

Peer reviewed papers 2016

Parallel simulated annealing using an adaptive resampling interval

Z. Lou, J. Reinitz

Parallel Computing; 53: 23-31. *PMCID:PMC4770898*

The Cardiac TBX5 Interactome Reveals a Chromatin Remodeling Network Essential for Cardiac Septation

L. Waldron, J.D. Steimle, T.M. Greco et al.

Developmental Cell 2016; 36(3):262–275. *PMCID:PMC4920128*

Multiscale Simulations Reveal Key Aspects of the Proton Transport Mechanism in the CIC-ec1 Antiporter

S. Lee, J.M. Swanson, G.A. Voth

Biophys J. 2016; 110(6):1334-45. *PMCID:PMC4816718*

Computationally Efficient Multiscale Reactive Molecular Dynamics to Describe Amino Acid Deprotonation in Proteins

S. Lee, R. Liang, G.A. Voth, J.M. Swanson

J Chem Theory Comput. 2016; 12(2):879-91. *PMCID:PMC4750100*

Computational Study of the W260A Activating Mutant of Src Tyrosine Kinase

Y. Meng, B. Roux

Protein Science; 25(1):219-30. *PMCID:PMC4815304*

A Decision-Theoretic Phase I-II Design for Ordinal Outcomes in Two Cycles

J. Lee, P.F. Thall, Y Ji, P. Müller

Biostatistics;17(2): 304-19. *PMCID:PMC4834949*

Conference proceedings and abstracts 2016

Supercomputing ulcerative colitis-associated cancer simulations to bridge mechanism with epidemiology

R.C. Cockrell, M. E. Stack, G. An

Digestive Disease Week, San Diego, CA, 5/21/2016

Characterizing the behavioral landscape of sepsis: supercomputing simulation of 40 million in silico patients

R.C. Cockrell, G. An
Society of Critical Care Medicine Annual Congress, Orlando, FL, 02/20/2016

Supercomputing sepsis simulations for in silico outcome prediction

R.C. Cockrell, G. An
Academic Surgical Congress 2016, Jacksonville, FL 02/03/2016

Investigating the development of ulcerative colitis-associated cancers through an agent-based model

R.C. Cockrell, G. An
Academic Surgical Congress 2016, Jacksonville, FL 02/03/2016

Peer reviewed papers 2015

***Large-scale spatiotemporal spike patterning consistent with wave propagation in motor cortex**

K.Takahashi, S. Kim, T. P. Coleman, K. A. Brown, A. J. Suminski, M.D. Best, N.G. Hatsopoulos
Nature Communications ;6:7169.PMCID:PMC4443713

****Stochastic integrated assessment of climate tipping points indicates the need for strict climate policy**

T.S. Lontzek, Y. Cai, K. L. Judd, T.M. Lenton
Nature Climate Change; 5: 441-444

Identification of epigenetic modifications that contribute to pathogenesis in therapy-related AML: Effective integration of genome-wide histone modification with transcriptional profiles

X. H. Yang, B. Wang, J.M. Cunningham
BMC Medical Genomics ;8 Suppl 2:S6.PMCID:PMC4460748

An analysis of biomolecular force fields for simulations of polyglutamine in solution

A.M. Fluitt, J.J. de Pablo
Biophysical Journal; 109(5):1009-1018. PMCID:PMC4564678

Zodiac: A comprehensive depiction of genetic interactions in cancer by integrating TCGA data

Y. Zhu, Y. Xu, D.L. Helseth, K. Gulukota, S. Yang, L.L. Pesce, R. Mitra, P. Müller, S. Sengupta, W. Guo, J.C. Silverstein, I. Foster, N. Parsad, K.P. White, Y. Ji
Journal of The National Cancer Institute;107(8). PMCID:PMC4554190

Environmental tipping points significantly affect the cost-benefit assessment of climate policies

Y. Cai, K.L. Judd, T.M. Lenton, T.S. Lontzek, D. Narita
PNAS U S A ;112(15):4606-11.PMCID:PMC4403162

Computational study of the "DFG-flip" conformational transition in c-Abl and c-Src tyrosine kinases

