Tim P. Schulze
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Positions held:

1999-present	Associate Head/Director of Graduate Studies (fall 2022-present) Professor (fall 2010 – present) Associate Professor (fall 03 – spring 2010) Assistant Professor (fall 99 – spring 03) Department of Mathematics, University of Tennessee
1997-1999	Associate Research Scientist Courant Institute of Mathematical Sciences, New York University Scientific Advisors: Professor Robert V. Kohn and Professor Weinan E
1995-1997	NSF-NATO Postdoctoral Research Fellow (1996-1997, awarded 1995) Postdoctoral Research Associate (1995-1996) Department of Applied Mathematics and Theoretical Physics (DAMTP), University of Cambridge Scientific Advisor: Dr. M. Grae Worster

Education:

1991-1995	Ph.D. in Applied Mathematics, Northwestern University Thesis Title: *Shear stabilization of morphological instability during directional solidification* Thesis Advisor: Professor Stephen H. Davis
1987-1991	B.S.E. in Interdisciplinary Engineering, University of Washington, Seattle

Extended visits to other institutions:

Spring 2020	Department of Applied Mathematics and Theoretical Physics, U. of Cambridge, UK Visiting Fellow Commoner (VFC) Trinity Colllege
Fall 2012	Institute for Pure and Applied Mathematics (IPAM), UCLA Co-chair of organizing committee for long program “Materials Defects: Mathematics, Computation, and Engineering”
Spring 2006	Courant Institute of Mathematical Sciences, NYU Program in Applied and Computational Mathematics, Princeton Industrial Research Limited/Victoria University, Wellington NZ Department of Mathematics, University of Michigan, Ann Arbor
Fall 2005	Institute for Pure and Applied Mathematics (IPAM), UCLA
May 2005	Institute for Mathematics and its Applications (IMA), University of Minnesota
Spring 2002	Program in Applied and Computational Mathematics, Princeton

Publications:

M. Abramson, H.J.Coleman, P. J. Simmonds, T.P. Schulze, and C. Ratsch, “Kinetic Monte Carlo simulations of quantum dot self-assembly,” *J. Crystal Growth,* Available online Aug. 27, 2022.

J. Hicks and T.P. Schulze, “Examining Exhaustive Saddle Point Searches in the Context of Off-Lattice Kinetic Monte Carlo”, *Communications In Computational Physics,* **30** *(2021) 749-770.*

T. Krumwiede, K. Dinh, C. Ratsch and T.P. Schulze, "The influence of edge energy on step flow instability for crystals with bravais versus non-bravais lattice structures”, *Communications In Computational Physics,* **27** *(2020) 70-86.*

H. Ruzayqat and T.P. Schulze, “A rejection scheme for off-lattice kinetic Monte Carlo Simulation,” *Journal of Chemical Theory and Computation,* **14** (2018) 48-54.

T. Krumwiede and T.P. Schulze, "Dendritic Growth Shapes in Bond-Counting Models," *Modeling and Simulation in Materials Science and Engineering* **25** *(2017) Art. no. 025009.*

K. L. Golenbiewski and T.P. Schulze, "Analysis of an Energy Localization Approximation Applied to Three-Dimensional Kinetic Monte Carlo Simulations of Heteroepitaxial Growth," *Journal of the Mechanics and Physics of Solids, **95** (2016) 708-718*.

D. Schebarchov, T.P. Schulze and S.C. Hendy, “Degenerate Ising model for atomistic simulation of crystal-melt interfaces,” *J. Chem. Phys.* **140** (2014) Art. no. 074704.

H.A. Boateng, T.P. Schulze and P. Smereka, “Approximating Off-Lattice Kinetic Monte Carlo,” *Multiscale Modeling and Simulation* **12** (2014) 181-199.

W. Chen, H. Chen, H. Lan, P. Cui, T. P. Schulze, W. Zhu and Z. Zhang, "Suppression of Grain Boundaries in Graphene Growth on Superstructured Mn-Cu(111) Surface"
Physical Review Letters **109** (2012) Art. no. 265507.

T.P. Schulze and P. Smereka, “Kinetic Monte Carlo Simulation of Heteroepitaxial Growth: Wetting Layers, Quantum Dots, Capping, and Nano-rings,” *Phys. Rev. B* **86** (2012) Art. no. 235313.

