CURRICULUM VITAE (FULL VERSION) September 2019

Thomas E. Cheatham, III

http://scholar.google.com/citations?user=fCEXKK4AAAAJ&hl=en

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Education and Work Experience

Professor 7/14 to present
Department of Medicinal Chemistry, Director of Graduate Studies (FY 2014-2017)
College of Pharmacy, University of Utah

Director, Research Computing / Center for High Performance Computing 7/14 to present
University Information Technology, University of Utah

Associate Professor (with tenure) and Director of Graduate Studies (DOG) 7/11 to 7/14
Department of Medicinal Chemistry
College of Pharmacy, University of Utah

Associate Professor (with tenure) 7/09 to 7/11
Assistant Professor 7/02 to 7/09
Department of Medicinal Chemistry (60%)
Department of Pharmaceutics and Pharmaceutical Chemistry (40%)
College of Pharmacy, University of Utah

Adjunct Professor 7/19 to 7/22
Adjunct Associate Professor 7/09 to 7/19
Adjunct Assistant Professor 7/00 to 7/09
Department of Biomedical Engineering (formerly Dept. of Bioengineering)
University of Utah

Research Assistant Professor, Department of Medicinal Chemistry, U Utah 1/00 to 7/02

National Research Council Research Associate 3/97 to 12/99
Laboratory of Biophysical Chemistry, NHLBI
National Institutes of Health **Advisor: Bernard R. Brooks**

PhD in Pharmaceutical Chemistry 9/90 to 3/97
Department of Pharmaceutical Chemistry
University of California at San Francisco **Advisor: Peter A. Kollman**

Programmer/Analyst 6/88 to 8/90
Aiken Computation Laboratory, Division of Applied Sciences
Harvard University

Middlebury College, Middlebury Vermont **March 1989**

B.A. Chemistry (honors)
Thesis: The Structure of Function of the Active Oxygen Intermediate of Cytochrome P450

B.A. Mathematics and Computer Science
Senior Project: The Fourier Transform and Applications in Digital Signal Processing

Minor: Personality and Social Psychology

Active Grants

- **National Institutes of Health, R01-GM-081411-06** 9/23/19-8/30/23
  Biomolecular simulation for the end-stage refinement of nucleic acid structure
  PI: Cheatham

  Core NIH grant for assessment, validation and improvement of force fields for nucleic acids and experimental and computational ensembles of model RNA systems.

- **National Science Foundation, OAC-1919667** 10/01/19-9/30/22
  MRI: Development of ACCORD, a Community Cyberinstrument for Broadening Access to Research on Sensitive Data
  PI: Ron Hutchins, Co-PIs: Sosonkina, Crawford, Midkiff, and Cheatham.

  This $2.5M equipment grant is for a compute infrastructure for U of Virginia for research on protected or sensitive data and Cheatham serves as a consultant.

- **National Science Foundation, OAC-1659425** 4/01/17-3/31/20
  CC Cyber Team: Creating a Community of Regional Data and Workflow Cyberinfrastructure Facilitators*
  PI: Hauser, Co-PIs: Burns, Williams, Siegel, and Cheatham.

  This is a collaborative grant for data facilitation in the region with Colorado State U and U Colorado Boulder as partners.

- **National Science Foundation, ACI-1443054** 10/01/14-9/30/19
  CIF21 DIBBS: Middleware and high performance analytics libraries for scalable data science.
  PI: Fox, Co-PIs: Wang, Qiu, Jha, Marathe; Cheatham is significant personnel.

  This is a data infrastructure building blocks award for the development of SPIDAL (spidal.org) and middleware. In no-cost-extension.

Completed Grants (Utah)

- **National Science Foundation, ACI-1515572** 9/01/15-7/31/19
  PRAC – Ensembles of molecular dynamics engines for assessing force fields, conformational change, and free energies of proteins and nucleic acids.
  PI: Cheatham, Co-PIs: Simmerling (Stony Brook U), Roitberg (UFl), and Case (Rutgers)

  This travel award allowed requests for allocations on Blue Waters and the team was awarded 12 million node hours on Blue Waters per year for three years. Currently in no cost extension.

- **National Institutes of Health, S10OD021644** 4/01/17-3/30/18
  From genomics to natural language processing: A protected environment for research computing in the health sciences.
  PI: Cheatham.

  This is a major equipment grant to replacement of the protected environment for restricted data at Utah.

- **National Science Foundation, ACI-1341935** 3/01/14-8/31/18
  Advanced Cyberinfrastructure – Research and Educational Facilitation: Campus-based computational research support.
  PI: Bottum (Clemson), Co-PIs: Jacobs (Hawaii), Wilson (Wisconsin), Cuff (Harvard), Dougherty (USC).

  This award supporting facilitators at six universities and advocated for the need for research computing and data facilitation on campuses; http://aci-ref.org. Cheatham PI of subcontract to U of Utah and PI Chair 2016-2018.

- **National Science Foundation, CNS-1338155** 8/30/13-6/30/17
  MRI: Development of Apt, A Testbed Instrument with Adaptable Profiles for Network and Computational Science.
  PI: Ricci, Co-PIs: Facelli, Cheatham, Eide, van der Merwe

  This major research equipment grant is for the bare metal testbed hardware Apt. In no cost extension.

- **NSF Cyberinfrastructure Partnership / TeraGrid / XSEDE** 10/01/16-9/30/17
  XRAC/LRAC MCA01S027: Insight into biomolecular structure, dynamics, interactions and energetics from simulation.
  PI: Cheatham, Computer time award: ~7M core hours awarded in 2017, award since 2002.

- **National Science Foundation, ACI-1521728** 4/01/15-3/31/17
  RAPID: Optimizing experimental approaches to Ebola membrane fusion inhibitor peptide design through high-throughput biomolecular simulation workflows on Blue Waters. PI: Cheatham

  Computational protein design using simulation of Ebola membrane fusion inhibitor peptides.