Y. Meng, Y.L. Lin, B. Roux
Journal of Physical Chemistry B ;119(4):1443-56.PMCID:PMC4315421

Ethnic-specific associations of rare and low-frequency DNA sequence variants with asthma

C. Igartua, R.A. Myers, R.A. Mathias, et al. C. Ober
Nature Communication;6:5965.PMCID:PMC4309441

Structural Refinement Methodology from Multiple Non-Interacting Fragments

R. Shen, W. Han, G. Fiorin et al., B. Roux
PLOS Comput. Biology; 11(10).PMCID: PMC4624691

Efficient Determination of Free Energy Landscapes in Multiple Dimensions from Biased Umbrella Sampling Simulations Using Linear Regression

Y. Meng, B. Roux
J Chem. Theory Comput; 11(8),pp 3523–3529

Simulating the distance distribution between spin-labels attached to proteins

S. M. Islam, B. Roux
J Phys Chem B; 119(10),pp3901–3911.PMCID:PMC4509421

DeepCNF-D: Predicting Protein Order/Disorder Regions by Weighted Deep Convolutional Neural Fields

S. Wang, S. Weng, J. Ma, Q. Tang
Int Journal of Molecular Sciences ;16(8):17315-30. PMCID:PMC4581195

The social cost of carbon with economic and climate risks

Y. Cai, K.L. Judd, T.S. Lontzek
(under review) in Journal of Political Economy, arXiv preprint arXiv:1504.06909

Supercomputing simulation of 40 million in silico patients to characterize the landscape of sepsis

G. An, C. Cockrell
(submitted) to the Society of Critical Care Medicine

A Subgroup Cluster Based Bayesian Adaptive Design for Precision Medicine

W. Guo, Y. Ji, D. Catenacci
(submitted to JASA)

Activation pathway of Src kinase reveals intermediate states as novel targets for drug design

Y. Meng, D. Shukla, V.S. Pande, B. Roux
Nature Commun. PMID: PMC4465921

Structural and functional characterization of a calcium-activated cation channel from *Tsukamurella paurometabola*

B. Dhakshnamoorthy, L. Blachowicz, H. Rui, B. Roux
(in preparation & to be submitted)

Monitoring H⁺-driven structural changes in a CLC chloride-proton antiporter using computationally-guided double electron-electron resonance spectroscopy

S.M. Islam, R. Cheng, A. R. Stein, et al., M. C. Maduke
(in preparation & to be submitted)

The Complete Activating Transition in c-Src Kinases

M. Fajer, Y. Meng, B. Roux
(in preparation & to be submitted)

Conference proceedings and abstracts 2015

Causal Network in a Deafferented Non-Human Primate Brain

K. Balasubramanian, K. Takahashi, N. Hatsopoulos
37 th Annual international conference of IEEE Engineering in Medicine and Biology Society (EMBC), Milan, August 2015

Intrinsic plasticity "set point", network stability, and sensory feedback processing as an early error detection mechanism in the HVC of zebra finches

A. Daou, P. Malonis, D. Margoliash
Society for Neuroscience, poster, November 2015 Chicago

Factors determining the degeneracy of the relationship between the parameters and dynamics of conductance model neurons

P. Malonis, A. Daou, D. Margoliash

Society for Neuroscience, poster, November 2015 Chicago

In silico construction of a host/pathogen patient cohort using HPC parameter sweeps on an agent-based model of sepsis

C. Cockrell, G. An

Mind Bytes: Research Computing Expo and Symposium, Chicago, IL 10/27/2015

Examining the pathogenesis of pouchitis using tissue-realistic computational model: SEGMENT_HPC

C. Cockrell, S. Christley, E. Chang, G. An

Academic Surgical Conference 2015, Las Vegas, NV, 2/3/2015

Peer reviewed papers 2014

Finding chemical reaction paths with a multilevel preconditioning protocol

S. Kale, O. Sode, A.R. Dinner, J. Weare

J Chem Theor Comp 10, 5467-5475. PMID:PMC4263463

Targeted analysis of whole genome sequence data to diagnose genetic cardiomyopathy