N.R. Gewecke and T.P. Schulze, “Solid-Mush Interface Conditions for Mushy Layers,” *Journal of Fluid Mechanics* **689** (2011) 357-375 *.*

N.R. Gewecke and T.P. Schulze, "The Rapid Advance and Slow Retreat of a Mushy Zone," *Journal of Fluid Mechanics* **674** *(2011) 227-243.*

T.P. Schulze and P. Smereka, “Simulation of Three-Dimensional Strained Heteroepitaxial Growth using Kinetic Monte Carlo,” *Communications in Computational Physics* **10** *(2011) 1089-1112.*

T.P. Schulze and P. Smereka, “ An Energy Localization Principle and its Application to Fast Kinetic Monte Carlo Simulation of Heteroepitaxial Growth,” *Journal of the Mechanics and Physics of Solids* **57** (2009) 521-538.

M. Saum, T.P. Schulze and C. Ratsch, “Inverted List Kinetic Monte Carlo with Rejection Applied to Directed Self-Assembly During Epitaxial Growth,” *Communications in Computational Physics* **6** (2009) 553-564.

M. Saum and T.P. Schulze, “The Role of Processing Speed in Determining Step Patterns during Directional Epitaxy," *Discrete and Continuous Dynamical Systems B* **11** *(2009) 443-457.*

T.P. Schulze, “Simulation of Dendritic Growth using Kinetic Monte Carlo,” *Physical Review E* **78** (2008) *:* Art. No. 020601(R) .

T.P. Schulze, "Efficient Kinetic Monte Carlo Simulation," *Journal of Computational Physics* **227** *(2008) 2455-2462.*

P. Zoontjens, T.P. Schulze and S. Hendy, “Hybrid Method for Modeling Epitaxial Growth: Kinetic Monte Carlo plus Molecular Dynamics,” *Physical Review B* ***76*** (2007): Art. No. 245418.

W. Guo, T.P. Schulze, and Weinan E, “Simulation of Impurity Diffusion in a Strained Nanowire Using Off-lattice KMC,” *Communications in Computational Physics* **2** (2007) 164-176.

T.P. Schulze, “Morphological Instability during Directional Exitaxy,” *Journal of Crystal Growth* **296** (2006) 188-201.

D.M. Anderson and T.P. Schulze, “Linear and Nonlinear Convection in Solidifying Ternary Alloys,” *Journal of Fluid Mechanics* **545** (2005) 213-243.

T.P. Schulze and M.G. Worster, "A Time-Dependent Formulation of the Mushy Zone Free Boundary Problem," *Journal of Fluid Mechanics* **541** (2005) 193-202.

T.P. Schulze, "A Hybrid Method for Simulating Epitaxial Growth," *Journal of Crystal Growth* **263** (2004) 605-615.

T.P. Schulze, P. Smereka and Weinan E, "Coupling Kinetic Monte-Carlo and Continuum Models with Application to Epitaxial Growth," *Journal of Computational Physics* **189** (2003) 197-211.

T.P. Schulze, "Kinetic Monte-Carlo with Minimal Searching," *Phys. Rev. E* **65** (2002) Art. No. 036704.

T.P. Schulze and M.G. Worster, "Mushy Zones with Fully Developed Chimneys," *Interactive Dynamics of Convection and Solidification,* edited by P. Ehrhard Kluwer Academic Publishers (2001) 71-80.

T.P. Schulze and Weinan E, "A Continuum Model for Epitaxial Growth," *Journal of Crystal Growth* **222** (2001) 414-425.

T.P. Schulze, "A Note on Subharmonic Instabilities," *Physics of Fluids* **11** no.12 (1999) 3573-3576.

T.P. Schulze and R.V. Kohn, "A Geometric Model for Coarsening During Spiral-Mode Growth of Thin Films," *Physica D* **132** (1999) 520-542.

T.P. Schulze and M.G. Worster, "Weak Convection, Liquid Inclusions and the Formation of Chimneys in Mushy Layers," *Journal of Fluid Mechanics* **388** (1999) 197-215.

T.P. Schulze and M.G. Worster, "A Numerical Investigation of Steady Convection in Mushy Layers During the Directional Solidification of Binary Alloys," *Journal of Fluid Mechanics* **356** (1998) 199-220.

T.P. Schulze and S.H. Davis, "Shear Stabilization of a Solidifying Front: Weakly Nonlinear Analysis in a Long-Wave Limit," *Physics of Fluids* **8** no. 9 (1996) 2319-2336.

S. H. Davis and T.P. Schulze, "Effects of Flow on Morphological Stability During Directional Solidification," *Metallurgical and Materials Trans. A---Physical Metallurgy and Material Science* **27** no. 3 (1996) 583-593.