- **National Science Foundation, ACI-1341034** 10/01/13-9/30/16
  CC-NIE Integration: Science slices converting network research innovation into enhanced capability for computational science and engineering at the University of Utah.
  PI: Cheatham, Co-PIs: Bolton, van der Merwe, Ricci

  Development of a research computing and data science DMZ to bypass campus firewalls for large scale data transfers.

- **National Science Foundation, CHE-1266307** 10/01/13-9/30/16
  CDS&E: Tools to facilitate deeper data analysis, exploration, management, and sharing of ensembles of molecular dynamics trajectory data.
  PI: Cheatham

  Development of software and tools for annotating, analyzing, managing and sharing of ensembles of molecular dynamics simulation data.

- **National Institutes of Health, R01 GM098102** 9/30/11-8/31/16
  RNA-ligand interactions: simulation and experiment.
  M-PIs: Cheatham, Kathleen Hall (Wash U, contact), Carlos Simmerling (Stony Brook).

  Combined experiment and theory to understand RNA and RNA-ligand interactions.

- **National Science Foundation, OCI-1440031** 9/01/14-8/31/16
  PRAC – Hierarchical molecular dynamics sampling for assessing pathways and free energies of RNA catalysis, ligand binding, and conformational change.
  PI: Cheatham, Co-PIs: Simmerling (Stony Brook U), Roitberg (UFl), Case (Rutgers), and York (Rutgers)

  This travel award allowed requests for allocations on Blue Waters and the team was awarded 7 million node hours on Blue Waters for half of 2014-2015.

- **National Science Foundation, OCI-1036208** 2/01/11-9/30/15
  PRAC – Hierarchical molecular dynamics sampling for assessing pathways and free energies of RNA catalysis, ligand binding, and conformational change.
  PI: Cheatham, Co-PIs: Simmerling (Stony Brook U), Roitberg (UFl), and York (Rutgers)

  This travel award allowed requests for allocations on Blue Waters and the team was awarded 14 million node hours on Blue Waters in 2013-2014.

- **National Institutes of Health, R01 GM074249** 1/01/11-12/31/14
  P450-mediated dehydrogenation mechanisms.
  PI: Gary Yost, Co-PIs: Cheatham, Reilly

- **National Institutes of Health, R01 GM081411** 2/01/08-1/31/14
  Biomolecular simulation for the end-stage refinement of nucleic acid structure.
  PI: Cheatham. No cost extension 2013-2014.
- **Pittsburgh Supercomputing Center, PSC12038P** 11/01/12-7/31/13
  Converging simulations of a DNA duplex and explorations of a DNA minicircle on the microsecond timescale using MD on Anton
  PI: Cheatham, Computer time award: 100,000 hours on DE Shaw's Anton machine.
- **National Institutes of Health, R01 GM079383** 9/28/07-8/31/12
  AMBER force field consortium: A coherent biomolecular simulation platform.
  PI: Yong Duan (UC Davis)
  Co-PIs: Cheatham, Carlos Simmerling (Stony Brook), Ray Luo (UC Irvine), Piotr Cieplak (Burnham Inst), Junmei Wang (Incisive, Inc.).
- **Pittsburgh Supercomputing Center, PSCA00033P** 4/01/11-12/31/11
  Molecular dynamics of DNA and protein-DNA complexes: A proposal for obtaining microsecond trajectories using Anton.
  PI: Cheatham, Computer time award: ~50K node hours awarded in 2011 on DE Shaw's Anton machine at PSC supported by an NIH Go grant. This will support the ABC consortium.
- **Pittsburgh Supercomputing Center, PSCA00067P** 4/01/11-12/31/11
  Development and testing of improved fixed-charge force fields for proteins
  PI: Case, Co-PIs: Cheatham, Simmerling, Merz. Computer time award: ~50K node hours awarded in 2011 on DE Shaw's Anton machine at PSC supported by an NIH Go grant.
- **DARPA, BAA-09-29** 4/01/10-3/31/11
  Modeling and optimization of hemostatic peptide sequences for SAIC Wound Stasis System, sub-contract to *Rapid hemostasis via a wound-targeting nanodelivery system.*
  Sub-contract PI: Darrell Davis, Co-PI: Cheatham
- **Office of Naval Research, N00014-05-1-0457** 4/01/05-9/30/08
  A new research tool for the computer simulation of chemical dynamics in complex systems.
  PI: Greg Voth (Chemistry); Co-PIs: Cheatham (10%), Dave Case (Scripps), Bill Miller (Berkeley) and Bernie Schlegel (Wayne State).
- **University of Utah, PID2502088.** 6/1/05-5/31/06
  Funding Incentive Seed Grant: Integration of computer-aided drug-design tools with biomolecular simulation: Flexibility and scoring through iterative molecular dynamics and docking simulations on computational grids
  PI: Cheatham ($30,500)
- **ACS-Petroleum Research Fund.** 1/1/05-10/1/05
  Summer school on computation, simulation, and theory in chemistry, biological chemistry and materials chemistry
  PI: Jack Simons (Chemistry), Co-PIs: Cheatham, T. Seideman (Northwestern U), K. Jordon (U Pitt), E. Carter (UCLA), J.E. Shea (UCSB), J. Tully (Yale), E. Heller (Harvard), M. Head-Gordon (Berkeley), J. Doll (Brown), and B. Garrison (Penn State)
  Travel funds for students and teachers to Park City, Utah.
- **National Science Foundation, CHE-0326027** 9/01/03-8/31/07
  ITR: Development of a Web-based Grid-computing Environment for Research and Education in Computational Science and Engineering
  PI: Thanh Truong (Chemistry), Co-PIs: Cheatham (10%), Julio Facelli (CHPC), James Lewis (WVU)

