Eric Barth

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Research Interests

Scientific Computing

- Biomolecular modeling and simulation
- Numerical algorithms for statistical mechanics
- Computational Musicology

Education

PostDoc 1994-1997 Courant Institute and NYU Chemistry, with Tamar Schlick
Ph.D. 1994 University of Kansas, Mathematics, with R. Byers and B. Leimkuhler
M.A. 1991 University of Kansas, Mathematics, with John Bunce
B.Mus. 1986 University of Kansas, Saxophone

Publications

[13] Barth, E., "Composing" , "Harmonics", "Scales", "Geometry of Music", "Wind Instruments", "Percussion Instruments", Essays in Encyclopedia of Mathematics and Society, Sarah Greenwald and Jill Thomley, editors, Salem Press, (2011)

[12] Cardenas, A., and Barth, E., Extending the Timescale in Atomically Detailed Simulations, Reviews in Computational Chemistry, Kenny B. Lipkowitz and Thomas R. Cundari, Eds., VCH Publishers, New York, Vol. 26, pp. 367–420, (2008)

[11] Barth, E.J., Leimkuhler, B.L., Sweet, C.R., Approach to Thermal Equilibrium in Biomolecular Simulation, Lecture Notes In Computer Science and Engineering, Volume 49, pp. 125–139 (2006)

[10] Barth, E.J., Laird, B.B., Leimkuhler, B.L., Generating Generalized Distributions from Dynamics Simulation, *Journal of Chemical Physics*, 118: 5759–5768 (2003)

[9] Barth, E., Leimkuhler, B. and Reich, S., A Test Set for Molecular Dynamics, Computational Methods for Macromolecules: Challenges and Applications, Tamar Schlick and Hin Hark Gan, editors, Lecture Notes in Computational Science and Engineering volume 24, Springer. pp. 73–103 (2002),

[8] Benner, P., Byers, R. and Barth, E., Fortran 77 Subroutines for Computing the Eigenvalues of Hamiltonian Matrices I: The Square-Reduced Method, *ACM Transactions on Mathematical Software*, 26:49–77 (2000)

[7] Barth, E., Leimkuhler, B. and Reich, S., A Semi-Explicit, Time-Reversible, Variable-Stepsize Integrator for Constrained Dynamics, *SIAM Journal of Scientific Computing*, 21:1027-1044 (1999)

[6] Barth, E. and Schlick, T., Overcoming Stability Limitations in Biomolecular Dynamics: Combining Force Splitting via Extrapolation with Langevin Dynamics in LN. *Journal of Chemical Physics*, 109: 1617-1632 (1998)

[5] Barth, E. and Schlick, T., Extrapolation versus Impulse in Multiple-Timestepping Schemes: Linear Analysis and Applications to Newtonian and Langevin Dynamics. *Journal of Chemical Physics*, 109: 1633-1642 (1998)

[4] Schlick, T., Barth, E., and Mandziuk, M., Biomolecular Dynamics at Long Timesteps: Bridging the Timescale Gap Between Simulation and Experimentation, in *Annual Review of Biophysics and Biomolecular Structure*, Volume 26, Robert M. Stroud, Editor (1997).

[3] Barth, E., Mandziuk, M. and Schlick, T., A Separating Framework for Increasing the Timestep in Molecular Dynamics, in *Computer Simulation of Biomolecular Systems: Theoretical and Experimental Applications*, Volume 3, W.F. van Gunsteren, P.K. Weiner and A. J. Wilkinson, Editors, ESCOM, Leiden, The Netherlands, (1996).

[2] Barth, E. and Leimkuhler, B., Symplectic Methods for Conservative Multibody Systems, in *Integration Algorithms for Classical Mechanics*, Fields Institute Communications, vol. 10, pp. 25–43, American Mathematical Society, (1996).

[1] Barth, E., Kuczera, K., Leimkuhler, B. and Skeel, R.D., Algorithms for Constrained Molecular Dynamics, *Journal of Computational Chemistry* 16:1192–1209 (1995).

