011	Statics	UG	UMN	S2008, S2011, F2012
AEM3031	Deformable Body Mechanics	UG	UMN	S2012, S2016, S2017
AEM4502	Computational Structural Analysis	UG	UMN	F2008, F2010, F2012, F2015, F2019, F2020, F2022, F2023
AEM5501	Continuum Mechanics	G	UMN	F2006, F2007, F2008, F2009, F2013, F2014, F2016, F2018, F2024
AEM8531	Fracture Mechanics	G	UMN	S2008, S2010, S2012, S2014, S2016, S2018, S2020, S2022
AEM8551	Multiscale Methods for Bridging Length and Time Scales	G	UMN	S2008, S2011, S2013, S2015, S2017, S2019, S2021, S2023
AEM8553	Data-Drive Molecular Simulation	G	UMN	S2025
HSEM3511H	Science Court: Strengthening Democracy through Rational Discourse	UG	UMN	F2018, F2019, S2021, S2022

Boards, Committees and Leadership Roles

2024–	Chair, Education and Infrastructure Committee, NSF NRT Program on Data-Driven Discovery and Engineering from Atoms to Processes (3DEAP), University of Minnesota
2024–	DSI Ambassador to AEM, Data Science Initiative, College of Science and Engineering, University of Minnesota.
2022–	Chair, Committee for Establishing Minimal Metadata Standards for Computational Materials Science (MatCore), National Science Foundation.
2022–	Principal Investigator, Data Driven Discovery and Design Program (4D), IPRIME, College of Science and Engineering, University of Minnesota.
2022–	Executive Committee Member, Data Science Initiative, College of Science and Engineering, University of Minnesota.
2018–	International Expert Member of the EU Scientific Network on the Assessment of Atomistic Simulations.
2017–	Organizer, AEM Solid Mechanics Research Seminar.
2015–	Leading the NSF "Rise of Data" program aimed at developing a strategy for the increasing prominence of data in materials research.
2020–2021	Member, Review Committee for AEM Head Reappointment, College of Science and Engineering, University of Minnesota
2014–2017	Promotion and Tenure Advisory Committee Member, College of Science and Engineering, University of Minnesota
2013–	Academic Excellence Committee Member, Nova Classical Academy (K-12 Charter School), St. Paul, MN
2013	Guest Editor, *Proceedings of the National Academy of Sciences*
2012–	Advisory Board Member, Cyberinfrastructure for Atomistic Materials Science
2009–	Director, Knowledgebase of Interatomic Models (KIM) Project
2009–	Associate Editor, *Journal of Elasticity*
2004–2006	Associate Editor, *Communications in Mathematical Sciences (CMS)*

Academic and Professional Honors

- Russell J. Penrose Professorship (2023–), Aerospace Engineering and Mechanics, University of Minnesota.
- Keynote Speaker (2023), Computational Technology Symposium, 3M.
- Nominated for an Einstein Foundation Award for Promoting Quality in Research for the OpenKIM project (2022).
- Invited Speaker, Computational Materials Science and Engineering, Gordon Research Conference (2022).
- Keynote Speaker, CSE Public Lecture (2020), University of Minnesota.
- Semi-Plenary Speaker (2019), 15th U.S. National Congress on Computational Mechanics.
- Plenary Speaker (2017), Res Metallica Symposium.
- Plenary Speaker (2014), Second Annual Mach Conference.
- Plenary Speaker (2012), The 32nd Israeli Conference on Mechanical Engineering.
- Plenary Speaker (2012), 52nd Sanibel Symposium.
- Visiting Erasmus Mundus Scholar (2007), European Commission Erasmus Mundus Masters Program ATOSIM, Ecole Normale Supérieure de Lyon, France
- ME Student Council Award for Best Lecturer (2003), Student Council, Faculty of Mechanical Engineering, Technion.
- Salomon Simon Manu Award for Excellence in Teaching (2001), Technion – Israel Institute of Technology.
- Award for Excellence in Teaching (Spring 1999, Spring 2001, Fall 2003), Technion – Israel Institute of Technology.
- MRS Graduate Student Award for Outstanding Performance in the Conduct of Research (1995), Materials Research Society.
- Professional Excellence Award (1990), RAFAEL – Israel Armament Development Authority.

Students

Postdoctoral Fellows and Research Scientists

2001–2003	Atul Kumar Agrawal, *The Mesh-Free Quasi-Continuum Method: Development of a novel, fast and accurate computational tool for 3D atomic-scale calculations.*
2003–2006	Leonid Kucherov, *Multiple-Scale Modeling of Materials: Theoretical and Computational Approaches.*
2006–2008	Marcel Arndt, *Multiscale Design of Advanced Materials based on Hybrid Ab Initio and Quasicontinuum Methods.*
2006–2009	Slava Sorkin, *Multiscale Design of Advanced Materials based on Hybrid Ab Initio and Quasicontinuum Methods.*

2008-2010	Tsvetanka Sendova, *Non-Uniqueness in Energy Minimization of Atomistic and Multiscale Problems: A Branch-Following and Bifurcation Investigation.*
2010–2012	Valeriu Smiricinschi, *Knowledgebase of Interatomic Models.*
2010–2012	Yeranuhi Hakobyan, *Objective Quasicontinuum.*
2010–2013	Woo Kyun Kim, *Hyper-QC: Accelerating time in a spatial multiscale method.*
2014–2015	Ilia Nikiforov, *Multiscale modeling of 2D layered heterostructures.*
2015–2016	Alexandros Anastassiou, *Atomistic simulation of polymer-polymer interfaces (Collaboration with 3M).*
2015–2018	Kuan Zhang, *Multiscale modeling of 2D layered heterostructures.*
2016–2018	Subrahmanyam Pattamatta, *Accelerated Quasicontinuum under Nonequilibrium Conditions.*
2019–2021	Yaser Afshar, *Knowledgebase of Interatomic Models and Cyberloop System R&D.*
2016–2022	Daniel Karls, *Knowledgebase of Interatomic Models R&D.*
2022–2024	Kyusic Park, *Open Knoledgebase of Reduced Order Models (OpenKROM) for Structural Dynamics.*
2021–	Amit Gupta, *ColabFit Machine Learning Potentials Development.*
2022–	Ilia Nikiforov, *Knowledgebase of Interatomic Models and Cyberloop Protocol Development.*
2022–	Claire Waters, *Knowledgebase of Interatomic Models Core Infrastructure Development.*
2022–	Eric Fuemmeler, *ColabFit Core Infrastructure Development.*

Ph.D. Students

2007–2014	Nikhil C. Admal *A unified interpretation of stress in molecular systems.* (WPE 04/2007, POE 01/2012, FOE 08/2014) Awarded UMN Doctoral Dissertation Fellowship.
2007–2015	Amit Singh *Nonstationary Heat Conduction in Atomistic Systems.* (WPE 04/2008, POE 07/2013, FOE 06/2015)
	Daniel S. Karls
2009–2016	*Transferability of Empirical Potentials and the Knowledgebase of Interatomic Models (KIM).* (WPE 04/2010, POE 09/2012, FOE 06/2016) Awarded UMN Doctoral Dissertation Fellowship.
2011–2016	Subrahmanyam Pattamatta *Equilibrium Maps: Characterizing the complex and stochastic behavior of nanosystems subjected to proportional loading.* (WPE 05/2011, POE 09/2013, FOE 11/2016)
2014–2019	Mingjian Wen *Development of Interatomic Potentials with Uncertainty Quantification Ability: Applications to Two-dimensional Materials.* (WPE 04/2014, POE 11/2016, FOE 06/2019) Awarded UMN Doctoral Dissertation Fellowship.

2014–2020	Jiadi Fan *Atomistically-Informed Finite Element Simulations of Phase Transformations and Fracture in Materials.* (WPE 04/2015, POE 12/2016, FOE 01/2020)
2018–2023	Moon-Ki Choi *Atomistic and Continuum Simulations of 2D Materials with Environmental Effects.* (WPE 04/2019, POE 11/2021, FOE 08/2023) Awarded UMN Doctoral Dissertation Fellowship.
2008–2023	Stephen M. Whalen (full time HP/Cray employee) *Parallelization and Optimization of Concurrent Multiscale Methods.* (WPE 03/2013, POE 03/2013, FOE 08/2023, Scientific Computation Program)
2014–2021	Min Shi *Aspets of Atomic Level Stress Computations for Fracture.* (WPE 04/2015, POE 08/2019, on leave)
2019–	James Hickenbotham *An Atomistic View of Stress Based on a Classically-Emergent Quantum Mechanics.* (POE 12/2021)
2022–	Chloe Zeller *Multiscale Modeling of Fracture of Refractory High Entropy Alloys.* Awarded NASA Space Technology Graduate Research Opportunities (NSTGRO22) Fellowship. (WPE 04/2023, POE 03/2025)
2023–	Pámela Bóveda-Aguirre *Information theoretic approaches to dataset pruning in machine learning models for materials applications.*
2024–	Sai Bodi *Multiscale modeling of fracture in nitinol medical devices.* (WPE 04/2024)
2025–	Winston Sullivan (co-advised with Sapna Sarupria) *Accelerated Sampling of Molecular Dynamics Trajectories.*

Visiting Ph.D. Students and Interns

2016	Guy Kovel, Technion – Israel Institute of Technology *Bridging the gap between atomistic simulations and fracture mechanics.*
2019–2020	Ye Feng, Tongji University *Atomistically-informed phase field modeling of fracture.*
2021–2022	Joshua Vita, DIGI-MAT Program, University of Illinois, Urbana-Champaign *Tools and Standards for Archving and Processing First Principles Materials Data*
2022–2024	Ben Jasperson, DIGI-MAT Program, University of Illinois, Urbana-Champaign *Training Interatomic Models on Canonical Properties*

M.Sc. Students (Thesis)

1999-2001	Shimon Hai, 1999-2001, *summa cum laude* (completed) *A Computational and Theoretical Investigation of Deformation Twinning at Aluminum Crack Tips* (summa cum laude). Shimon was awarded First Prize by the *Aharon and Ovadia Barazani Memorial Fund for Excellence* for this thesis.