- **National Science Foundation, CHE-0218739.** 9/1/02-8/31/05
  ITR: Multiscale simulation of Biomolecular Assemblies on a Computational Grid
  PI: Voth (Chemistry), Co-PI's: Cheatham, Ayton (Chemistry).
  < 1 mo. Salary/year for 1 year.
- **National Institutes of Health, 1 R21 EB002880** 9/23/03-8/31/05
  Molecular docking and imaging devices for drug delivery
  PI: Y. Bruce Yu (Pharmaceutics), Collaborator: Cheatham, 5% effort.
- **National Institutes of Health, 1 S10 RR017214-01** 10/1/03-9/30/05
  High End Instrumentation Program-- Proteins to Populations: A metacluster for bioinformatics
  PI: Facelli, Co-PIs: L. Canon-Albright (Medical Informatics), Cheatham, DM Grant (Chemistry), GA Voth (Chemistry), JA Weiss (Bioengineering), RB Weiss (Genetics).
  $1,531,008 + $500,000 UofU match; equipment only (no overhead).
- **University of Utah**, **College of Pharmacy** 7/1/01-6/30/02
  Research Support Grant: Bioinformatics of Bio-molecular Simulation
  PI: Cheatham (~$5,000)

Fellowships, Honors and Awards

- University of Utah College of Pharmacy P2 Teacher of the year, 2013.
- Plenary speaker, eScience 2009, Oxford, U.K.
- Keynote speaker, TeraGrid 09, 2009
- Keynote speaker, Mercury conference at Hamilton College, 2009
- Nominated for the College of Pharmacy, University of Utah, Teaching Award (2006-2012).
- Chosen to present a Telluride Town Talk on the Science of Recreational Drugs, 2008
- Recipient of "Hewlett-Packard Outstanding Junior Faculty Award" from the American Chemical Society COMP division for outstanding work in computational chemistry, 2007.
- Member, NSF CyberInfrastructure User Advisory Committee, 2006-2007.
- Associate Editor, *Molecular Modeling and Computational Chemistry Results*, MMCC, Inc. (Editor: D. Busath, BYU), 2004-2005; Assistant Editor 2000-2004.
- National Research Council Research Associate, March 1997 to December 2000.
- National Science Foundation Travel Award, September 1997 (CECAM).
- Finalist, Computerworld-Smithsonian Awards in the category of Science, 1998.
- DNA simulation research was featured in the 1996 annual report and the 1998 PSC multimedia collection, see http://www.psc.edu/science/Kollman/kollman.html
- UCSF Chancellor's Graduate Research Fellow, September 1995 to June 1996.
- UCSF Pharmacy School, Frank Goyan Award for Excellence in Achievement in Phys. Chemistry, 1995.
- UCSF Dept. Pharmaceutical Chemistry Award for Outstanding Service, 1994-1995.

Professional Service / Review Panels

Internet2 E-CAS "Exploring Cloud for Acceleration of Science" Advisory Board (2018-)
Center for Computational Engineering and Sciences, UNICAMP, Brazil, Intl Advisory Board (2018-)
Campus Research Computing Consortium (CaRCC), Chair (2016-2017), Council Chair (2017-2019), Acting Chair (2019-)
Rocky Mountain Advanced Computing Consortium (RMACC), Vice-Chair (2017-2018), Board Member (2018-)
Advanced Research Computing on Campuses (ARCC) @ PEARC17, Chair (2017)
NSF XSEDE Science Advisory Board (2016-)
NSF XSEDE User Requirements Evaluation and Prioritization Committee (2016-)
Advanced Cyberinfrastructure Research and Educator Facilitator (ACI-REF), PI Chair (2016-2018)
Practice and Experience in Research Computing on Campuses (PEARC) annual meeting steering committee (2016-)
External Thesis Examiner and Opponent, KTH Royal Institute of Technology, Stockholm Sweden (4/2016)
Utah Education Network Advisory Council (2015-2021)