S.H. Davis and T.P. Schulze, "Shear Stabilization of a Solidifying Front," *Proc. 3rd Microgravity Fluid Physics Conf.* (1996).

M.G. Worster, D.M. Anderson and T.P. Schulze, "Nonlinear Convection in Mushy Layers," *Proc. 3rd Microgravity Fluid Physics Conf.* (1996).

T.P. Schulze and S.H. Davis, "Shear Stabilization of Morphological Instability During Directional Solidification," *Journal of Crystal Growth* **149** (1995) 253-265.

T.P. Schulze and S.H. Davis, "The Influence of Oscillatory and Steady Shears on Interfacial Stability During Directional Solidification," *Journal of Crystal Growth* **143** (1994) 317-333.

S.H. Davis and T.P. Schulze, "Shear Stabilization of Solidification Fronts," *Proc. 2nd Microgravity Fluid Physics Conf.* (1994) 181-186.

Volumes edited:

T.P.Schulze, X. Feng, V. Alexiades and T. Tang, editors, “Multiscale Modeling and Simulation in Materials Science,’’ *Proceedings of the 2007 John H. Barrett Memorial Lectures, Journal of Scientific Computing,* **37,** 2008.

Xiaobing Feng and Tim P. Schulze, editors, "Recent Advances in Numerical Methods for Partial Differential Equations and Applications," *Proceedings of the 2001 John H. Barrett Memorial Lectures, Trends in Computational Mathematics*, May 10-12, 2001, The University of Tennessee.

Grants:

2016 NSF DIVISION OF MATHEMATICAL SCIENCES, Applied Mathematics, $245,180 (3 years)
“Kinetic Monte Carlo Simulation of Nanoalloy Crystal Growth”

2011 NSF DIVISION OF MATHEMATICAL SCIENCES, Applied Mathematics, $211,763 (3 years)
“Kinetic Monte Carlo Modeling and Simulation of Phase Boundaries and Polycrystals”

2009 UTK/ORNL Joint Institute for Advanced Materials (JIAM) Seed Project Proposal, with Z. Zhang (Physics), J. Shen (Physics) and W. Zhu (Physics), $35,000
“*Development of Dynamic -Zone Monte Carlo (DZ-KMC) Simulations for Predictive Modeling of Interface Evolution During Nonequilibrium Growth”*

2009 NSF DIVISION OF MATHEMATICAL SCIENCES, with P. Smereka (Michigan) and V. Shenoy (Brown), Applied Mathematics, $1,006,764 (3 years)
“FRG: Modeling and Computation of Crystalline Nanostructures”

2007 NSF DIVISION OF MATHEMATICAL SCIENCES, Applied Mathematics, $126,068 (3 years)
“Fast Kinetic Monte Carlo Simulation of Crystal Growth and Evolution”

2007 NSF Conference Proposal with Alexiades and Feng, Computational Mathematics, $15,000
“Conference proposal: Multi-Scale Modeling and Simulation in Materials Science ”

2004 NSF DIVISION OF MATHEMATICAL SCIENCES, Applied Mathematics, $115,352 (3 years)
“The mushy-zone free-boundary problem”

2003 DEPARTMENT OF ENERGY, $400,000 (5 years)
“Integrated multiscale modeling of molecular computing devices”

2001 NSF DIVISION OF MATHEMATICAL SCIENCES, Applied Mathematics, $76,000 (3 years)
“Modeling, simulation and analysis of epitaxial film growth”

Post docs:
Weidong Guo (spring 04 – spring 05),Mike Saum (fall 06 – spring 08), Henry Boateng (fall 2010-spring 2013)

Current and former PhD students:
John Hicks (Ph.D. Summer 2020), Khoa Dinh (Ph. D. Spring 2019), Hamza Ruzayqat (Ph.D. Spring 2018), Tim Krumweide (Ph.D. Spring 2017), Kyle Golenbiewski (Ph.D. Spring 2016), Holly Clark (Ph.D. Spring 2014), Nick Gewecke (Ph. D. Spring 2011), Hua Chen (Physics, joint with Zhenyu Zhang, Spring 2012).