M.E. Students (No Thesis)

1999	Isaac Pickholtz, *Parallel Tempering Method for the Determination of Optimal Transition Paths.*
2000	Israel Yonah, *Surface-Tension Effects in Fracture Mechanics.*

Undergraduate Students

2009–2012	Daniel Gerbig (UROP, Blue Waters). *Hybrid Hessian/Verlet Nudged Elastic Band Algorithm.*
2012–2014	Adam Ludvik (UROP). *Visualization software development for OpenKIM project.*
2014–2016	John Hooper. *In-page visualizer development for OpenKIM project.*
2015–2016	Alexander Halaszyn. *CB-ANSYS finite element simulations of diamond anvil cell experiments.*
2020–2020	Ambrose Dukek. *Dynamics of twisted graphene bilayer reconstructions.*
2021–2021	Manix White. *Knowledge, Dissent, and Influence Within a Heterogeneous Jury.*
2021–2022	Chloe Zeller. *Multiscale QC Simulation of Fracture Toughness of Amorphous Carbon.*
2022–2023	Ebise Teshale. *Defect Dynamics in 2D Colloidal Crystals.*
2024	Lainey Oliphant. *Stress Calculation using Machine Learning Interatomic Potentials.*
2025	Sofia Gerasimchuk. *3D visualization of anisotropic fracture envelopes.*

Grants

Funded Research — Active

[11] NVIDIA Academic Grant
Novel Nonlinear Optical Crystals from Atomistic Stochastic Interpolants
E. B. Tadmor (PI), E. Femmeler (UMN)
04/1//2025–09/30/2025

[10] National Science Foundation (SIR) (CMMI-2428667)
NSF/FDA SiR: Improving the Safety Evaluation of Nitinol Medical Devices with AI-Based Multiscale Modeling
. B. Tadmor (PI), S. Ravindran (UMN)
09/01/2024–08/31/2026

[9] National Science Foundation (NRT-2345719)
NRT-HDR: Data-Driven Discovery and Engineering from Atoms to Processes (3DEAP)
P. Daoutidis (PI), C. Bartel, Q. Zhang, S. Sarupria, E. B. Tadmor (UMN)
09/01/2024–08/31/2029

[8] National Science Foundation (DMR-2404283)
Conference: Community Development of the Material Core Metadata (MatCore) Standard
Ellad B. Tadmor (PI), K. Persson (UC Berkeley), F. Guistino (UT Austin)
06/01/2024–05/31/2025

[7] National Science Foundation (CSSI) (OAC-2311632)
GOALI: Frameworks: At-Scale Heterogeneous Data based Adaptive Development Platform for

Machine-Learning Models for Material and Chemical Discovery
S. Martiniani (PI) (NYU), **Ellad B. Tadmor (UMN Lead)**, R. Hennig (UFL), E. Fuemmeler, (UMN), A. Gupta (UMN), G. Karypis (UMN), M. Liu (UFL), A. E. Roitberg (UFL), H. Rangwala (AWS), M. Transtrum (BYU)
10/01/2023–09/30/2028

[6] University of Minnesota, Data Science Initiative
Learning Using Privileged Information (LUPI) for Materials Discovery
Vladimir Cherkassky (PI), Tony Low, Ellad B. Tadmor, Eric Fuemmeler
09/01/2023–08/31/2024

[5] U.S. Department of Energy by Lawrence Livermore National Laboratory (LLNL) under Contract DE-AC52-07NA27344, Laboratory Directed Research and Development Program, Strategic Initiative (23-SI-006)
Infrastructure for the LDRD-SI Automated Framework for Predictive Atomistic Materials Simulations with Uncertainty Quantification
E. B. Tadmor (PI)
10/01/2022–09/30/2025

[4] National Aeronautics and Space Administration (NASA), 2022 NASA Space Technology Graduate Research Opportunities (NSTGRO22) (21-NSTGRO22-0159)
Quasicontinuum Fracture Modeling and Development of Refractory High Entropy Alloys
E. B. Tadmor (PI); NASA Space Technology Graduate Research fellowship for Chloe Zeller
09/01/2022–08/31/2026

[3] National Science Foundation (CESER) (OAC-2039575)
Data CI Pilot: CI-Based Collaborative Development of Data-Driven Interatomic Potentials for Predictive Molecular Simulations
E. B. Tadmor (PI), R. S. Elliot (UMN), S. Martiniani (UMN)
10/01/2020–09/30/2025

[2] National Science Foundation (CSSI) (OAC-1931304)
Collaborative Research: Framework: Cyberloop for Accelerated Bionanomaterials Design
E. B. Tadmor (PI), H. Heinz (U. Colorado), W. Im (Lehigh)
10/01/2019–09/30/2025

[1] National Science Foundation (DMR) (DMR-1834251)
Collaborative Research: Reliable Materials Simulation based on the Knowledgebase of Interatomic Models (KIM)
E. B. Tadmor (PI), R. S. Elliott (UMN), G. Karypis (UMN), M. K. Transtrum (BYU)
10/01/2018–03/31/2025

Publications

Theses

[T1] E. B. Tadmor. Plastic failure of pressurized multilayered cylinders. Master's thesis, Technion – Israel Insitute of Technology, Haifa, Israel, June 1991. Thesis advisors: Profs. David Durban and Miles Rubin.

[T2] E. B. Tadmor. *The Quasicontinuum Method. Modeling Microstructure on Multiple Length Scales: A Mixed Continuum and Atomistics Approach*. PhD thesis, Brown University, Providence, RI, USA, May 1996. Thesis advisors: Profs. Michael Ortiz and Rob Phillips.

Books

[B1] Ellad B. Tadmor and Ronald E. Miller. *Modeling Materials: Continuum, Atomistic and Multiscale Techniques*. Cambridge University Press, Cambridge, 2011 (786 pages).

[B2] Ellad B. Tadmor, Ronald E. Miller, and Ryan S. Elliott. *Continuum Mechanics and Thermodynamics: From Fundamental Principles to Governing Equations*. Cambridge University Press, Cambridge, 2012 (372 pages).

Invited Chapters in Books

[CB1] E. B. Tadmor. A peierls criterion for deformation twinning at a mode II crack. In S. Attinger and P. Koumoutsakos, editors, *Multiscale Modelling and Simulation*, volume 39 of *Lecture Notes in Computational Science and Engineering*. Springer-Verlag, New York, 2004.

[CB2] E. B. Tadmor and R. E. Miller. The theory and implementation of the quasicontinuum method. In S. Yip, editor, *Handbook of Materials Modeling, Part A - Methods*. Springer-Verlag, New York, 2005.

[CB3] N. C. Admal and E. B. Tadmor. A unified interpretation of stress in molecular systems. In R. Fosdick and E. Fried, editors, *Statistical Mechanics, Molecular Modeling, and the Notion of Stress - An Invited Collection*. Springer, 2010.

[CB4] W. K. Kim and E. B. Tadmor. Temporal acceleration in coupled continuum-atomistic methods. In W. Andreoni and S. Yip, editors, *Handbook of Materials Modeling, Volume 1 Methods: Theory and Modeling*. Springer, Cham, Second edition, 2018.

Original Papers in Refereed Journals (Most Recent First)

[P83] B. A. Jasperson, I. Nikiforov, A. Samanta, B. Runnels, H. T. Johnson, and E. B. Tadmor. Fundamental microscopic properties as predictors of grain boundary energy trends. *Acta Materialia*, 286:120722, 2025.

[P82] B. A. Jasperson, I. Nikiforov, A. Samanta, F. Zhou, E. B. Tadmor, V. Lordi, and V. V. Bulatov. Cross-scale covariance for material property prediction. *npj Computational Materials*, 11:1, 2025.

[P81] M. Choi, S. H. Sung, R. Hovden, and E. B. Tadmor. Elastic plate basis for the deformation and electron diffraction of twisted bilayer graphene on a substrate. *Physical Review B*, 110:024116, 2024. PRB Editors' Suggestion.

[P80] J. R. Gissinger, I. Nikiforov, Y. Afshar, B. Waters, M. Choi, D. S. Karls, A. Stukowski, W. Im, H. Heinz, A. Kohlmeyer, and E. B. Tadmor. Type label framework for bonded force fields in LAMMPS. *The Journal of Physical Chemistry B*, 128:3282–3297, 2024.

[P79] K. Kanhaiya, M. Nathanson, P. in 't Veld, C. Zhu, I. Nikiforov, E. B. Tadmor, Y. K. Choi, W. Im, R. Mishra, and H. Heinz. Accurate force fields for atomistic simulations of oxides, hydroxides, and organic hybrid materials up to the micrometer scale. *Journal of Chemical Theory and Computation*, 19:8293–8322, 2023.

[P78] J. A. Vita, E. G. Fuemmeler, A. Gupta, G. P. Wolfe, A. Q. Tao, R. S. Elliott, S. Martiniani, and E. B. Tadmor. ColabFit Exchange: open-access datasets for data-driven interatomic potentials. *Journal of Chemical Physics*, 159:154802, 2023.

[P77] B. Waters, D. S. Karls, I. Nikiforov, R. S. Elliott, E. B. Tadmor, and B. Runnels. Automated determination of grain boundary energy and potential-dependence using the OpenKIM framework. *Computational Materials Science*, 220:112057, 2023.

[P76] M. Choi, M. Pasetto, Z. Shen, E. B. Tadmor, and D. Kamensky. Atomistically-informed continuum modeling and isogeometric analysis of 2D materials over holey substrates. *Journal of the Mechanics and Physics of Solids*, 170:105100, 2023.

[P75] S. H. Sung, Y. M. Goh, H. Yoo, R. Engelke, H. Xie, K. Zhang, Z. Li, A. Ye, P. B. Deotare, E. B. Tadmor, A. J. Mannix, J. Park, L. Zhao, P. Kim, and R. Hovden. Torsional periodic lattice distortions and diffraction of twisted 2D materials. *Nature Communications*, 13:7826, 2022.

[P74] W. K. Kim, A. Kavalur, S. M. Whalen, and E. B. Tadmor. Free energy calculation and ghost force correction for hot-QC. *International Journal for Numerical Methods in Engineering*, 123:4916–4934, 2022.

[P73] Y. Kurniawan, C. Petrie, K. Williams Jr., M. K. Transtrum, E. B. Tadmor, R. S. Elliott, D. S. Karls, and M. Wen. Bayesian, frequentist, and information geometry approaches to parametric uncertainty quantification of classical empirical interatomic potentials. *Journal of Chemical Physics*, 156:214103, 2022.