NSF XSEDE User Advisory Committee (2015-)
Blue Waters Science and Engineering Team Advisory Committee – SETAC (2014-)
International HPC Summer School, Organizing Committee & Presenter (2012-)
NIH ZRG1 MSFD Study Section (charter member 7/11-6/15)
External PhD Thesis Examiner and Opponent, IRB Barcelona, Spain (10/14)
NSF Review Panel, CHE (3/14)
Great Lakes Consortium for Petascale Computation Blue Waters Allocations Review Panel (1/14)
Supercomputing 14/15/16 Education Program Executive Committee (2014-2016)
Scientific Advisory Committee of the Swedish National Infrastructure for Computing (SNIC) (10/2013-10/2016)
XSEDE14 Science Track Chair (2013-2014)
NIH ZRG1 MID-B NIAID Study Section (10/13)
Referee for CECAM workshops (2013)
National Academies Committee on Proposal Evaluation for Allocation of Supercomputing Time on Anton (2013, 2014)
NSF XSEDE User Advisory Committee, Chair (2012-4/2015)
NSF XSEDE Science Advisory Board (2012-4/2015)
NSF XSEDE Senior Management Team (2012-4/2015)
PRACE Supercomputing reviews (2015, 2013, 2012)
NSF Review Panel OCI/CHE (11/12, 5/13)
Supercomputing 12 Program Committee (2011-2012)
Swiss Supercomputing Center proposal reviews (2011, 2012)
NSF Site Visit Team, Engineering/CI (3/12)
NIH ZRG F04 Fellowship: Chemistry, Biochemistry, Biophysics, and Bioengineering F30-F33 Study Section (3/12)
External PhD Thesis examiner and Opponent, University of Bergen, Norway (4/11)
NIH NCI intramural lab site review (3/11)
NSF Teragrid Science Advisory Board (6/07-7/11, Chair 7/10-7/11)
NSF Review Panels (10/10, 5/10)
University of Toronto, visit as external thesis examiner (9/10)
NIH ZRG1 MSFD Study Section (Computational Biophysics) (ad hoc 2/09, 6/09, 6/10)
AAAS review, University of Southern Florida neuroscience seed grants (2/10)
National Institute of Computational Sciences User Advisory Committee (2010-2011)
NIH ZRG1 BCMB-P (58) RRFA-09-003: Challenge Grants Panel 7 mail reviews (6/09)
NIH ZRG1 BCMB-B 90 (Special Topics in Biological Sciences) (ad hoc 7/08)
TeraGrid Resource Allocations Committee/LRAC/MRAC, NSF Review Panels for computer time, (3/04-6/08, 4x/year), Chair 6/07, 9/07, 12/07, 3/08, 6/08.
External PhD Thesis Examiner and Opponent, Karolinska Institute, Stockholm Sweden (2/08)
External PhD Thesis Examiner and Opponent, Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy (1/08)
NIH ZRG1 MSFD Study Section (Computational Biophysics) (ad hoc 10/07)
NSF Cyberinfrastructure User Advisory Committee (6/06-6/07)
NIH ZRG1 F04B-A (20) Study Section (Biophysics Fellowships) (ad hoc 3/06)
NIH ZRG1 BCMB-Q (02) Study Section (Computational Biophysics) (ad hoc 10/05, 3/06)
NSF Chemistry Division, mail review (10/05, 3/06, 8/06, 9/06, 8/07)
Ad hoc reviewer for the University of Utah Funding Incentive Seed Grant, (10/04, 3/05)
Universitat Innsbruck, Austria; External PhD thesis review (2004, 2005)
NIH Special Emphasis Panel ZAI1 AR-M (M1), Cooperative Research for Development of Vaccines, Adjuvants, Therapeutics, Immunotherapeutics and Diagnostics for Biodefense and SARs (ad hoc 2/04)
Cooperative Grants Program of the U.S. Civilian Res. Dev. Foundation, mail reviewer, (12/03)
NIH BBCA Study Section, (ad hoc 2/03)
Fonds zur Forderung der Wissenschaftlichen Forschung (Austria), mail reviewer, (3/02)
Alliance Allocations Board/NRAC (NSF/Computer time) (3/02-9/04, 4x/year)
DOE Site review team, Environmental Health Sciences Laboratory, PNNL (11/01)

Publications

(1) DA Pearlman, DA Case, JW Caldwell, WS Ross, TE Cheatham, III, S DeBolt, DM Ferguson, GL Seibel & PA Kollman. "AMBER, a package of computer programs applying molecular mechanics, normal mode analysis, molecular dynamics and free energy calculations to simulate the structural and energetic properties of molecules." *Comp. Phys. Comm*. 91, 1-41 (1995).

(2) TE Cheatham, III, JL Miller, T Fox, TA Darden & PA Kollman. "Molecular dynamics simulations on solvated biomolecular systems: The particle mesh Ewald method leads to stable trajectories of DNA, RNA and proteins." *J. Amer. Chem. Soc*. 117, 4193-4194 (1995).

(3) TE Cheatham, III & PA Kollman. "Observation of the A-DNA to B-DNA transition during unrestrained molecular dynamics simulations in aqueous solution." *J. Mol. Biol*. 259, 434-444. (1996).

(4) TE Cheatham, III & PA Kollman. "Molecular dynamics simulations highlight the structural differences among DNA:DNA, RNA:RNA and DNA:RNA hybrid duplexes." *J. Amer. Chem. Soc*. 119, 4805-4825 (1997).

(5) P Cieplak, TE Cheatham, III & PA Kollman. "Molecular dynamics simulations find that 3' phosphoramidate modified DNA duplexes undergo a B to A transtion and normal DNA duplexes an A to B transition." *J. Amer. Chem. Soc*. 119, 6722-6730 (1997).

(6) T Spector, TE Cheatham, III & PA Kollman. "Unrestrained molecular dynamics of photodamaged DNA in aqueous solution." *J. Amer. Chem. Soc*. 119, 7095-7104 (1997).

(7) TE Cheatham, III, MF Crowley, T Fox & PA Kollman. "A molecular level picture of the stabilization of A-DNA in mixed ethanol-water solutions." *Proc. Nat. Acad. Sci*. 94, 9626-9630 (1997).

(8) TE Cheatham, III & PA Kollman. "Insight into the stabilization of A-DNA by specific ion association: Spontaneous B-DNA to A-DNA transitions observed in molecular dynamics simulations of d[ACCCGCGGGT]$_2$ in the presence of hexaamminecobalt(III)." *Structure* 5, 1297-1311 (1997).

(9) MF Crowley, TA Darden, TE Cheatham, III & D Deerfield. "Adventures in improving the scaling and accuracy of a parallel molecular dynamics program." *J. Supercomputing*. 11, 255-278 (1997).

(10) TA Darden, LG Pedersen, AY Toukmaji, MF Crowley & TE Cheatham, III. "Particle-mesh based methods for fast Ewald summation in molecular dynamics simulations". *Proceedings of the Eighth SIAM Conference on Parallel Processing for Scientific Computing*. Eds: M. Heath *et al.*, (Minn, MN). March (1997).

(11) TE Cheatham, III, JL Miller, TI Spector, P Cieplak & PA Kollman. "Molecular dynamics simulations on nucleic acid systems using the Cornell *et al*. force field and particle mesh Ewald electrostatics." in *Modeling and Structure Determination of Nucleic Acids*. Eds: NB Leontis & J Santa Lucia, Jr (ACS Press: Washington, DC) p. 285-303 (1998).

(12) SC Harvey, RK-Z Tan & TE Cheatham, III. "The flying ice cube: Velocity rescaling in molecular dynamics leads to violation of energy equipartition." *J. Comp. Chem*. 19, 726-740 (1998).