Employment

Mathematics and Computer Science Department Chair
Kalamazoo College, 2006–present

Professor of Mathematics
Kalamazoo College, 2010–present

Courses Taught:

- Quantitative Reasoning
- Calculus I, II and III
- Intermediate Calculus
- Linear Algebra I and II
- Differential Equations and Numerical Methods
- Complex and Vector Variables
- Real Analysis I
- Probability
- Mathematical Statistics
- Special Topics: Numerical Methods
- Special Topics: Numerical Methods in Environmental Modeling
- Introductory Physics 1, discussion and lab sections
- Introductory Physics 2, discussion and lab sections
- Thermal Physics with Lab

College and Community Service: * indicates chairmanship

- Educational Policies Committee, 2002-2003, 2003-2004*, 2013-2015
- Board Member, National Alliance of El Sistema Inspired Programs (El Sistema U.S.A.). 2013-2014
- President, Kalamazoo Junior Symphony Board of Directors, 2008-2011*
- Faculty Personnel Committee, 2006-2008, 2008-2012*
- Chinese Search Committee, 2009, 2012
- Department Chair, Mathematics and Computer Science, 2005-present*
- Mathematics Search Committee, 2005-2006*, 2006-2007*, 2007-2008*, 2009*, 2012*
- Faculty Development Committee, 2005-2006*
- Division Chair, Natural Sciences and Mathematics, 2003-2004*
- College Forum Committee, 1998-2002
- Art Search Committee, 1999
- Statistics Search Committee, 1998-1999,
- Mathematics Search Committee, 1998-1999, 2002
- Computer Science Search Committee, 1999, 2002, 2004
- Luce Professor Search Committee, 2001
- Howard Hughes Medical Institute Grant Steering Committee, 2000-present
- HHMI proposal working group, 1999
- Henry R. Luce proposal working group, 2000
- First Year Experience panelist, 2000
- New faculty orientation speaker, 1998, 1999

Curriculum Director, Kalamazoo Kids in Tune
Kalamazoo Symphony Orchestra, 2012–present

Design curriculum integrating math, music, humanities for an intensive after-school orchestra immersion program serving 85 elementary students each year
Compose and arrange music for student symphony orchestra
Lead student orchestra in rehearsals and performances

GLCA New Directions Initiative Faculty Liaison
Kalamazoo College, 2012–2015

Associate Professor of Mathematics
Kalamazoo College, 2003–2010

Natural Science and Mathematics Division Chair
Kalamazoo College, 2003–2004

Assistant Professor of Mathematics
Kalamazoo College, 1997–2003

Subject Matter Expert
McGraw-Hill Higher Education, 2006-2012

Check accuracy of online mathematics courses
Compose narration notes for online mathematics courses
Develop lesson plans and learning objectives
Coordinate online resources with traditional paper textbooks

Faculty Consultant
The College Board A.P. Calculus Reading, 2001

Honorary Academic Visitor
University of Leicester, England, 2001, 2004

Howard Hughes Medical Institute Research Associate
Courant Institute of Mathematical Sciences and Department of Chemistry,
New York University, 1994–1997

Grants and Awards

- Great Lakes Colleges Association New Directions Initiative Grant, 2010, 2011
- Mellon Strategic Planning Grant, 2009
- Howard Hughes Medical Institute, curriculum grant, 2006-2007
- Dr. Winthrop S. and Lois A. Hudson Award, Kalamazoo College, 2004
- Sabbatical Leave, Kalamazoo College, 2004
- National Institutes of Health, NIGMS AREA research grant, 2003-2006
- Petroleum Research Fund, research grant, 2001-2004
- Howard Hughes Medical Institute, curriculum grant, 2000-2003
- American Mathematical Society Project NExT Fellow, 1998-1999
- Pharmacia and Upjohn, research grant, 1998-2000
- Faculty/Student Grant for developing online resources, Kalamazoo College, 1997
- Kalamazoo College Faculty Development Travel awards,
  1998-1999, 1999-2000, 2000-2001, 2001-2002, 2004, 2010, 2014

Current Projects

- Computer simulation of molecular flexibility in drug transport
- Generalized Density Dynamics
- New generation thermostatting techniques in molecular modeling
- Computational approaches to musicological analysis
- Assessment of student outcomes with web-based Calculus Mastery Exams