[P72] Y. K. Choi, N. R. Kern, S. Kim, K. Kanhaiya, Y. Afshar, S. H. Jeon, S. Jo, B. R. Brooks, J. Lee, E. B. Tadmor, H. Heinz, and W. Im. CHARMM-GUI Nanomaterial Modeler for modeling and simulation of nanomaterial systems. *ACS Journal of Chemical Theory and Computation*, 18(1):479–493, 2022.

[P71] Y. Feng, J. Fan, and E. B. Tadmor. A rigorous universal model for the dynamic strength of materials across loading rates. *Journal of the Mechanics and Physics of Solids*, 159:104715, 2022.

[P70] M. Wen, Y. Afshar, R. S. Elliott, and E. B. Tadmor. KLIFF: A framework to develop analytic and machine learning interatomic potentials. *Computer Physics Communications*, 272:108218, 2022.

[P69] Y. Zhang, M.-K. Choi, G. Haugstad, E. B. Tadmor, and D. J. Flannigan. Holey substrate-directed strain patterning in bilayer MoS_2. *ACS Nano*, 15:20253–20260, 2021.

[P68] J. Fan, A. Anastassiou, C. W. Macosko, and E. B. Tadmor. Molecular dynamics based cohesive law for epoxy–graphene interfaces. *Tribology Letters*, 69:55, 2021.

[P67] M. Wen and E. B. Tadmor. Uncertainty quantification in molecular simulations with dropout neural network potentials. *npj Computational Materials*, 6:124, 2020.

[P66] D. S. Karls, M. Bierbaum, A. A. Alemi, R. S. Elliott, J. P. Sethna, and E. B. Tadmor. The OpenKIM Processing Pipeline: A cloud-based automatic materials property computation engine. *Journal of Chemical Physics*, 153:064104, 2020.

[P65] M. Shi, N. C. Admal, and E. B. Tadmor. Noise filtering in atomistic stress calculations for crystalline materials. *Journal of the Mechanics and Physics of Solids*, 144:104083, 2020.

[P64] J. Fan, A. Anastassiou, C. W. Macosko, and E. B. Tadmor. Molecular dynamics predictions of thermomechanical properties of an epoxy thermosetting polymer. *Polymer*, 196:122477, 2020.

[P63] Erik van der Giessen, Peter A. Schultz, Nicolas Bertin, Vasily V. Bulatov, Wei Cai, Gábor Csányi, Stephen M. Foiles, M. G. D. Geers, Carlos González, Markus Hütter, Woo Kyun Kim, Dennis M. Kochmann, Javier LLorca, Ann E. Mattsson, Jörg Rottler, Alexander Shluger, Ryan B. Sills, Ingo Steinbach, Alejandro Strachan, and Ellad B. Tadmor. Roadmap on multiscale materials modelling. *Modelling and Simulations in Materials Science and Engineering*, 28:043001, 2020.

[P62] M. Wen and E. B. Tadmor. Hybrid neural network potential for multilayer graphene. *Physical Review B*, 100(19):195419, 2019.

[P61] H. Yoo, R. Engelke, S. Carr, S. Fang, K. Zhang, P. Cazeaux, S. H. Sung, R. Hovden, A. Tsen, T. Taniguchi, K. Watanabe, G.-C. Yi, M. Kim, M. Luskin, E. B. Tadmor, E. Kaxiras, and P. Kim. Atomic and electronic reconstruction at the van der Waals interface in twisted bilayer graphene. *Nature Materials*, 18(5):448–453, 2019.

[P60] J. Fan and E. B. Tadmor. Rescaling cohesive element properties for mesh independent fracture simulations. *Engineering Fracture Mechanics*, 213:89–99, 2019.

[P59] M. Wen, S. Carr, S. Fang, E. Kaxiras, and E. B. Tadmor. Dihedral-angle-corrected registry-dependent interlayer potential for multilayer graphene structures. *Physical Review B*, 98(23):235404, 2018.

[P58] K. Zhang and E. B. Tadmor. Structural and electron diffraction scaling of twisted graphene bilayers. *Journal of the Mechanics and Physics of Solids*, 112:225–238, 2018.

[P57] M. Wen, S. N. Shirodkar, P. Plecháč, E. Kaxiras, R. S. Elliott, and E. B. Tadmor. A force-matching Stillinger-Weber potential for MoS_2: Parameterization and Fisher information theory based sensitivity analysis. *Journal of Applied Physics*, 122(24):244301, 2017.

[P56] W. W. Gerberich, E. B. Tadmor, J. Kysar, J. A. Zimmerman, A. M. Minor, I. Szlufarska, J. Amodeo, B. Devincre, E. Hintsala, and R. Ballarini. Review article: Case studies in future trends of computational and experimental nanomechanics. *Journal of Vacuum Science & Technology A*, 35:060801, 2017.

[P55] E. B. Tadmor and R. E. Miller. Benchmarking, validation and reproducibility of concurrent multiscale methods are still needed. *Modelling and Simulations in Materials Science and Engineering*, 25:071001, 2017.

[P54] W. K. Kim and E. B. Tadmor. Accelerated quasicontinuum: A practical perspective on hyper-QC with application to nanoindentation. *Philosophical Magazine*, 97(26):2284–2316, 2017.

[P53] P. Cazeaux, M. Luskin, and E. B. Tadmor. Analysis of rippling in incommensurate one-dimensional coupled chains. *Multiscale Modeling and Simulation*, 15(1):56–73, 2017.

[P52] M. Wen, J. Li, P. Brommer, R. S. Elliott, J. P. Sethna, and E. B. Tadmor. A KIM-compliant *Potfit* for fitting sloppy interatomic potentials: Application to the EDIP model for silicon. *Modelling and Simulations in Materials Science and Engineering*, 25:014001, 2017.

[P51] K. Zhang and E. B. Tadmor. Energy and moiré patterns in 2D bilayers in translation and rotation: A study using an efficient discrete–continuum interlayer potential. *Extreme Mechanics Letters*, 14:16–22, 2017.

[P50] A. Singh and E. B. Tadmor. Simulating the superheating of nanomaterials due to latent heat release in surface reconstruction. *International Journal of Heat and Mass Transfer*, 107:792–804, 2017.

[P49] M. M. Salary, S. Inampundi, K. Zhang, E. B. Tadmor, and H. Mosallaei. Mechanical actuation of graphene sheets via optically induced forces. *Physical Review B*, 94:235403, 2016.

[P48] N. C. Admal and E. B. Tadmor. The non-uniqueness of the atomistic stress tensor and its relationship to the generalized Beltrami representation. *Journal of the Mechanics and Physics of Solids*, 93:72–92, 2016.

[P47] R. E. Miller, E. B. Tadmor, J. S. Gibson, N. Bernstein, and F. Pavia. Molecular dynamics at constant Cauchy stress. *Journal of Chemical Physics*, 144(18):184107, 2016.

[P46] N. C. Admal and E. B. Tadmor. Material fields in atomistics as pull-backs of spatial distributions. *Journal of the Mechanics and Physics of Solids*, 89:59–76, 2016.

[P45] A. Singh and E. B. Tadmor. Thermal parameter identification for non-Fourier heat transfer from molecular dynamics. *Journal of Computational Physics*, 299:667–686, 2015.

[P44] M. Wen, S. M. Whalen, R. S. Elliott, and E. B. Tadmor. Interpolation effects in tabulated interatomic potentials. *Modelling and Simulations in Materials Science and Engineering*, 23:074008, 2015.

[P43] A. Singh and E. B. Tadmor. Removing artificial Kapitza effects from bulk thermal conductivity calculations in direct molecular dynamics. *Journal of Applied Physics*, 117(18):185101, 2015.

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[P20] N. Bernstein and E. B. Tadmor. Tight-binding calculations of stacking energies and twinnability in fcc metals. *Physical Review B*, 69(9):094116, 2004.

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[P6] R. Miller, M. Ortiz, R. Phillips, V. B. Shenoy, and E. B. Tadmor. Quasicontinuum models of fracture and plasticity. *Engineering Fracture Mechanics*, 61(3–4):427–444, 1998.

[P5] R. Miller, E. B. Tadmor, R. Phillips, and M. Ortiz. Quasicontinuum simulation of fracture at the atomic scale. *Modelling and Simulation in Materials Science and Engineering*, 6(5):607–638, 1998.

[P4] V. B. Shenoy, R. Miller, E. B. Tadmor, R. Phillips, and M. Ortiz. Quasicontinuum models of interfacial structure and deformation. *Physical Review Letters*, 80(4):742–745, 1998.

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Refereed Papers in Conference Proceedings

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[C11] J. Greenberg, P. Bóveda-Aguirre, J. Allison, P. Asinari, M. Chan, A. Chandrasekaran, E. Ertekin, E. Garoufallou, G. Galli, P. Giannozzi, F. Giustino, G. Goldbeck, H. Heinz, A. Jayaraman, V. Lordi, K. A. Persson, G.-M. Rignanese, A. Thompson, E. Toberer, S. McClellan, and Ellad B. Tadmor. Towards MatCore: A unified metadata standard for materials science. In Emmanouel Garoufallou, editor, *Metadata and Semantic Research*. Springer Nature Switzerland, 2024. Accepted.

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[C9] Jay Alameda, Claire Stirm, Gregory Bauer, Timothy Boerner, Brett Bode, Maytal Dahan, William Gropp, Marlon Pierce, Cynthia Yewdall Grigorescu, Michael Zentner, Meghna Babbar-Sebens, Michael Barton, Daniele Bianchi, Michael Bell, Michel Boufadel, Michael Cianfrocco, Sean Cleveland, Cosan Daskiran, Kjiersten Fagnan, Geoffrey Fox, Eleftherios Garyfallidis, Jerome Hajjar, Gerhard Klimeck, Mark Miller, Mark Perri, Victor Pinks II, Mohan Ramamurthy, Michel Regenwetter, Amy Roberts, Aldo Romero, Carol Song, Alejandro Strachan, Ellad Tadmor, and Greg Tucker. The Delta gateway: Exploring community use of GPU resources through a science gateway. In *Gateways 2022 Conference*, San Diego, CA, USA, 2022. Science Gateways Community Institute.