(13) S Bogusz, TE Cheatham, III & BR Brooks. "Removal of pressure and free energy artifacts in charged periodic systems via net charged corrections to the Ewald potential." *J. Chem. Phys*. 108, 7070-7084 (1998).

(14) TE Cheatham, III & PA Kollman. "Molecular dynamics simulation of nucleic acids in solution: How sensitive are the results to small perturbations in the force field and environment?" in *Structure, Motion, Interactions and Expression of Biological Macromolecules*. Eds: R.H. Sarma & M.H. Sarma (Adenine Press: Albany, NY) p. 99-116 (1998).

(15) TE Cheatham, III & BR Brooks. "Recent advances in molecular dynamics simulation towards realistic representation of biomolecules in solution". *Theor. Chem. Acc*. 99, 279-288 (1998).

(16) M Hodoscek, EM Billings, TE Cheatham, III & BR Brooks. "High performance computing in biophysics: Recent experiences and developments of CHARMM." *Proceedings of the International Symposium on Supercomputing: New Horizons of Computational Science*. (Kluwer Academic) (1998).

(17) JL Miller, TE Cheatham, III, & PA Kollman. "Simulation of Nucleic Acid Structure." in *Oxford Handbook of Nucleic Acid Structure*. Ed: S. Neidle (Oxford University Press) p.95-115 (1999).

(18) J Srinivasan, TE Cheatham, III, P Cieplak, PA Kollman & DA Case. "Continuum solvent studies of the stability of DNA, RNA and phosphoramidate-DNA helices". *J. Amer. Chem. Soc*. 120, 9401-9409 (1998).

(19) PA Kollman, DA Pearlman, DA Case, JW Caldwell, WS Ross, TE Cheatham, III, S DeBolt, DM Ferguson & G Seibel. "AMBER." in *Encyclopedia of Computational Chemistry* (Wiley-Interscience: NY) (1998).

(20) MF Crowley, TA Darden, TE Cheatham, III & D Deerfield. "Fine- and coarse-grain parallel AMBER and particle mesh Ewald on MPP's" in *Parallel Computing for Industrial and Scientific Applications*, Eds: J Jenness (Morgan-Kaufmann: NY) (1999).

(21) TE Cheatham, III, J Srinivasan, DA Case & PA Kollman. "Molecular dynamics and continuum solvent studies of the stability of polyG-polyC and polyA-polyT DNA duplexes in solution." *J. Biomol. Struct. Dyn.* 16, 265-280 (1998).

(22) TE Cheatham, III, BR Brooks & PA Kollman. "Molecular modeling of nucleic acid structure" in *Current Protocols in Nucleic Acid Chemistry*. (Wiley: New York) 7.5.1-7.5.13 (1999).

(23) DE Konerding, TE Cheatham, III, PA Kollman & TL James. "Unrestrained and restrained PME MD on NMR-derived DNA decamer and dodecamer sequences." *J. Biomol. NMR*. 13, 119-131 (1999).

(24) TE Cheatham, III, P Cieplak & PA Kollman. "A modified version of the Cornell *et al*. force field with improved sugar pucker phases and helical repeat." *J. Biomol. Struct. Dyn*. 16, 845-862 (1999).

(25) TE Cheatham, III & PA Kollman. "Molecular dynamics simulations of nucleic acids". *Ann. Rev. Phys. Chem.* 51, 435-471 (2000).

(26) PA Kollman, I Massova, C Reyes, B Kuhn, S Huo, L Chong, M Lee, T Lee, Y Duan, W Wang, O Donini, P Cieplak, J Srinivasan, DA Case & TE Cheatham, III. "Calculating structures and free energies of complex molecules: Combining molecular mechanics and continuum methods." *Acc. Chem. Res.* 33, 889-897 (2000).

(27) TE Cheatham, III, BR Brooks & PA Kollman. "Molecular modeling of nucleic acid structure: Energy and sampling" in *Current Protocols in Nucleic Acid Chemistry*. (Wiley: New York) 7.8.1-7.8.21 (2001).

(28) TE Cheatham, III, BR Brooks & PA Kollman. "Molecular modeling of nucleic acid structure: Electrostatics and solvation" in *Current Protocols in Nucleic Acid Chemistry*. (Wiley: New York) 7.9.1-7.9.22 (2001).

(29) TE Cheatham, III, BR Brooks & PA Kollman. "Molecular modeling of nucleic acid structure: Setup and analysis" in *Current Protocols in Nucleic Acid Chemistry*. (Wiley: New York) 7.10.1-7.10.18 (2001).

(30) TE Cheatham, III and MA Young. "Molecular dynamics simulations of nucleic acids: Successes, limitations and promise." *Biopolyers Nuc. Acid Sci.* 56, 232-256 (2001).

(31) F Lankas, TE Cheatham, III, P Hobza, J Langowski, N Spackova, and J Sponer. "Critical effect of the N2 amino group on structure, dynamics and elasticity of DNA polypurine tracts" *Biophys. J.* 82, 2592-2609 (2002).

(32) JP Lewis, J Pikus, TE Cheatham, III, EB Starikov, H Wang, J Tomfohr, and OF Sankey. "A comparison of electronic states in periodic and aperiodic poly(dA)-poly(dT) DNA." *Phys. Stat. Sol. (b)* 233, 90-100 (2002).

(33) N Spackova, TE Cheatham, III, F Ryjacek, F Lankas, L van Meervelt, P Hobza, and J Sponer. "Molecular dynamics simulations and thermodynamics analysis of DNA-drug complexes. Minor groove binding between 4'-6-diamino-2-phenylindole and DNA duplexes in solution." *J. Amer. Chem. Soc.* 125, 1759-1769 (2003).