Current and former Masters students:
Dragos Ilas (masters Fall 2014), Aaron Craig (Spring 2015), Kevin Huerto (Spring 2022)

Honors Thesis students:

Presentations:

7/21 SIAM annual meeting, online.
2/20 Institute for Theoretical Geophysics Seminar, University of Cambridge, Cambridge, UK
10/19 Numerical Analysis Seminar, Worcester Polytechnics Institute
3/19 Applied and Comp. Math. Seminar, U. of South Carolina, Columbia, SC
7/18 Particle-based Methods in Materials Science, Edinburgh, Scotland
Invited Talk: *Lattice and off-lattice kinetic Monte Carlo*
7/18 Advances in Applied & Computational Mathematics: In Memory of Peter Smereka, Ann Arbor, MI
Invited Talk: *In Memory of Peter Smereka: Kinetic Monte Carlo---A Look Back and a Step Forward*
5/18 CNLS 38th Annual Conference Rate Theory and Long Timescale Simulations, Santa Fe, NM
Invited Talk: *A Rejection Scheme for Off-Lattice Kinetic Monte Carlo*
11/17 Materials Research Society Fall Meeting, Boston.
10/16 Physics Colloquium, Oakland University, Rochester, MI
9/16 Junior Colloquium, University of Tennessee
6/16 The Magma/Mantle Dynamics of Earth, Isaac Newton Institute, Cambridge, UK
Invited Talk: *The rapid advance and slow retreat of a mushy zone*
5/16 SIAM Meeting of Material Science, Philadelphia, PA
Materials Defects session
5/16 SIAM Meeting of Material Science, Philadelphia, PA
Peter Smereka memorial session
6/15 Materials Defects Reunion Conference, Lake Arrowhead, CA
Invited Talk: *Crystal growth shapes in bond-counting and continuum models*
12/14 IAS Multiscale Modeling & Simulation of Defect Problems in Materials Science, Hong Kong
Invited Talk: *A degenerate Ising model for atomistic simulation of crystal-melt interfaces*
10/14 The 7th International Conference on Multiscale Materials Modeling, Berkeley, CA
6/14 Materials Defects Reunion Conference, Lake Arrowhead, CA
Invited Talk: *A degenerate Ising model for atomistic simulation of crystal-melt interfaces*
6/14 IPAM Reunion Conference joint session, Lake Arrowhead, CA
Invited Talk: *The mathematics of poker*
6/13 SIAM Meeting of Material Science, Philadelphia, PA
5/13 Applied Mathematics Seminar, University of Delaware
2/13 SIAM Conference on Computational Science and Engineering, Boston, MA
12/12 Materials Defects Culminating Workshop, Lake Arrowhead, CA
10/12 Workshop II: Atomistic and Mesoscale Modeling of Materials Defects, UCLA
9/12 Materials Defects: Mathematics, Computation, and Engineering (Tutorials), UCLA
5/12 Heterostructured Nanocrystalline Materials Workshop, ICERM/Providence
12/11 Applied Mathematics Seminar, Purdue
7/11 7th International Congress on Industrial and Applied Mathematics, Vancouver, Canada (mini-symposium)
6/11 Coarse-Graining of Many-Body Systems: Analysis, Computations and Applications, Heraklion Crete, Greece
Invited Talk: *Simulation of three–dimensional strained heteroepitaxial growth using kinetic Monte Carlo*
3/11 Junior Colloquium, University of Tennessee
1/11 Multiscale Simulation of Heterogeneous Materials & Coupling of Thermodynamic Models, Leuven, Belgium
Invited Talk: *Kinetic Monte Carlo simulation of heterostructured nanocrystalline growth*
7/10 9th World Congress on Computational Mechanics, Sydney (minisymposium)
5/10 SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia (minisymposium)
3/10 AMS Spring Southeastern Sectional Meeting, Lexington, KY
11/09 6th Annual Clusters and Nanoparticles Meeting, Lake Tekapo, New Zealand
Invited Talk: *Kinetic Monte Carlo Simulation of Quantum Dots*
10/09 Dept. of Chemical and Biomolecular Engineering Graduate Seminar, UTK
10/09 2nd US-China Workshop on Nanostructured Materials for Global Energy & Environmental Challenges Changzhou, China
8/09 The 17th American Conference on Crystal Growth and Epitaxy, Lake Geneva, WI
Invited talk: *Using Kinetic Monte Carlo to Simulate Dendritic Growth*
5/09 Eurotherm Seminar 84: Thermodynamics of Phase Change, Namur, Belgium.
7/08 Applied Mathematics Colloquium, Northwestern University
7/08 8th World Congress on Computational Mechanics, Venice
6/08 Bridging Time & Length Scales in Materials Science & Bio-Physics Reunion Conf., IPAM