[C8] Z. Shui, D. S. Karls, M. Wen, I. A. Nikiforov, E. B. Tadmor, and G. Karypis. Injecting domain knowledge from empirical interatomic potentials to neural networks for predicting

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[C6] D. S. Karls, S. M. Clark, B. A. Waters, R. S. Elliott, and E. B. Tadmor. HPC extensions to the OpenKIM Processing Pipeline. In *2022 IEEE 18th International Conference on e-Science (e-Science)*, pages 278–283, 2022.

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[C2] R. Miller, M. Ortiz, V. Shenoy, and E. B. Tadmor. Quasi-atomistic models of fracture and plasticity. In B. L. Karihaloo, Y. W. Mai, M. I. Ripley, and R. O. Ritchie, editors, *Proceedings of the Ninth International Conference on Fracture*, page 2817. Sydney, Australia, April 1997.

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Reports

[R1] E. B. Tadmor. ANSYS finite element analysis of sandwich structures [in hebrew]. Technical Report 1989/46/684, RAFAEL, Haifa, Israel, November 1989.

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Media Appearances/Interviews (Most Recent First)

[M7] May 16, 2024, "Opinion: Could 'Science Courts' Help Build Public Trust?," Arik Shams, Leana King, and Joy Liu, *Undark*.
https://undark.org/2024/05/16/opinion-science-courts-public-trust-science/

[M6] February 17, 2022, "UMN class, Science Court, set to debate S/N grading this semester," Madison Roth, *Minnesota Daily*.
https://mndaily.com/271034/news/umn-class-science-court-set-to-debate-s-n-grading-this-semester

[M5] October 8, 2020, "Can Truth Save Democracy? We're Trying in Science Court," CSE Public Lecture, Curiosity Drives Progress Lecture Series: Impacting Communities, College of Science and Engineering, University of Minnesota.
https://cse.umn.edu/college/cse-public-lecture

[M4] Winter 2020, "Ellad Tadmor: Defending Science," Kermit Pattison, *Inventing Tomorrow*, College of Science and Engineering, University of Minnesota.
https://cse.umn.edu/college/inventing-tomorrow-archive

[M3] November 10, 2019, "University professor Ellad Tadmor is using science to fight polarization," Niamh Coomey, *Minnesota Daily*.
https://mndaily.com/222147/news/adtadmor/

[M2] March 16, 2019, "Aerospace engineer takes civility to court at University of Minnesota," Gail Rosenblum, Inspired Section, *Star Tribune*.
https://www.startribune.com/aerospace-engineer-takes-civility-to-court-at-university-of-minnesota/507205152

[M1] December 6, 2018, "Debating issues with science," MPR News with Keri Miller, *Minnesota Public Radio*.
https://www.mprnews.org/story/2018/12/06/miller-debating-issues-with-science

Conference and Workshop Participation

Plenary, Keynote and Invited Talks (Most Recent First)

[80] Invited panelist, GenAI Day, University of Minnesota, Minneapolis Data Science Initiative, College of Science and Engineering, University of Minnesota, Minneapolis, MN, May 20, 2025.

[79] "Open Materials Generation (OMG): Open-Source Generative AI for Crystalline Material Discovery" (invited), 2025 Spring Meeting of the Materials Research Society, Seattle, WA, April 7–11, 2025.

[78] "Efficient Rigorous Stress Calculations for Machine Learning Interatomic Potentials" (invited), CECAM Workshop on "Fulfilling the Multiscale Promise in Materials: Getting Information out of the Atomistic Scale" (invited), Lausanne, Switzerland, March 31–April 3, 2025.

[77] "The Stress of Machine Learning Force Fields" (invited), 64th Sanibel Symposium, St. Augustine Beach, FL, February 23–28, 2025.

[76] "Towards Machine Learning based Materials Discovery" (keynote), 8th i-CoMSE workshop, Minneapolis, MN, July 22–26, 2024.

[75] "ColabFit: Data for Training Machine Learning Interatomic Potentials" (invited), Open Databases Integration for Materials Design (OPTIMADE), CECAM Flagship Workshop, June 10–14, 2024 [Online].

[74] "The data revolution in molecular simulation: Machine learning, uncertainty quantification, and cyberinfrastructures" (invited), IPRIME Annual Meeting, Minneapolis, MN, May 30–June 1, 2023.

[73] "A Material Modeler's Guide to Living in the Age of Data" (keynote), Computational Technology Symposium, 3M Company, Saint Paul, MN, April 11, 2023.

[72] "Data Management and Sharing for Advanced Materials and Chemistry Discovery" (invited), Peter O. Stahl Advanced Design Forum, Inaugural Meeting, Department of Chemical Engineering and Materials Science (CEMS) and IPRIME, University of Minnesota, Minneapolis, MN, March 6, 2023.

[71] Invited panelist, Workshop on Advancing Materials and Molecules via Data Science, Data Science Initiative, College of Science and Engineering, University of Minnesota, Minneapolis, MN, February 17, 2023.

[70] "OpenKIM and ColabFit Infrastructure for Interatomic Model Selection and Training" (invited), Charting Large Materials Dataspaces, CECAM Flagship Workshop, October 10–12, 2022 [Online].

[69] "Accelerated Quasicontinuum Methods and Some Related Open Source Efforts" (invited), Computational Materials Science and Engineering, Gordon Research Conference, Newry, ME, August 1–5, 2022.

[68] "QC3D: High-Performance Quasicontinuum for Multilattice 3D Systems" (invited), 2021 Virtual Fall Meeting of the Materials Research Society, December 6–8, 2021 [Online].

[67] "Atomistically-Informed Multiscale Modeling" (invited), ChiMaD Phase Field Methods Workshop XII, Center for Hierarchical Materials Design (ChiMaD), Evanston, Il, November 2–4, 2021 [Online].

[66] "Standard Access to Datasets for Training Interatomic Potentials" (invited), Ontologies for Materials-Databases Interoperability (OMDI2021), Linköping University, Sweden, October 5–7, 2021 [Online].

[65] "ColabFit: Collaborative development and exchange of Data-Driven Interatomic Potentials" (invited), Open Databases Integration for Materials Design (OPTIMADE), CECAM Flagship Workshop, June 7–11, 2021 [Online].

[64] "When not to trust the predictions of machine learning interatomic potentials" (invited), Nanomaterials 2021, March 25–26, 2021 [Online].

[63] "OpenKIM as an Enabling Infrastructure for Atomistic Workflows" (invited), POTENTIALS Workflows for Atomistic Simulation, March 10–12, 2021 [Online].

[62] "Addressing Industrial Needs for Atomistic Simulations through OpenKIM" (invited), European Materials Modelling Council (EMMC) International Workshop 2021, March 2–4, 2021 [Online].

[61] "OpenKIM's role in Models and Workflows Driven by Data" (invited panelist), Materials Research Data Alliance (MaRDA) Annual Meeting, February 23–25, 2021 [Online].

[60] "Molecular Simulations you can Trust and Reproduce: The OpenKIM Framework" (invited), NIST Workshop on Atomistic Simulations for Industrial Needs, August 5–7, 2020 [Online].

[59] "OpenKIM Bringing Standards to Molecular Simulations" (invited), Digital Event – Open Databases Integration for Materials Design (OPTIMADE), CECAM Flagship Workshop, June 8–12, 2020.

[58] "Molecular Simulations you can Trust and Reproduce: The OpenKIM Framework" (invited), TMS 2020: Annual Meeting & Exhibition, San Diego, CA, February 24–28, 2020.

[57] "Molecular Stress: Uniqueness and Filtering" (invited), MolStress Workshop, Heidelberg Institute for Theoretical Studies, Heidelberg, Germany, November 4, 2019.

[56] "Moiré Mechanics in 2D Materials" (semi-plenary), 15th U.S. National Congress on Computational Mechanics (USNCCM15), Austin, Texas, July 28–August 1, 2019.

[55] "Multiscale Modeling of 2D Heterostructures" (keynote), 13th World Congress on Computational Mechanics (WCCM 2018), New York City, July 22–27, 2018.

[54] "Hyperdynamics + Quasicontinuum = Hyper-QC" (invited), 2017 Fall Meeting of the Materials Research Society, Boston, November 27 – December 1, 2017.

[53] "Climbing up from atoms" (plenary), Res Metallica Symposium, KU Leuven, Heverlee, Belgium, May 17, 2017.

[52] "A Coupled Continuum-Atomistic Framework for 2D Layered Heterostructures: Incommensurate-Commensurate Transformations in Bilayer Graphene" (invited), 2017 Spring Meeting of the Materials Research Society, Phoenix, AX, April 17–21, 2017.

[51] "Making interatomic potentials reliable and portable: the Knowledgebase of Interatomic Models (OpenKIM.org)" (invited), CECAM Workshop in "Multiscale Simulation: From Materials to Industrial Usage", Dublin, Ireland, September 5–7, 2016.

[50] "OpenKIM and the Future of Empirical Interatomic Models: Citability, Portability and Transferability" (invited), Nano Korea 2016, Seoul, South Korea, July 13–16, 2016.

[49] "Modeling the Mechanics of 2D Layered Heterostructures" (invited), SIAM Meeting on Mathematical Aspects of Materials Science, Philadelphia, PA, May 8–11, 2016.

[48] "Open KIM and the Future of Force Fields: Citability, Portability and Transferability" (invited), Workshop on Force Fields 2014, Jülich, Germany, November 3–5, 2014.

[47] "Accelerated Multiscale Simulations of Incipient Plasticity using Hyper-QC" (invited), MMM 2014, Berkeley, CA, October 6–10, 2014.

[46] "MiniMol: A Minimal Molecular Dynamics Program using the Knowledgebase of Interatomic Models (invited)", SES 2014 Annual Technical Meeting, West Lafayette, IN, October 1–3, 2014.

[45] 'Ensuring Reliability, Reproducibility and Transferability in Atomistic Simulations: The Knowledgebase of Interatomic Models (openKIM.org) (invited)", SES 2014 Annual Technical Meeting, West Lafayette, IN, October 1–3, 2014.

[44] "Faster, Bigger, Longer: Spanning Length *and* Time Scales in Materials Simulations" (plenary), 2014 Mach Conference, Annapolis, MD, April 9–11, 2014.