(34) R Stefl, TE Cheatham, III, N Spackova, E Fadrna, I Berger, J Koca, and J Sponer. "Formation pathways of a guanine-quadruplex DNA revealed by molecular dynamics and thermodynamical analysis of the substates." *Biophys. J.* 85, 1787-1804 (2003). PMCID: PMC1303352

(35) JP Lewis, TE Cheatham, III, H Wang, E Starikow, and OF Sankey. "Dynamically amorphous character of electronic states in poly(dA)-poly(dT) DNA." *J. Phys. Chem. B* 107, 2581-2587 (2003).

(36) F Lankas, J Sponer, J Langowski & TE Cheatham, III. "DNA base-pair step deformability inferred from molecular dynamics simulation" *Biophys. J.* 85, 2872-2883 (2003). PMCID: PMC1303568

(37) E Fadrna, N Spackova, R Stefl, J Koca, TE Cheatham, III, and J Sponer. "Molecular dynamics simulations of guanine quadruplex loops: Advances and force field limitations." *Biophys. J.* 87, 227-242 (2004). PMC1304345.

(38) F Lankas, J Sponer, J Langowski, and TE Cheatham, III, "DNA deformability at the base pair level." *J. Amer. Chem. Soc.* 126, 4124-4125 (2004).

(39) DL Beveridge, G Barreiro, KS Byun, DA Case, TE Cheatham III, SB Dixit, E Giudice, F Lankas, R Lavery, J Maddocks, R Osman, H Sklenar, G Stoll, KM Thayer, P Varnai, and MA Young "Molecular dynamics simulations of the 136 unique tetranucleotide sequences of DNA oligonucleotides. I. Research design, informatics, and results on d(CpG) steps." *Biophys. J.* 87, 3799-3813 (2004). PMCID: PMC1304892

(40) TE Cheatham, III "Simulation and modeling of nucleic acid structure, dynamics and interactions" *Curr. Opin. Struct. Biol.* 14, 360-367 (2004).

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Abstracts:

MA Munger, FS Albright, JE Buskupiak, DK Blumenthal, TE Cheatham, III, FM Creekmore. "Utility of the foreign graduate equivalency examination to assess pharmacy curricula". 107th annual meeting AACP (2006).

JE Buskupiak, DK Blumenthal, TE Cheatham, III, FS Albright, MA Munger. "An employer survey as a pharmacy curriculum assessment tool". 108th annual meeting AACP (2007).

Recent technical training and teaching experience

- **PharmD Recitation,** Pharm 5151: Spring 2018, 2019
  2 credits; 26 contact hours, Course Master
- **Organic Medicinal Chemistry,** MDCH 5210: 1st half Fall semester
  2 credits; 16-20 contact hours, 2002-2015, Course Master.
- **Principles of Medicinal Chemistry**, MDCHEM 6990: ½ Spring semester.
  2 credits, ~3-6 contact hours, Spring 2006-2013.
- **Mechanisms and Kinetics of Drug Degradation and Stabilization / Biotechnology,** PHCEU 7040
  Fall 2002-2011. 8-12 hours in 2002-2011, 4 hours in 2013.
- **Molecular Modeling and Biomolecular Simulation from a Pharmaceutical Perspective**, PHCEU/MDCHEM 7095: 2nd half Spring semester.
  2 credits, ~30 contact hours, Spring 2004, 2005, 2006, 2011, 2012, 2013; Course Master.
- **Introduction to Bioinformatics**, MDINF 6600.
  3 lectures on structure prediction, Spring 2002-2006.
- **RNA/DNA as a Drug Target Journal Club**, PHCEU 5660.
  1 credit/15 hours, Fall 2004, Course Master.
- **Fundaments of Pharmaceutical Sciences**, PHSCI 7113.
  2 lectures on drug development, 1 on solutions; Fall 2004-present.

Selected Presentations and Workshops (2007-present)

- CaRCC Sustainability workshop, DFW, October 2019 [organizer]
- Research Computing and Data Maturity model workshop, EDUCAUSE, October 2019 [organizer]
- CASC meeting, Arlington VA, September 2019 [invited]
- National Research Platform Workshop, Minneapolis MN, September 2019 [organizing committee]
- NSF CI for Large Facilities Workshop, Arlington VA, September 2019 [organizing committee]
- TACC Frontera Dedication, Austin TX, September 2019 [invited]
- RMACC Systems Administrator meet-up, Tempe AZ, August 2019
- PEARC19, Chicago IL, July 2019 [workshop organizer, BoF, Town Hall, keynote, panels]
- International HPC Summer School, Kobe Japan, July 2019 [invited]
- NSF CI Coordination Workshop, Arlington VA, June 2019 [facilitator/organizer]
- BioExcel/PRACE HPC for Life Sciences, Stockholm Sweden, June 2019 [invited]
- Blue Waters Symposia, Sun River OR, June 2019 [invited]