Invited talk: *Simulation of Dendritic Growth using Kinetic Monte Carlo*
5/08 SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia
3/08 Applied Mathematics & Computation Seminar, University of Massachusetts, Amherst
12/07 Mathematical & Computational Nanoscience Workshop, Victoria Univ., Wellington, New Zealand
Invited Talk: *Extending the Capabilities of Kinetic Monte Carlo*
11/07 AMS Regional Meeting, Middle Tennessee State University, Murfreesboro, TN.
7/07 6th International Congress on Industrial & Applied Mathematics, Zurich (minisymposium)
6/07 Bridging Time & Length Scales in Materials Science & Bio-Physics Reunion Conf., IPAM
Invited talk: *Efficient Kinetic Monte Carlo*
11/06 Differential Equations and Computational Math Seminar, University of Tennessee
11/06 Junior Colloquium, University of Tennessee
10/06 Meeting on Kinetic Monte Carlo and Micro Fluidics, Princeton
Invited talk: *KMC with O(1) Event Selection*
05/06 Applied Mathematics Seminar, Courant Institute, New York University
04/06 Mechanical and Aerospace Engineering Seminar, Princeton
04/06 Applied Math Colloquium, New Jersey Institute of Technology
02/06 Nanotechnology Seminar, Industrial Research Limited, Wellington, New Zealand
01/06 Applied and Interdisciplinary Mathematics Seminar, University of Michigan
11/05 IPAM Multiscale Analysis and Computation Workshop, IPAM, University of California, Los Angeles
Invited talk: *Kinetic Monte Carlo: Building a Bridge to Larger Length Scales*
10/05 IPAM Applicable Mathematics Seminar, IPAM, University of California, Los Angeles
5/05 Materials Science Seminar, IMA, University of Minnesota
11/04 Workshop on Nanoscale Material Interfaces: Experiment, Theory & Simulation, Nat. Univ of Singapore
Invited talk: *Off-Lattice Kinetic Monte Carlo Simulation*
5/04 SIAM Meeting on Material Science, Los Angeles (minisymposium)
5/04 Applied Math & Computational Science Seminar, NIST, Gaithersburg, Maryland
10/03 Bio-math Seminar, Vanderbilt University
9/03 Applied Mathematics Colloquium, Northwestern University
8/03 Workshop on Continuum Models for Epitaxial Growth, CEASAR research institute , Bonn
Invited talk: *Coupling Kinetic Monte Carlo and Continuum Models with Applications to Epitaxial Growth*
7/03 5th International Congress on Industrial & Applied Mathematics, Sydney (minisymposium)
5/03 SIAM Conference on Applications of Dynamical Systems, Snowbird, Utah (minisymposium)
3/03 Materials Science and Engineering Seminar, University of Tennessee
11/02 Mathematics Seminar, University of Tennessee
5/02 Fronts, Fluctuations and Growth Conference, University of Michigan
Invited talk: *Simulating Epitaxial Growth*
2/02 Applied Mathematics Seminar, Courant Institute, New York University

Miscellaneous service activities:

2018 Main organizer for “Particle Based Methods in Materials Science” meeting at ICMS in Edinburgh.

*2017,*2012, 2009, 2007, 2005, 2003 Served on NSF review panels

2016 Organizer for SIAM materials meeting memorial sessions in honor of Peter Smereka

2015 Organizer for IPAM ``Material Defects'' second reunion conference.

2014 Organizer for IPAM “Materials Defects” reunion conference.

2011-12 Co-chair of organizing committee for IPAM long program “Materials Defects: Mathematics, Computation, and Engineering”

2012 Co-organized ICERM workshop on “Heterostructured Nanocrystalline Nanomaterials”

2010 Co-organized mini-symposium at 2010 SIAM meeting in Philadelphia

2009 2nd US-China Workshop on Nanostructured Materials for Global Energy and Environmental Challenges, NSF sponsored workshop in Suzhou, October 17-18, 2009.

2009 Co-organizing mini-symposium at 2010 SIAM materials meeting in Philadelphia

2008 Supervised Fulbright New Zealand student Dmitri Schebarchov

2007-2008 Coedited 2007 Barrett Lectures proceedings

2007 co-organized (with S Hendy) nanotechnology meeting in Wellington, NZ for Dec 2007

2007 Co-organized mini-symposium at 2007 ICIAM meeting in Zurich

2007 Barrett Lectures (conference held at UT, Knoxville) organizing committee chair

2006-2012 Editorial board of *Discrete and Continuous Dynamical Systems B*

Review of manuscripts for various journals (e.g. *Journal of Fluid Mechanics, Journal of Computational Physics, Journal of Crystal Growth,* ...)