[43] "Mapping the Stochastic Response of Nanostructures" (invited), TMS 2014: Annual Meeting & Exhibition, San Diego, CA, February 16–20, 2014.

[42] "Hyper-QC: A method for spanning space and time" (invited), PIRE Workshop on "Evolution Problems for Material Defects: Dislocations, Plasticity, and Fracture", PIRE-SISSA, Trieste, Italy, September 30–October 4, 2013.

[41] "V&V of Interatomic Potentials: The Knowledgebase of Interatomic Models (KIM)" (invited), Grand Challenges in Computational Materials Design, NCSU, Raleigh, NC, January 15–16, 2013.

[40] "10,000,000,000,000,000,000,000 atoms" (plenary), ICME 2012, The 32nd Israeli Conference on Mechanical Engineering, Tel-Aviv University, Tel-Aviv, Israel, October 17–18, 2012.

[39] 'Knowledgebase of Interatomic Models" (invited), Foundations of Molecular Modeling and Simulation (FOMMS) 2012, Mt. Hood, OR, July 20–26, 2012.

[38] "Ensuring reliability, reproducibility and transferability in atomistic simulations: the Knowledgebase of Interatomic Models (openKIM.org)" (plenary), 52nd Sanibel Symposium, St. Simons Island, GA, February 19–24, 2012.

[37] "Interatomic potentials, forces and the uniqueness of stress" (invited), Institute for Applied Computational Science (IACS) Seminar Series, Harvard University, February 10, 2012.

[36] "Interatomic Potentials, Forces and the Uniqueness of Stress" (invited), Future Directions in Mechanics Research, NSF Workshop and Symposium in honor of Professor L. B. Freund, Providence, June 1–3, 2011.

[35] "From discrete atoms to continuum fields for arbitrary many-body potentials" (invited), Department of Mechanical Engineering, University of Houston, Houston, TX, April 21, 2011.

[34] "Ensuring reliability, reproducibility and transferability in atomistic simulations: the Knowledgebase of Interatomic Models (openKIM.org)" (invited), Department of Mechanical Engineering, University of Houston, Houston, TX, April 21, 2011.

[33] "From discrete atoms to continuum fields for arbitrary many-body potentials" (invited), Center for Advanced Scientific Computing and Modeling (CASCaM), University of North Texas, Denton, TX, April 11–14, 2011.

[32] "Knowledgebase of Interatomic Models (openKIM.org): an online platform for testing and archiving interatomic potentials" (invited), USC-DOE Workshop on Materials for Energy Applications: Experiment, Modeling and Simulations, Ranchos Palos Verdes, March 30–April 1, 2011.

[31] "Interatomic Potentials, Forces and Stress" (invited), Institute for Multiscale Materials Distinguished Lecture Series, Los Alamos National Laboratory, November 2, 2010.

[30] "Open Knowledgebase of Interatomic Models (openKIM.org): an online platform for testing and archiving empirical potentials" (invited), 2010 NIST Workshop on Atomistic Simulations for Industrial Needs, NIST Gaithersburg, July 27–28, 2010.

[29] "Non-uniqueness in Energy Minimization of Atomistic and Multiscale Problems: A Branch-Following and Bifurcation Investigation" (invited), 2010 March Meeting of the American Physical Society (APS), Portland, March 15–19, 2010.

[28] "A Quasicontinuum for Multilattice Phase Transforming Materials (invited talk opening the CSCAMM Spring 2008 Lecture Series), Center for Scientific Computation and Mathematical Modeling (CSCAMM), University of Maryland, College Park, January 30, 2008.

[27] "Application of the Cauchy-Born Rule to Phase Transforming Materials: Cascading Cauchy-Born Kinematics" (invited), 2007 Meeting of the Society for Natural Philosophy, Houston, October 26–28, 2007.

[26] Invited speaker (one of five) at a Summer School on "Multiscale Methods for Materials Science", Co-sponsored by CEA, EDF and INRIA, Paris, FRANCE. Target audience are engineers at CEA and EDF and researchers at INRIA. Nine hours of lectures and six hours "hands-on" sessions. Paris, June 25–July 5, 2007.

[25] "The Cascading Cauchy-Born Rule" (invited), 2006 Fall Meeting of the Materials Research Society, Boston, November 27 – December 1, 2006.

[24] "Multiscale Modeling of Material Response" (invited), Army High Performance Computing Research Center (AHPCRC) Workshop on "Verification and Validation", Aberdeen, October 5–6, 2006.

[23] "A Quasicontinuum for Complex Crystals" (invited), Third International Conference on Multiscale Materials Modeling, Freiburg, September 18–22, 2006.

[22] Invited three-lecture series opening the Institute for Mathematics and its Applications (IMA) Thematic Year on "Mathematics of Materials and Macromolecules: Multiple Scales, Disorder, and Singularities", Minneapolis, September 20–22, 2004. Lecture titles: (1) "Materials and Multiple Scales", (2) "The Theoretical Foundations of the Quasicontinuum Method", (3) "Quasicontinuum Applications and Future Directions".

[21] "A Meshless Quasicontinuum" (invited), SIMU 2004 conference on "Bridging the Scale", Genova, August 29–31, 2004.

[20] "An Analysis of Deformation Twinning in FCC Metals" (invited), Third GAMM Seminar on Microstructures, Stuttgart, January 9–10, 2004.

[19] "Theory and Simulation of Deformation Twinning in FCC Metals" (invited), Army High Performance Computing Research Center (AHPCRC) Workshop on "The Mechanical Behavior of Materials From Atoms to Structures", Minneapolis, November 6–7, 2003.

[18] Invited participant to the "XIII Workshop on Computational Materials Science (CMS2003)", organized by the Physics Department of Università di Cagliari and the Cagliari Research Unit of Istituto Nazionale per la Fisica della Materia, Sardinia, September 13–18, 2003. Lecture titles: (1) "Multiple-Scale Modeling of Materials using the Quasicontinuum Method", (2) "A First-Principles Analysis of Deformation Twinning in FCC Metals".

[17] Invited faculty to the "Summer School in Multi-Scale Modeling and Simulation", organized by the Computational Laboratory (CoLab) at ETH Zurich, the Swiss Center for Scientific Computing in Manno (CSCS) and the Università della Svizzera Italiana (USI), Lugano, August 15–30, 2003. Lecture title: "Deformation Twinning at Crack Tips: A Case Study in Multiscale Modeling"

[16] "Multiple-Scale Modeling of Materials using the Quasicontinuum Method" (plenary), Workshop on Computational Challenges in Scientific and Engineering Computation, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, January 20–25, 2003.

[15] "Linking Across Scales: An Overview of the Quasicontinuum Method" (invited), 19th General Conference of the European Physical Society – Condensed Matter Division, Brighton, England, April 7–11, 2002.

[14] "Theory and Simulation of Deformation Twinning at Crack Tips" (invited), CECAM Workshop on Multiscale Modelling of Materials, Heraklion, Crete, Greece, July 2–7, 2001.

[13] "A Novel Approach for the Determination of Activation Barriers for Physical Processes" (invited) 2001 Spring Meeting of the Materials Research Society, San Francisco, April 16–20, 2001.

[12] "Coarsening Atomistics: The Quasicontinuum Method" (invited), US National Congress on Computational Mechanics, University of Colorado, Boulder, August 4–6, 1999.

[11] "What is Dislocation Dynamics?" (invited), Workshop on Dislocation Dynamics, Brown University, Providence, December 5, 1998.

[10] "Quasicontinuum Models for Complex Bravais Crystals" (invited), 1998 Fall Meeting of the Materials Research Society, Boston, November 30 – December 4, 1998.

[9] "Multiple-Scale Modeling of Microsystems using the Quasicontinuum Method" (invited), Mardi Gras Conference on "Materials and Microsystems for Extreme Environments: Experimental and Computational Challenges" , Louisiana State University, Baton Rouge, Louisiana, February 19–21, 1998.

[8] "Atomistically Driven Continuum Mechanics" (invited), Mini-workshop on Interatomic Potentials and Linking of Scales, Institute for Theoretical Physics, University of California, Santa Barbara, June 5–7, 1997.

[7] "Bridging the Atomistic and Continuum Scales" (invited), Workshop on Multi-Scale Modeling of Polycrystal Plasticity, Institute for Mechanics and Materials, University of California, San Diego, April 9–11, 1997.

[6] "Quasi-Continuum Models for Mesoscopic Mechanics" (invited), 1997 Spring Meeting of the Materials Research Society, San Francisco, March 31 – April 4, 1997.

[5] "Multiple-Scale Quasi-Continuum Models for Metals and Directionally Bonded Solids" (invited), Mini-workshop on Fracture and Interfaces, Institute for Theoretical Physics, University of California, Santa Barbara, February 13–15, 1997.

[4] Invited participant to the workshop: "Quantitative Methods in Materials Research", Institute for Theoretical Physics, University of California, Santa Barbara, January 13 – June 27, 1997.

[3] "Quasicontinuum Analysis of Mesoscopic Deformation" (invited), Combined Workshop on Fracture, Friction and Deformation, Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, April 19–24, 1996.

[2] "An Introduction to the Finite Element Method" (invited), Combined Workshop on Fracture, Friction and Deformation, Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, April 19–24, 1996.

[1] "Quasicontinuum Analysis of Defects in Crystals" (invited), Graduate Student Awards Program, 1995 Fall Meeting of the Materials Research Society, Boston, November 27 – December 1, 1995.

Contributed Talks (Most Recent First)

[47] "Cross-scale covariance for material property prediction", APS March Meeting, March 17–21, 2025, Anaheim, CA.

[46] "Reproducible high-fidelity molecular simulation through OpenKIM and ColabFit", 2023 SES Annual Technical Meeting, October 9, 2023, Minneapolis, MN.

[45] "New from OpenKIM: Machine Learning Based Tools to Develop, Test, Select and Deploy Advanced Interatomic Potentials", LAMMPS Virtual Workshop and Symposium, August 9, 2023 [Online].

[44] "OpenKIM for the LAMMPS User", LAMMPS Users' Workshop, August 10–13, 2021 [Online].

[44] "OpenKIM for the LAMMPS User", LAMMPS Users' Workshop, August 10–13, 2021 [Online].