J.R. Golbus, M.J. Puckelwartz, L. Dellefave-Castillo, et al., E.M. McNally

Circ Cardiovascular Genetics ;7(6):751-9.PMID:PMC4270910

****Investigation of inflammation and tissue patterning in the gut using a spatially explicit general-purpose model of enteric tissue (SEGMENT)**

C. Cockrell, S. Christley, G. An

PLoS Computational Biology 10, no. 3 : e1003507. PMID:PMC3967920

****Towards Anatomic Scale Agent-Based Modeling with a Massively Parallel Spatially Explicit General-Purpose Model of Enteric Tissue (SEGMENT_HPC)**

R.C. Cockrell, S. Christley, E. Chang, G. An

PloS one 10, no. 3 : e0122192-e0122192. PMID:PMC4373890

Loss of conformational entropy in protein folding calculated using realistic ensembles and its implications for NMR-based calculations

M.C. Baxa, E.J. Haddadian, J.M. Jumper, K.F. Freed, T.R. Sosnick

PNAS U S A ;111(43):15396-401.PMID:PMC4217416

Foxf Genes Integrate Tbx5 and Hedgehog Pathways in the Second Heart Field for Cardiac Septation

A. D. Hoffmann, X. H. Yang, O. Burnicka-Turek, et al., I.P. Moskovitz
PLOS Genetics ;10(10):e1004604.PMCID:PMC4214600

Molecular mechanism for differential recognition of membrane phosphatidylserine by the immune regulatory receptor Tim4

G.T. Tietjen, Z. Gong, C.H. Chen, et al., E.J. Adams
PNAS U S A ;111(15):E1463-72.PMCID:PMC3992656

Escherichia coli peptidoglycan structure and mechanics as predicted by atomic-scale simulations

J.C. Gumbart, M. Beeby, G.J. Jensen, B. Roux
PLOS Computational Biology ;10(2):e1003475.PMCID:PMC3930494

Constraints and potentials of future irrigation water availability on agricultural production under climate change

J. Elliott, D. Deryng, C. Müller, et al. D. Wisser
PNAS U S A ;111(9):3239–3244.PMCID: PMC3948288

Locking the active conformation of c-Src kinase through the phosphorylation of the activation loop

Y. Meng, B. Roux
Journal of Molecular Biology ;426(2):423–435.PMCID:PMC3947352

Supercomputing for the parallelization of whole genome analysis

M.J. Puckelwartz, L.L. Pesce, V. Nelakuditi, et al., E.M. McNally
Bioinformatics ;30(11):1508–1513.PMCID: PMC4029034

Subgroup-Based Adaptive (SUBA) Designs for Multi-Arm Biomarker Trials

Y. Xu, L. Trippa, P. Muller, Y. Ji
(submitted) *Statistics in Biosciences*

Molecular Dynamics Studies of Ion Conduction in a Prokaryotic Channel

K.M. Callahan, B. Roux
Biophysical Journal ;106(2),p37a.

'N-of-1-pathways' unveils personal deregulated mechanisms from a single pair of RNA-Seq samples: towards precision medicine

V. Gardeux, I. Achour, J. Li, et al. Y.A. Lussier
J Am Med Inform Assoc;21(6):1015-25.PMCID:PMC4215042

Determinants of fluidlike behavior and effective viscosity in cross-linked actin networks

T. Kim, M.L. Gardel, E. Munro
Biophysical Journal ;106(3):526-34.PMCID:PMC3944977

Experiences Building Globus Genomics: A Next-Generation Sequencing Analysis Service using Galaxy, Globus, and Amazon Web Services

R.K. Madduri, D. Sulakhe, L. Lacinski, et al. I.T. Foster
Concurr Comput ;26(13):2266-2279.PMCID:PMC4203657

Computational Study of Gleevec and G6G Reveals Molecular Determinants of Kinase Inhibitor Selectivity

L. Lin, Y. Meng, L. Huang, B. Roux
J Am Chem Soc ;136(42):14753-62.PMCID:PMC4210138

Multiscale Reactive Molecular Dynamics for Absolute pK_a Predictions and Amino Acid Deprotonation