- RMACC, U Colorado Boulder, May 2019
- Sealy Symposium, Galveston TX, May 2019 [invited]
- CaRCC Ecosystem of Research Computing and Data Workshop, St. Louis, April 2019 [organizer]
- ACS National Meeting, Orlando FL, April 2019 [1 invited, 1 contributed]
- AMBER Developers Meeting, Safety Harbor FL, March 2019 [invited]
- CASC, Arlington VA, March 2019 [invited]
- Theory-Software Workshop, New Orleans LA, February 2019 [invited]
- Internet2 Research Computing Maturity Model Workshop, December 2018 [invited]
- University of Missouri, State of Research Computing at Utah, November 2018 [invited]
- APLU-AUU Workshop on Accelerating Public Access to Research Data, October 2018 [invited]
- CASC, Arlington VA, October 2018 [invited]
- Georgia State University, Department of Chemistry, September 2018 [invited]
- RMACC, U Colorado Boulder, August 2018
- National Research Platform, U Montana Bozemann, August 2018
- PEARC18, Pittsburgh, PA, July 2018
- International HPC Summer School, Ostrava Czech Republic, July 2018 [invited]
- ISQBP, Barcelona Spain, June 2018 [invited]
- Blue Waters Symposia, Sun River OR, June 2018 [invited]
- CECAM on multiscale modeling of epigenetics, Laussane Switzerland, May 2018 [invited]
- RMACC System Administrators meet-up, Arizona State U, April 2018
- Sustainable Software Institute Workshop, Berkeley CA, April 2018 [invited]
- Open Science Grid all-hands meeting, University of Utah, March 2018 [invited]
- CASC, Arlington VA, March 2018 [invited]
- CI Professionalization Workshop, Arlington VA, March 2018 [invited]
- CENIC, Monterey CA, March 2018 [invited]
- AMBER Developers Meeting, Florida, February 2018 [invited]
- WestNet, Tucson AZ, January 2018 [invited]
- CASC, Arlington VA, October 2017 [invited]
- 7th iCatse International Conference on IT Convergence and Security, Seoul Korea, September 2017 [invited]
- Lucian Symposium, St Edwards College, Austin TX, September 2017 [invited]
- National Research Platform workshop, Bozeman MT, August 2017 [invited]
- RNA Dynamics @ Telluride, July 2017
- ARCC Tutorial and CaRC @ PEARC17. New Orleans, July 2017 [invited]
- International HPC Summer School, Boulder Co., June 2017 [invited]
- DE Shaw Research, New York, NY, June 2017 [invited]
- Utah Education and Telehealth Network Tech Summit, Salt Lake City, UT, June 2017 [invited]
- MolSSI workshop, Blacksburg VA, June 2017 [invited]
- DDN Best Practices in Data, Boston MA, May 2017 [invited]
- Blue Waters Symposia, Sun River OR, May 2017 [invited]
- NSF workshop in Big Data in Chemistry, Arlington VA, April 2017 [invited]
- PRACE workshop on Gromacs, AMBER and NAMD, Stockholm Sweden, April 2017 [invited]
- CI Practitioners workshop, Washington DC, March 2017 [invited]
- NSF Workshop on Integrating Computation into Biology and Chemistry, New Orleans, March 2017 [invited]
- OSG All Hands, San Diego CA, March 2017 [invited]
- NSF SI2 PI Meeting, Arlington VA, February 2017 [invited]
- AMBER Developers Meeting, Athens GA, February 2017 [invited]
- ACI-REF face to face meeting, Miami FL, February 2017 [invited]
- Westnet CIO meeting, Tempe AZ, January 2017 [invited]

- NSF Cloud workshop, Arlington VA, December 2016 [invited]
- SIGUCCS. Denver, Panel, November 2016 [invited]
- Pacific Rim Platform – ACI-REF joint meeting at Cal-IT2, October 2016 [invited]
- RMACC workshop, Colorado State U, August 2016 [invited]
- International HPC Summer School, Ljubljana, Slovenia, June 2016 [invited]
- ISQBP President's meeting, Bergen, Norway, June 2016 [invited]
- Blue Waters Symposia, Sun River, OR, June 2016 [invited]
- RNA: Structure, Dynamics and Function, SISSA, Trieste, Italy, May 2016 [invited]
- Stockholm University, Lindahl Lab, Stockholm, April 2016 [invited]
- Arizona State University, Computational Physics Seminar, April 2016 [invited]
- Advanced Research Computing on Campuses, UIUC, Urbana, March 2016 [invited]
- AMBER Developers Meeting, San Diego, March 2016 [invited]
- ACS National Meeting, San Diego, March 2016 [invited]
- RNA Structure Prediction workshop, Punta Cana, Dominican Republic, December 2015 [invited]
- SaintCon Utah's IT security conference, Weber State, October 2015 [invited]
- Mexico National Chemistry Congress, Queretaro, October 2015 [keynote]
- RMACC workshop, Boulder Colorado, August 2015 [invited]
- Zing Computational Biological Chemistry, Cairnes Australia, August 2015 [invited]
- RNA Dynamics, Telluride, July 2015 [invited]
- AMBER workshop at University College London, July 2015 [invited]
- International HPC Summer School, Toronto, June 2015 [invited]
- 19th Conversation, University of Albany, NY, June 2015 [invited]
- Blue Waters Symposium, Sunriver, OR, May 2015 [invited]
- ACS National Meeting, David Case Awards Symposia, Denver, CO, March 2015 [invited]
- Advanced Research Computing on Campuses, Researcher Perspectives Panel, Clemson, March 2015 [invited]
- AMBER developers meeting, University of Florida, February 2015
- National Academy of Sciences Future of NSF HPC testimony, Mountain View, December 2014 [invited]
- AMBER workshop at UNAM, Mexico City, October 2014 [organizer]
- CHANGES 2014, Chinese Academy of Sciences, Beijing, September 2014 [invited]
- XXVI IUPAP Conference on Computational Physics, Boston, August 2014 [invited]
- XSEDE14, Atlanta, July 2014 [Science Track Chair, Presenter]
- ISQBP Presidents Meeting, Telluride, June 2014 [President, Organizer]
- International HPC Summer School, Budapest, June 2014
- Sandia National Labs, Biomaterials Science, May 2014
- Blue Waters Symposia, U Illinois, May 2014
- CECAM Biomolecules in unnatural conditions, Stuttgart, March 2014
- American Physical Society National Meeting, Denver, March 2014
- St. Louis University, Department of Chemistry, January 2014
- AMBER Developers Meeting, Stony Brook U, January 2014
- Zing conference on RNA and protein structure prediction, Playa de Carmen, Mexico, Dec 2013 [invited]
- Louisiana Alliance for Simulation-Guided Materials Applications, LaTech, Oct 2013 [invited]
- ACS National Meeting, Fall 2013, Indianapolis [1 invited]
- RNA Dynamics @ Telluride, July 2013 [invited]
- NSF cCWCS Computational Chemistry and Theoretical Chemistry Summer School @ Westminster, July 2013 [invited]
- International HPC Summer School (XSEDE, PRACE, Riken), NYU, June 2013 [invited]
- Blue Waters NEIS-P2 / User Workshop, NCSA, May 2013 [invited]
- ACS National Meeting, Spring 2013, New Orleans [2 invited]