[43] "OpenKIM: Streamlining the use of Interatomic Models with LAMMPS", LAMMPS Users' Workshop, University of New Mexico, August 13–15, 2019, Albuquerque, NM.

[42] "OpenKIM: Reliable Interatomic Models for Atomistic and Multiscale Simulations", 15th U.S. National Congress on Computational Mechanics (USNCCM15), Austin, Texas, July 28–August 1, 2019.

[41] "Structural and electron diffraction scaling of twisted graphene bilayers", 2017 Fall Meeting of the Materials Research Society, Boston, November 27 – December 1, 2017.

[40] "The OpenKIM testing framework for interatomic potentials", LAMMPS Users' Workshop, University of New Mexico, August 1–3, 2017, Albuquerque, NM.

[39] "Coupled Continuum-Atomistic Simulations of Incommensurate to Commensurate Transformations in Twisted Graphene Bilayers", 14th US National Congress on Computational Mechanics (USNCCM-14), July 17–20, 2017, Montreal, Canada.

[38] "K-Dominance of Atomistic Cracks", SES 2016 Meeting, Hyattsville, MD, October 2–5, 2016.

[37] "Cauchy-Born Simulations of a Diamond Anvil Cell Experiment using ABAQUS", SES 2016 Meeting, Hyattsville, MD, October 2–5, 2016.

[36] "Modeling the Mechanics of 2D Layered Heterostructures", SES 2016 Meeting, Hyattsville, MD, October 2–5, 2016.

[35] "Mechanics of Weakly-Bonded Incommensurate Atomic Bilayers", SES 2015 Meeting, College Station, TX, October 26–28, 2015.

[34] "Cauchy-Born ANSYS", USNCCM-13, San Diego, CA, July 26–30, 2015.

[33] "The Knowledgebase of Interatomic Models (openKIM.org): Ensuring Reliability, Reproducibility and Transferability in Atomistic Simulations", MMM 2014, Berkeley, CA, October 6–10, 2014.

[32] "Ensuring Reliability, Reproducibility and Transferability in Atomistic Simulations: The Knowledgebase of Interatomic Models (openKIM.org)", TMS 2014: Annual Meeting & Exhibition, San Diego, CA, February 16–20, 2014.

[31] "Nanoindentation Simulation of a Thin Ni Film Using Hyper-QC", Society of Engineering Science (SES) 2013 Meeting, Providence, RI, July 28–31, 2013.

[30] "Mapping the Stochastic Response of Nanostructures", Society of Engineering Science (SES) 2013 Meeting, Providence, RI, July 28–31, 2013.

[29] "Hyper-QC: Accelerated Finite-Temperature Quasicontinuum Simulations Using Hyperdynamics", Society of Engineering Science (SES) 2012 Meeting, Atlanta, GA, October 10–12, 2012.

[28] "Unique Scale-Dependent Definition for Stress at the Atomic Scale", Society of Engineering Science (SES) 2012 Meeting, Atlanta, GA, October 10–12, 2012.

[27] "Ensuring Reliability, Reproducibility and Transferability in Atomistic Simulations: The Knowledgebase of Interatomic Models (openKIM.org)", 2011 AIChE Annual Meeting, Minneapolis, October 16–21, 2011.

[26] "Non-uniqueness in Energy Minimization of Atomistic and Multiscale Problems: A Branch-Following and Bifurcation Investigation", Minneapolis, July 25–29, 2011.

[25] "Open Knowledgebase of Interatomic Models (openKIM.org): an online platform for testing and archiving empirical potentials", MS& T'10 Conference, Houston, October 17–21, 2010.

[24] "Non-Uniqueness in Energy Minimization of Simulations of Defects", Society of Engineering Science (SES) 2010 Meeting, Ames, October 3–6, 2010.

[23] "Interatomic Potentials, Forces and Stress", Society of Engineering Science (SES) 2010 Meeting, Ames, October 3–6, 2010.

[22] "A Branch-Following and Bifurcation Investigation of Atomistic Scale Problems: A Study of Energy Minimization", 2009 ASME International Mechanical Engineering Congress (IMECE2009), Lake Buena Vista, November 13–19, 2009.

[21] "A Quasicontinuum for Multilattice Crystals Exhibiting Martensitic Phase Transformations: Cascading Cauchy-Born Kinematics", 2009 ASME International Mechanical Engineering Congress (IMECE2009), Lake Buena Vista, November 13–19, 2009.

[20] "A Quasicontinuum for Multilattice Phase Transforming Materials", Society of Engineering Science (SES) 2008 Meeting, Urbana-Champaign, October 12–15, 2008.

[19] "A Unified Interpretation of the Microscopic Stress Tensor", Society of Engineering Science (SES) 2008 Meeting, Urbana-Champaign, October 12–15, 2008.

[18] "Microscopic Foundations of Continuum Mechanics: Overview and Current Directions", SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, May 11–14. 2008.

[17] "Nano-scale Plasticity at Crack Tips: Deformation Twinning in FCC Metals", 2004 Meeting of the Israel Society for Theoretical and Applied Mechanics (ISTAM), Tel-Aviv, December 12, 2004.

[16] "Theory and simulation of deformation twinning in fcc metals", The 11th Israel Materials Engineering Conference, Haifa, December 24–25, 2003.

[15] "An efficient data structure for graded atomistic simulations", 2003 Mechanical Engineering Conference, Haifa, May 12–13, 2003.

[14] "Electromechanical coupling correction for piezoelectric layered beams", 2003 Mechanical Engineering Conference, Haifa, May 12–13, 2003.

[13] "Multiscale Simulation of Polarization Switching in Lead-Titanate", Ninth Israel Symposium on Computational Mechanics (ISCM-9), Department of Mechanical Engineering, Technion – Israel Institute of Technology, Haifa, October 26, 2000.

[12] "Quasicontinuum Simulation of Phase Transformations and Polarization Switching in Complex Bravais Crystals", James H. Belfer Memorial Symposium on Nonlinear Mechanics, Department of Mechanical Engineering, Technion – Israel Institute of Technology, Haifa, June 11, 2000.

[11] "Quasicontinuum Simulation of Nanoindentation in Complex Crystals", One-day symposium on the Multi-scale Problem of the Strength of Solids, Department of Mechanical Engineering, Ben-Gurion University, Beer Sheva, June 4, 2000.

[10] "Parallel Tempering Algorithm for the Determination of Lowest-Barrier Transition Paths", 1999 Fall Meeting of the Materials Research Society, Boston, November 29 – December 3, 1999.

[9] "Simulation of Resistance Measurements during Silicon Nanoindentation", Conversations about Computational Physics, Department of Physics, Technion – Israel Institute of Technology, Haifa, October 10–13, 1999.

[8] "Atomic-Scale Simulation of Hexagonal Void Formation in Zirconium", Sixth ASME International Conference on Nuclear Engineering (ICONE-6), San Diego, May 11–14, 1998.

[7] "Ab Initio Predictions of Macroscopic Piezoelectric Response" (poster), Fifth Williamsburg Workshop on First-Principles Calculations for Ferroelectrics, Williamsburg, February 1–4, 1998.

[6] "A Quasicontinuum Methodology for Small-Scale Engineering", 1997 Fall Meeting of the Materials Research Society, Boston, December 1–5, 1997.

[5] "Quasicontinuum Models of Crystalline Solids" (poster), MIT Workshop on Multiscale Materials Prediction: Fundamentals and Industrial Applications, Massachusetts Institute of Technology, Cambridge, September 14–16, 1997.

[4] "Multiple-Scale Quasi-Continuum Finite Element Analysis of Defects in Crystals", 1995 Fall Meeting of the Materials Research Society, Boston, November 27 – December 1, 1995.

[3] "Quasicontinuum Finite Element Analysis of Defects in Crystals", 1995 March Meeting of the American Physical Society, San Jose, March 20–24, 1995.

[2] "Quasicontinuum Finite Element Analysis of Inelastic Deformation in Crystals", 1994 Fall Meeting of the Materials Research Society, Boston, November 27 – December 2, 1994.

[1] "Analysis of Sandwich Structures using ANSYS Layered Elements", ANSYS Fifth International Conference and Exhibition, Pittsburgh, May 20–24, 1991.

Talks and Seminars (Most Recent First)

[62] "Revolutionizing Molecular Simulation of Materials: The Rise of Data", CEMS Seminar, Department of Chemical Engineering and Materials Science, University of Minnesota, April 24, 2025.

[61] "Machines Discovering New Materials", The Guild of Metalsmiths, Membership Meeting, Bloomington, MN, October 9, 2024.

[60] "When not to trust the predictions of molecular simulations", School of Mechanical Engineering, Tel Aviv University, Tel Aviv, Israel, June 22, 2022.

[59] "Data-Informed Molecular Simulations", 3M Technical Forum (TekEx), November 17, 2021 [Online].

[58] "Modeling Multilayer Graphene: Atomistics, Machine Learning and Multiscale Mechanics", Condensed Matter Seminar Series, Physics Division, LLNL, September 21, 2021 [Online].

[57] "Moiré Mechanics in 2D Materials", Computational Mechanics Seminar, ORNL, August 19, 2021 [Online].

[56] "Can Truth Save Democracy? We're trying in Science Court", Anoka County DFL Senior Caucus, April 14, 2021 [Online].

[55] "Moiré Mechanics in 2D Materials", MAE Research Seminar Series, Department of Mechanical and Aerospace Engineering, University of Colorado, Colorado Springs, April 1, 2021 [Online].

[54] "Can Truth Save Democracy? We're trying in Science Court", Pilgrim House, Unitarian Universalist Fellowship, February 6, 2021 [Online].

[53] "Can Truth Save Democracy? We're trying in Science Court", Instiute for Child Development, University of Minnesota, November 12, 2020 [Online].

[52] "Revolutionizing Molecular Simulation: Multiscale Modeling, Machine Learning, and OpenKIM", SE Special Seminar in Computational Mechanics, University of California, San Diego, CA, February 26, 2020.

[51] "Introducing OpenKIM to OpenFF", Online Webinar, February 19, 2020.

[50] "Revolutionizing Molecular Simulation: OpenKIM and Machine Learning", AEM Colloquium, University of Minnesota, Minneapolis, MN, January 31, 2020.