J.G. Nelson, Y. Peng, D.W. Silverstein, J.M. Swanson
J Chem Theory Comput. 10(7): 2729-37

Conference proceedings and abstracts 2014

Differences in dynamics and stability of the wild type β -Amyloid A β (1-40) and Δ E22-A β (1-39) (Japanese) protofibril structures, a Molecular Dynamics Study

K.W. Johnson, T.R. Sosnick, K.F. Freed, E.J. Haddadian
Biophysical society 58th annual meeting. February 2014. San Francisco, CA

About 20,000,000 core-hours of high throughput computations were conducted on the Beagle GLOBUS. The study was supported in part by the NIH grants UL1TR000050 (University of Illinois CTSA), 1S10RR029030-01 (BEAGLE Cray Supercomputer, K22LM008308), and NCI P30CA023074 grant of the University of Arizona Cancer Center.

H. Li, I. Achour, V. Gardeux, et al., Yves A. Lussier

Characterization of nonlinear propagation waves of local field potentials in motor cortical areas

J. Chemili, K. Takahashi
IEEE EMBC 2014

Spatiotemporal dynamics of motor cortical network using ECoG signals

H. Watanabe, K. Takahashi, T. Isa
IEEE EMBC 2014

Multi-modal Decoding: Identifying Information Redundancy between Spike Trains and Sub-dural Electrographic Signals

K. Balasubramanian, K. Takahashi, M. Slutzky, N. Hatsopoulos
IEEE EMBC 2014

Compiler Optimization for Extreme-Scale Scripting

T.G. Armstrong, J.M. Wozniak, M. Wilde, I.T. Foster
CCGrid 2014 Doctoral Symposium, 2014

Robust scaling of next-generation sequencing analyses using the modular SwiftSeq workflow.

J.J. Pitt, K.P. White
Biological Data Science. Cold Spring Harbor Laboratories, Cold Spring Harbor, NY, USA. November 6th, 2014

Compiler Optimization for Data-Driven Task Parallelism on Distributed Memory Systems Argonne National Laboratory

T.G. Armstrong, J.M. Wozniak, M. Wilde, I.T. Foster
Tech Report ANL/MCS-P5080-0214, 2014

Examining the pathogenesis of pouchitis using a multiscale model of the intestinal mucosa: Spatially Explicit General-purpose Model of Enteric Tissue (SEGMENT_HPC)

C. Cockrell, S. Christley, E. Chang, G. An
IMAG Multiscale Modeling Consortium Meeting 2014, Bethesda, MD, 09/05/2014

Investigation of inflammation and tissue patterning in the gut using a Spatially Explicit General-purpose Model of Enteric Tissue (SEGMENT)

C. Cockrell, S. Christley, G. An
Huggins Research Symposium 2014, Chicago, IL, 03/22/2014

Examining the dynamics of epithelial metaplasia and pouchitis in an ileal pouch with a Spatially-Explicit General Purpose Model of Enteric Tissue (SEGMENT)

C. Cockrell, S. Christley, E. Chang, G. An, M. Ward
Academic Surgical Conference 2014, San Diego, CA, 02/04/2014

Peer reviewed papers 2013

Computational analysis of the binding specificity of Gleevec to Abl, c-Kit, Lck, and c-Src tyrosine kinases

Y. Lin, B. Roux
J American Chemical Society;135(39):14741-53.PMCID:PMC4026022

Large-Scale Modeling of Epileptic Seizures: Scaling Properties of Two Parallel Neuronal Network Simulation Algorithms

L.L. Pesce, H.C. Lee, M. Hereld, S. Visser, R.L. Stevens, A. Wildeman, W. van Drongelen

Comp Math Methods in Medicine ;2013:182145.PMCID:PMC3876705

Simplified Protein Models: Predicting Folding Pathways and Structure Using Amino Acid Sequences

A. Adhikari, K.F. Freed, T.R. Sosnick

Phys Rev Lett ;111(2):028103.PMCID:PMC4047675

Fast and accurate pedigree-based imputation from sequenced data in a founder population

O.E. Livne, L. Han, G. Alkorta-Aranburu, et al., Carole Ober

American Society of Human Genetics ;11(3):e1004139.PMCID:PMC4348507

Explaining why Gleevec is a specific and potent inhibitor of Abl kinase

Y.L. Lin, Y. Meng, W. Jiang, B. Roux

Proc Natl Acad Sci USA ;110(5):1664-9.PMCID:PMC3562763

Computational study of the prokaryotic sodium channel

K. M.Callahan, B. Roux

Biophysical Journal ;104(2),p136a.