Software Developed

- ChemSolver: A MATLAB simulation environment for chemical reaction kinetics.
- Extensive algorithm development in CHARMM (Chemistry at HARvard Molecular Modeling): Langevin Normal mode (LIN/LN) dynamics, TNPACK truncated Newton minimization, and efficient nonlinear solvers for constrained molecular dynamics in Fortran 77.
- CSHAKE: A C language simulator for elastic rod dynamics, incorporating advanced timestepping schemes for constrained dynamics. (with B. Leimkuhler)
- MBLab: Toolbox for Conservative Multibody Dynamics in MATLAB.
- Fortran 77 implementations of the structure preserving eigenvalue algorithms HAMEV and SQRED (with P. Benners and R. Byers) in SLICOT numerical algorithms library
- LORAX: Parallel software for large banded symmetric eigenvalue problems, Fortran 77 with multiprocessor compiler directives.

Presentations and Media Appearances

- Television, WGVU "Kalamazoo Lively Arts", 2015
- Radio, WMUK hour-long live interview with Cara Lieurance, 2015
- Television, Kalamazoo Public Media Network "K-12 360", 2015
- Conference Talk, MAA Michigan Section, 2014
- Conference Talk, Michigan After-School Association Summer Summit, with Artrella Cohn, Lansing, 2013
- Online Media, Huffington Post, "Kids in Tune, Kalamazoo Music Program Changes Lives One Note At A Time", 2013
- Conference Talk, Michigan After-School Associations Collaborative Conference, with Elizabeth Youker, Kalamazoo, 2012
- Colloquium Talk, Albion College, 2011
- Colloquium Talks, Kalamazoo College, 2010
- Colloquium Talk, Calvin College, 2010
- Faculty Panel Discussion, "The Two Cultures", Kalamazoo College, 2009
- Colloquium Talks, Kalamazoo College, 2009
- "Molecular Dynamics Tutorial", Institute for Mathematics and its Applications, Minneapolis, 2007
- Invited Talk, Workshop on Molecular Modeling, Notre Dame, 2005
- Invited Talk, Banff International Research Station, 2005
- Applied Math Colloquium Talk, Purdue University, 2005
- Applied Math Seminar, University of Leicester, UK 2004
- Invited Talk, 4th Intl. Workshop on Methods in Macromolecular Modeling, Leicester, 2004
- Computational Neuroscience Seminar, KFKI, Budapest, 2001
- Applied Mathematics Seminar, University of Leicester, UK, 2001
- "Town and Gown" presentation for Lord Mayor of Leicester, 2001
- Minisymposium Talk, Intl. Conf. on Computer Science, San Francisco, 2001
- Seminar Talk, University of Michigan, 2000
- Poster, 3rd Intl. Workshop on Methods in Macromolecular Modeling, New York, 2000
- Invited Talk, Applicable Maths Seminar, University of Leicester, UK, 2000
- Invited Talk, CECAM Geometric Integrators Workshop, Lyon, France, 2000
- Mathematics Department Colloquium, Kalamazoo College, 2000
- Seminar Talk, University of Kansas, 1999
- Faculty Study Talk, Kalamazoo College, 1999
- Colloquium Talk, Alma College, 1998
- Invited Talk, Texas Tech University, 1997
- Invited Talk, Hofstra University, 1997

- Meeting Organizer, HPCC Grand Challenge Application Group, New York, 1996
- Minisymposium Presentation, SIAM Annual Meeting, Kansas City, 1996
- Invited Talk, Ellis B. Stouffer Colloquium, University of Kansas, 1996
- Session Organizer, HPCC Grand Challenge Application Group, Champaign, 1995
- Invited Talk, Multigrid Workshop, Weizmann Institute of Science, Israel, 1995
- Minisymposium Presentation, SciCADE '95, Stanford University, 1995
- Invited Talk, HPCC Grand Challenge Application Group, Yale University, 1994
- Invited Talk, Kansas Workshop on Algorithms for Macromolecular Modeling, 1994
- Minisymposium Presentation, SIAM Annual Meeting, San Diego, 1994
- Biomathematics Seminar, Courant Institute, New York University, 1994
- Physical Chemistry Colloquium, University of Kansas, 1994
- Contributed Talk, MAA Kansas Section Meeting, 1994 — *best paper award*
- K.I.T.C.S. Seminar, 1994
- Contributed Talk, First MATLAB Conference, Cambridge, 1993
- Wavelet and Multigrid Seminar, University of Kansas, 1993.