[49] "Knowledgebase of Interatomic Models (KIM): Reliable Interatomic Models for Molecular Simulations", University of Houston, Houston, TX, March 1, 2019.

[48] "Stacking 2D Materials: Bonding, Mechanics and Reconstructions", University of Houston, Houston, TX, February 28, 2019.

[47] "Understanding the Mechanics of 2D Heterostructures", All-MRSEC Meeting, University of Minnesota, Minneapolis, MN, January 31, 2019.

[46] "The Knowledgebase of Interatomic Models (openkim.org) Ensuring reliability, reproducibility and transferability in atomistic simulations", Los Alamos National Laboratory, Los Alamos, NM, August 1, 2017.

[45] "Structural and electron diffraction scaling of twisted graphene bilayers", Los Alamos National Laboratory, Los Alamos, NM, July 31, 2017.

[44] "Multiscale Simulation of 2D Heterostructures: Incommensurate to Commensurate Transformations in Twisted Graphene Bilayers", School of Mechanical Engineering, Tel Aviv University, Tel Aviv, Israel, June 28, 2017.

[43] "Multiscale Simulation of 2D Heterostructures: Incommensurate to Commensurate Transformations in Twisted Graphene Bilayers", Special Seminar, Faculty of Mechanical Engineering, Technion – Israel Institute of Technology, Haifa, Israel, June 21, 2017.

[42] "10 Sextillion Atoms", Warren Lecture, University of Minnesota, Department of Civil Engineering, November 18, 2016.

[41] "Hot and Hyper Quasicontinuum", Korea Advanced Institute of Science and Technology (KAIST), Daejeon, South Korea, July 15, 2016.

[40] "Rise of Data in Materials Research", Korea Institute of Science and Technology (KIST), Seoul, South Korea, July 12, 2016.

[39] "Ensuring reliability, reproducibility and transferability in atomistic simulations: The Knowledgebase of Interatomic Models (openkim.org)", Korea Institute of Science and Technology (KIST), Seoul, South Korea, July 12, 2016.

[38] "MURI Multiscale Mathematical Modeling and Design Realization of Novel 2D Functional Materials; Year 1 Review: Mechanics Progress", Harvard University, Cambridge, MA, December 8, 2015.

[37] "Multiscale Science: Coupling across length and time scales in mechanics", Dept. Aerospace Engineering, Iowa State University, Ames, Iowa, October 8, 2015.

[36] "Bridging time and length scales in atomistic simulations using hyper-QC", Dept. Metallurgy and Materials Engineering, Katholieke Universiteit Leuven, Heverlee, Belgium, November 7, 2014.

[35] "Mapping the Stochastic Response of Nanostructures", Mechanics Group Seminar, Faculty of Mechanical Engineering, Technion – Israel Institute of Technology, Haifa, Israel, June 25, 2014.

[34] "Mapping the Stochastic Response of Nanostructures", Mechanical Engineering and Applied Mechanics Colloquium, University of Pennsylvania, Philadelphia, PA, February 11, 2014.

[33] "Mapping the Stochastic Response of Nanostructures", MechSE Departmental Seminar, University of Illinois at Urbana-Champaign, January 21, 2014.

[32] "Bridging time and length scales in atomistic simulations using Hyper QC", CAM Colloquium, Penn State University, University Park, PA, October 21, 2013.

[31] "Mapping the Stochastic Response of Nanostructures", CCMA Luncheon Seminar, Penn State University, University Park, PA, October 21, 2013.

[30] "10,000,000,000,000,000,000,000 atoms", Dept. of Materials Science, Shanghai Jiao Tong University, Shanghai, China, June 28, 2013.

[29] "Why Things Break: From Atoms to Airplanes", Golden Centennial Talk, University of Minnesota, Minneapolis, MN, May 10, 2013.

[28] "10,000,000,000,000,000,000,000 atoms", Division of Engineering, Brown University, Providence, RI, March 8, 2013.

[27] "Introduction to Modeling Materials Short Courses", 3M Company, 3M Center, Saint Paul, MN, February 8, 2013.

[26] "Materials and Multiple Scales", Minnesota Clockmakers Guild, December 6, 2012.

[25] "Interatomic Potentials, Forces and the Uniqueness of Stress", IACS Seminar, Harvard University, Cambridge, MA, February 10, 2012.

[24] "Interatomic potentials, forces and stress", Computational Physics Seminar, Department of Physics, Technion – Israel Institute of Technology, January 2, 2011.

[23] "Knowledgebase of Interatomic Models (KIM)", Sandia National Laboratory, Albuquerque, November 3, 2010.

[22] "Knowledgebase of Interatomic Models (KIM)", Institute for Multiscale Materials, Los Alamos National Laboratory, Los Alamos, November 2, 2010.

[21] "Interatomic potentials, forces and stress", Institute for Multiscale Materials, Los Alamos National Laboratory, Los Alamos, November 2, 2010.

[20] "A unified interpretation of stress in molecular systems", Solid and Continuum Mechanics Research Seminar, Aerospace Engineering and Mechanics, University of Minnesota, April 14, 2009.

[19] "A Quasicontinuum for Phase Transforming Materials: Applications for high-speed machining", Third Wave Systems, Minneapolis, January 18, 2008.

[18] "A Multiscale Method for Phase Transforming Materials", École Normale Supérieure de Lyon, June 11, 2007.

[17] "Multiscale Materials Modeling: Why, How and What's Next?", AEM, University of Minnesota, February 24, 2006.

[16] "Is the virial stress a stress?", Solid and Continuum Mechanics Research Seminar, AEM, University of Minnesota, November 22, 2005.

[15] "Quasicontinuum challenges: Finite Temperature and Dynamics", Monday Focus Group on Multiscale Modeling and Computation, Institute for Math and its Applications (IMA), University of Minnesota, October 4, 2004.

[14] "Theory and simulation of deformation twinning in FCC metals", Faculty of Mechanical Engineering, Technion – Israel Institute of Technology, March 15, 2004.

[13] "Deformation Twinning at Crack Tips: A First-Principles Analysis" (invited), Division of Applied Mechanics, Stanford University, April 16, 2003.

[12] "Theory and Simulation of Deformation Twinning at Crack Tips", Dept. Metallurgy and Materials Engineering, Katholieke Universiteit Leuven, Heverlee, Belgium, December 6, 2002.

[11] "Theory and Simulation of Deformation Twinning at Crack Tips" (invited), Center for Computational Materials Science, Naval Research Lab, Washington, DC, October 1, 2001.

[10] "Quasicontinuum Simulation of Phase Transformations in Complex Bravais Crystals" (invited), Department of Mechanical and Aerospace Engineering, Princeton University, January 9, 2001.

[9] "Coarsening Atomistics", Department of Materials Engineering, Technion – Israel Institute of Technology, May 9, 1999.

[8] "Connecting Atomistics and Continuum: The Quasicontinuum Method", Interfaculty Seminar on Scientific Computing, Physics Department, Technion – Israel Institute of Technology, January 17, 1999.

[7] "A Combined Continuum and Atomistic Approach for Modeling Microsystems", 1998 Meeting of the Israel Society for Theoretical and Applied Mechanics (ISTAM), Tel-Aviv, December 20, 1998.

[6] "Atomic-Scale Modeling of MEMS devices", Microcosm Technologies, Cambridge, MA, December 7, 1998.

[5] "Multiple-Scale Modeling of Microsystems", Draper Laboratory, Cambridge, MA, July 28, 1998.

[4] "A Quasi-Continuum Method for Small-Scale Engineering and Materials Modeling" (invited), Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, April 24, 1997.

[3] "Bridging Length Scales in Materials Modeling" (invited), Division of Applied Mechanics, Stanford University, October 10, 1996.

[2] "Quasicontinuum Finite Element Analysis of Inelastic Deformation Processes in Crystals", Department of Aerospace Engineering, Technion – Israel Institute of Technology, June 29, 1994.

[1] "Plastic Failure of Pressurized Multilayered Cylinders", Department of Mechanical Engineering, Technion – Israel Institute of Technology, May 13, 1991.

Service

Participation in Organizing Workshops and Conferences (Most Recent First)

[30] Organizer of "Systematic Discovery and Characterization of Materials Across Compositions and Structures", MACH 2024 Conference, Annapolis, MD, April 2024. (Additional organizers: Ilia Nikiforov, Chris Bartel (University of Minnesota), Rodrigo Freitas (MIT))

[29] Organizer of "Interatomic Models in Materials Simulations: Theory, Standards, Infrastructure, and Applications", 2023 Society of Engineering Science (SES) Annual Technical Meeting, October 8–11, 2023, Minneapolis, MN. (Additional organizers: Ryan Elliott, Ronald Miller, Ilia Nikiforov)

[28] Organizer of the Symposium "Systems for Fitting, Uncertainty Quantification, Selection and Use of Interatomic Models", 2023 Mach Conference, April 5–7, 2023, Towson, MD. (Additional organizer: Ilia Nikiforov.)

[27] Organizer of the "NSF Workshop on the Knowledgebase of Mesoscale Modeling and Experimentation (KnoMME)", January 12–13, 2023, Houston, TX. (Additional organizer: Shailendra Joshi)

[26] Organizer of the "Cyberloop Workshop on Nano/Bio-Material Modeling and Validation", November 18–19, 2021, [Online]. (Additional organizers: Hendrik Heinz (U. Colorado, Boulder), Wonpil Im (Lehigh).)

[25] Co-organizer of three coding sprints:

- OpenKIM Sprint I: Development of OpenKIM Python Packages, August 6–10, 2018
- OpenKIM Sprint II: OpenKIM Packaging and Automated Continuous Integration, July 30–Aug 4, 2018.
- OpenKIM Sprint III: Simulator Support for KIM API 2.0 and Simulator Models, Aug 20–24, 2018.

Institute for Mathematics and its Applications (IMA), University of Minnesota, Minneapolis, MN. (Additional organizer: Ryan Elliott.)

[24] Co-organizer of the Symposium "Mechanics of Multifunctional 2D Materials – Graphene and Beyond", 18th U.S. National Congress for Theoretical and Applied Mechanics (USNCTAM 2018), June 4–9, 2018, Chicago, IL. (Additional organizers: Rui Huang (UT Austin), Kenneth Liechti (UT Austin), Harold Park (BU).)