- AMBER Developers Meeting, Salt Lake City, March 2013 [organizer]
- Department of Biochemistry, University of Rochester, March 2013 [invited]
- Department of Physics, University of Delaware, November 2012 [invited]
- Department of Bioinformatics, University of Kansas, October 2012 [invited]
- AMBER CECAM workshop, Laussane, Switzerland, October 2012 [invited]
- Skaggs Symposia, College of Pharmacy, U Colorado, September 2012 [invited]
- Department of Materials Science and Engineering, U Utah, September 2012 [invited]
- NSF Workshop on Community Codes, Chicago, IL, September 2012 [invited]
- Joint AMBER/CHARMM developers meeting, Rockville, MD, July 2012 [invited]
- 3rd annual European and U.S. School in High Performance Computing, Dublin, Ireland, June 2012 [invited]
- Department of Physics, University of Leeds, U.K., June 2012 [invited]
- School of Pharmacy, University of Nottingham, U.K., June 2012 [invited]
- International Society of Quantum Biology and Pharmacology, Stockholm, Sweden, June 2012 [invited]
- JICS/GRS workshop, Oak Ridge, TN, April 2012 [invited]
- AMBER Developers meeting, Piscataway, NJ, January 2012 [invited]
- DNA in disorders and disease, New Delhi, India, December 2011 [invited]
- CECAM Protein-nucleic acid interactions, Zurich, Switzerland, September 2011 [invited]
- CECAM Coarse-grained mechanics of DNA, Lausanne, Switzerland, August 2011 [invited]
- TeraGrid/Deisa HPC Summer School, Lake Tahoe, CA., August 2011 [invited]
- RNA dynamics Telluride Science meeting, July 2011 [invited, co-organizer]
- TeraGrid '11, Science Track, Salt Lake City, UT, July 2011
- 17th conversation in Biomolecular Stereodynamics, Albany, June 2011 [session chair]
- Computational Aspects of Biomolecular NMR GRC, Il Ciocco, May 2011 [poster]
- University of Bergen, Norway, April 2011 [invited]
- 51st Sanibel Symposia, St. Simons Island, Georgia, March 2011 [invited]
- AMBER developers meeting, Athens, Georgia, March 2011 [invited]
- Pharmaceutical Sciences seminar, U Maryland @ Baltimore, December 2010 [invited]
- Juan Diego High School Pre-Med Club, Draper, Utah, December 2010 [invited]
- TeraGrid/DEISA Summer School in HPC, Catania, Sicily, Italy, October 2010 [invited]
- Biomedical Informatics Departmental seminar, October 2010 [invited]
- NSF OCI task force meeting, Campus Bridging, Denver, CO, August 2010 [invited]
- Application Drivers for Exascale Computing and Data CI, Arlington VA, July 2010 [invited]
- ISQBP President's Meeting, Cetraro, Italy, June 2010 [invited]
- Medicinal Chemistry seminar, University of Minnesota, April 2010 [invited]
- Biochemistry seminar, University of Missouri, March 2010 [invited]
- 50th Sanibel Symposia, St. Simons Island, Georgia, March 2010 [invited]
- Department of Materials Science, University of Utah, February 2010 [invited]
- University of Kentucky, NSF CI Days, February 2010 [invited]
- AMBER developers meeting at Stony Brook, January 2010
- Plenary, E-science workshop at Oxford, Great Britain, December 2009 [invited, plenary]
- ABC Satellite Meeting, Barcelona, Spain, November 2009 [invited]
- Algorithms in MacroMolecular Modeling, Austin, November 2009 [invited]
- University of Florida, Physical Chemistry Seminar Series, October 2009 [invited]
- Pharm/Tox Seminar Series, U of Utah, October 2009 [invited]
- Mercury undergraduate research meeting at Hamilton, August 2009 [invited, keynote]
- RNA Dynamics meeting at Telluride, July 2009 [invited]
- TeraGrid '09 at Crystal City, VA, June 2009 [invited, keynote]
- Air Force Research Lab, March 2009 [invited]

Committee appointments (Utah)

University of Utah, Academic Senate (2019-2022)
University of Utah, Academic Senate Executive Committee (2019)
University of Utah, Senate Advisory Committee on Information Technology (2016-2019, 2019-2022)
University of Utah, Senate Ad Hoc Faculty Information Technology Committee (2015-2016)
University of Utah, Information Technology Research Portfolio Committee, Chair (2013-2015)
University of Utah, Operational Information Technology Committee (2013-2015)
University of Utah, Academic Senate (2012-2015)
University of Utah, Personnel and Elections Committee (2012-2015)
University of Utah, Director of Graduate Studies Medicinal Chemistry (2011-2017)
University of Utah, Graduate Council Review Committee, Dept. of Atmospheric Sciences (2017)
Center for High Performance Computing, User Advisory Committee (2001-)
College of Pharmacy, Outcomes Assessment Committee (2004-present)
College of Pharmacy, Computer Committee (2000-present, Chair 2007-2014, ad hoc 2014-)
College of Pharmacy, Mentoring Committee (2012-)
University of Utah, Cyberinfrastructure Council (2007-2012)
University of Utah Information Technology Council (2001-2012)
Medicinal Chemistry Seminar Coordinator (2003-2004, 2010-2011)
College of Pharmacy, PharmD Seminar Committee (2009-2010)
University of Utah, CyberInfrastructure Advisory Committee (2006-2007)
University of Utah, Bioinformatics Advisory Committee (2002-2004)
U Utah, Health Sciences Center Information Technology Projects Approval (2001-2003)