[23] Co-organizer of the Symposium "Computational Mechanics at the Atomistic and Electronic Scales", 54th Annual Meeting of the Society of Engineering Science (SES 2017), July 25–28, 2017, Boston, MA. (Additional organizers: Amartya Banerjee (LLNL), Phanish Suryanarayana (Georgia Tech), Kaushik Bhattacharya (Caltech).)

[22] Co-organizer of the Minisymposium on "Advances in Atomistic-to-Continuum Coupling Techniques", 14th US National Congress on Computational Mechanics (USNCCM-14), July 17–20, 2017, Montreal, Canada. (Additional organizers: Dennis Kochmann (Caltech), Jaime Marian (UCLA), Chuin-Shan (David) Chen (National Taiwan University), and Ron Miller (Carleton).)

[21] Co-organizer of the Symposium "Mechanics of Multifunctional 2D materials and 2D-based Nanostructures", 53rd Annual Meeting of the Society of Engineering Science (SES 2016), October 2–5, 2016, Hyattsville, MD. (Additional organizers: Shuze Zhu (MIT), Cemal Basaran (U. Buffalo), Wei Gao (Northwestern), Kuan Zhang (UMN)).

[20] Organizing Committee for the SIAM Meeting on Mathematical Aspects of Materials Science, May 8-11, 2016, Philadelphia, PA.

[19] Organizer of the "TMS Town Hall Meeting on the Rise of Data in Materials Research", February 16, 2016, Nashville, TN. (Additional organizers: Ryan Elliott (U. Minnesota)).

[18] Organizer of the Symposium "Mechanics of 2D Materials", 52nd Annual Meeting of the Society of Engineering Science (SES 2015), October 26–28, 2015, College Station, TX. (Additional organizers: Ilia Nikiforov (UMN)).

[17] Co-organizer of a tutorial on "Techniques and Best Practices for Performing High-Quality MD Simulations," LAMMPS Users' Worshop, University of New Mexico, August 5–7, 2015, Albuquerque, NM. (Additional organizers: Ryan Elliott (U. Minnesota)).

[16] Co-organizer of the Minisymposium on "Quasicontinuum and Other Atomistic-to-Continuum Coupling Techniques", 13th US National Congress on Computational Mechanics (USNCCM-13), July 26–30, 2015, San Diego, CA. (Additional organizers: Dennis Kochmann (Caltech), Jaime Marian (UCLA), and Chuin-Shan (David) Chen (National Taiwan University).)

[15] Organizer of the "NSF Workshop on the Rise of Data in Materials Science", June 29–30, 2015, Arlington, VA. (Additional organizers: Ryan Elliott (U. Minnesota)).

[14] Organizer of the Symposium "Interatomic Models in Materials Simulations: Theory, Standards, Infrastructure and Applications", 51st Annual Meeting of the Society of Engineering Science (SES 2014), October 1–3, 2014, West Lafayette, IN. (Additional organizers: Ryan Elliott (U. Minnesota) and Jim Sethna (Cornell)).

[13] Organizer of the "KIM Content Carnival", August 18–21, 2014, University of Maryland, College Park, MD. (Additional organizers: Ryan Elliott (U. Minnesota)).

[12] Organizer of the Symposium "From Atomistics to Reality: Spanning Scales in Simulations and Experiments", 50th Annual Meeting of the Society of Engineering Science (SES 2013), July 28–31, 2013, Providence, RI. (Additional organizers: Derek Warner (Cornell) and Ron Miller (Carleton University)).

[11] Organizer of the Symposium "Continuum Mechanics of Solids and Fluids: A Symposium in Honor of Roger Fosdick", XIII Pan-American Congress of Applied Mechanics (PACAM-XIII), May 22–24, 2013, Houston, TX. (Additional organizers: Ryan Elliott (U. Minnesota), and Adair Aguiar (University of São Paulo)).

[10] Organizer of the "KIM Content Carnival", October 9–12, 2012, Institute for High Performance Computing, A*Star, Singapore. (Additional organizers: Ryan Elliott (U. Minnesota)).

[9] Organizer of the "KIM Content Carnival", August 20–23, 2012, AICES, RWTH Aachen University, Aachen, Germany. (Additional organizers: Ryan Elliott (U. Minnesota)).

[8] Organizer of the "KIM Content Carnival", March 13–16, 2012, University of Minnesota, Minneapolis. (Additional organizers: Ryan Elliott (U. Minnesota)).

[7] Organizer of the "KIM Inaugural Workshop", February 26–27, 2011, San Diego, CA. (The workshop is integrated with the TMS 2011 Annual Meeting and Exhibition.) (Additional organizers: Ryan Elliott (U. Minnesota))

[6] Co-organizer of the Minisymposium on "Recent Advances in the Quasicontinuum Method and other Atomistic/Continuum coupling Techniques", 11th US National Congress on Computational Mechanics (USNCCM-11), July 25–29, 2011, Minneapolis, MN. (Additional organizers: Jaime Marian (LLNL), Chuin-Shan (David) Chen (National Taiwan University) and Ronald Miller (Carleton University)).

[5] Co-organizer of the Symposium on "Atomistic Aspects of Fracture", 12th International Conference on Fracture, July 12–17, 2009, Ottawa. (Additional organizers: R. E. Miller, W. A. Curtin and P. Gumbsch.)

[4] Organizer of the Minisymposium on the "Microscopic Foundations of Continuum Mechanics", SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, May 11–14, 2008.

[3] Co-organizer of the Symposium on "Bridging Scales for the Strength of Materials", Third International Conference on Multiscale Materials Modeling, September 18–22, 2006, Freiburg. (Additional organizer: M. Ortiz, Caltech.)

[2] Twelfth Annual Workshop of the Israel Association for Computational Method in Mechanics (ISCM-12), Haifa, April 11, 2002. Coordinated and chaired the morning session on computational modeling of MEMS devices.

[1] North Carolina – Israel Partnership (NCIP) Workshop on MEMS Technology, Design and Application, Haifa, May 22–24, 2000. Involved in writing the funding proposal, contacting academics and industry both in Israel and NC to ensure participation, and organizing workshop.

Short Courses (Most Recent First)

[16] Modeling Materials Short Course, Weizmann Institute of Science, August 16–27, 2020, Rehovot, Israel [Online].

[15] "A 'How-To' Tutorial on Using OpenKIM with LAMMPS," NIST Workshop on Atomistic Simulations for Industrial Needs, August 5–7, 2020, Gaithersburg, MD, USA [Online].

[14] Two-part lecture series on "Predicting Behavior from the Ground Up: Molecular and Multiscale Simulations of Materials," Computational Chemistry and Materials Science (CCMS) Summer Institute, Lawrence Livermore National Laboratory, July 23–24, 2020, Livermore, CA, USA [Online].

[13] Modeling Materials Short Course, National University of Singapore, August 18-22, 2016, Singapore.

[12] Modeling Materials Short Course, Friedrich-Alexander-Universität and Engineering of Advanced Materials (EAM) Cluster of Excellence, August 17-21, 2015, Erlangen-Nürnberg, Germany.

[11] Modeling Materials Short Course, Hamburg University of Technology (TUHH), March 17-21, 2014, Hamburg, Germany.

[10] Modeling Materials Short Course, Argonne National Laboratory, November 18-22, 2013, Argonne, IL, USA.

[9] Modeling Materials Short Course, 3M Company, November 11-15, 2013, Saint Paul, MN, USA.

[8] Modeling Materials Short Course, Shanghai Jiao Tong University, July 1-5, 2013, Shanghai, China.

[7] Modeling Materials Short Course, DoD High Performance Computing Modernization Program's PETTT Program, Army Research Laboratory, June 3-7, 2013, Aberdeen, MD.

[6] Modeling Materials Short Course, Friedrich-Alexander-Universität and Engineering of Advanced Materials (EAM) Cluster of Excellence, February 18-22, 2013, Erlangen-Nürnberg, Germany.

[5] Modeling Materials Short Course, Aachen Institute for Advanced Study in Computational Engineering Science (AICES), August 14-17, 2012, Aachen, Germany.

[4] Modeling Materials Short Course, DoD High Performance Computing Modernization Program's PETTT Program, Army Research Laboratory, July 9-13, 2012, Aberdeen, MD.

[3] Tutorial on Atomistic Simulations using Standardized Interatomic Potentials (openKIM workshop), TMS 2012, 141st Annual Meeting & Exhibition, March 11, 2011, Orlando, FL.

[2] Tutorial on Atomistic Simulations using Standardized Interatomic Potentials (openKIM workshop), 11th US National Congress on Computational Mechanics (USNCCM-11), July 24, 2011, Minneapolis, MN.

[1] Three-day Tutorial on the Quasicontinuum Method, Centre Européen de Calcul Atomique et Moléculaire (CECAM), Lyon, France, June 9–11, 2004. The tutorial was co-taught with R. Miller (Carleton University).

Outreach – Websites

[1] https://kim-initiative.org: Portal to efforts organized under the "KIM Initiative" that provide tools and resources to researchers in materials science and chemistry who are using molecular simulations to revolutionize technologies across the sciences.

[2] https://openkim.org: Tadmor is the Founding Director of the Open Knowledgebase of Interatomic Models (OpenKIM). OpenKIM is a core NSF cyberinfrastructure established in 2009. OpenKIM develops and maintains a curated repository of interatomic potentials and force fields, an API connecting the potentials to all major MD codes, and a testing and curation workflow with rigorous transferability and uncertainty estimation of interatomic potentials.

[3] https://colabfit.org: The ColabFit project aims to create a framework to facilitate the training and use of machine learning (ML) models in materials science including interatomic potentials. This includes an online exchange for datasets used to train ML models and a portable format for deploying ML models to simulation platforms using the OpenKIM system.

[4] http://modelingmaterials.org: This website is associated with the two books "Modeling Materials" and "Continuum Mechanics and Thermodynamics" co-authored by Tadmor (see above under "BOOKS"). The website provides general information, resources for readers and instructors, and errata.

[5] http://qcmethod.org: Information for users of the quasicontinuum (QC) method, which includes the complete QC source code, example problems, a library of atomistic potentials, and a user's manual and tutorial.