Discovering RNA-Protein Interactome by Using Chemical Context Profiling of the RNA-Protein Interface

M. Parisien, X. Wang, G. Perdrizet, et al. T. Pan

Cell Reports ;3(5):1703-13.PMCID:PMC3769137

Architecture and assembly of the Gram-positive cell wall

M. Beeby, J.C. Gumbart, B. Roux, G.J. Jensen

Molecular Microbiology ;88(4):664-72.PMCID:PMC3663049

Self-Learning Adaptive Umbrella Sampling Method for the Determination of Free Energy Landscapes in Multiple Dimensions

W. Wojtas-Niziurski, Y. Meng, B. Roux, S. Bernèche

J Chem Theory Comput;9(4):1885–1895.PMCID: PMC3694627

***Two gene co-expression modules differentiate psychotics and controls**

C. Chen, L. Cheng, K. Grennan, et al. C. Liu

Molecular Psychiatry ;18(12):1308-14.PMCID:PMC4018461

Conference proceedings and abstracts 2013

Kinematically defined state dependent changes in functional connectivity of neurons and in local field potentials in orofacial motor cortex during chewing and swallowing

K. Takahashi in Motor control of feeding behaviors session
Neuro2013 (2013)

Wave propagation of beta oscillations in motor cortex and its relation to spatiotemporal spiking patterns and behavior

K. Takahashi
CiNet (2013)

Validation of bootstrap-based comparison of ROC curves on partially-paired data sets

Y. Peng, L. Pesce, Y. Jiang
SPIE (2013)

Atomistic simulation of polyglutamine in solution

A.M. Fluitt, J.J. de Pablo
Conf Proc American Institute of Chemical Engineers Annual Meeting. San Francisco, CA 2013

Development of the Charmm Drude Polarizable Force Field for the Study of Ion Interactions in Biological Systems

H. Li, K. Callahan, A.D. Mackerell, B. Roux
Biophysical Journal ;104(2),p.507a

Spatially explicit multi-scale model of intestinal epithelial metaplasia

C. Cockrell, S. Christley, E. Chang, G. An, M. Ward
qBio 2013, Santa Fe, NM, 8/8/2013

Examining the dynamics of epithelial metaplasia and pouchitis in an ileal pouch with a spatially-explicit computational multi-scale gut model (MSGM)

C. Cockrell, S. Christley, E. Chang, G. An, M. Ward
SpringSim Multiconference 2013, San Diego, CA, 4/7/2013

Examining the dynamics of inflammatory bowel disease with a spatially-explicit computational multi-scale gut model (MSGM)

C. Cockrell, S. Christley, E. Chang, G. An, M. Ward
Huggins Research Symposium 2013, Chicago, IL, 2/20/2013

Peer reviewed papers 2012

Coarse-Graining Provides Insights on the Essential Nature of Heterogeneity in Actin Filaments

J. Fan, M.G. Saunders, G.A. Voth

Biophysical Journal ;103(6):1334-42.PMCID:PMC3446683

A statistically defined anthropomorphic software breast phantom

B.A. Lau, I. Reiser, R.M. Nishikawa, P.R. Bakic

Medical Physics ;39(6):3375-85.PMCID:PMC3371078

Complex-disease networks of trait-associated single-nucleotide polymorphisms (SNPs) unveiled by information theory

H. Li, Y. Lee, J.L. Chen, E. Rebman, J. Li, Y.A. Lussier

J Am Med Inform Assoc.;19(2):295–305.PMCID: PMC3277620

Granger causality analysis of functional connectivity of spiking neurons in orofacial motor cortex during chewing and swallowing

K. Takahashi, L. Pesce, J. Iriarte-Díaz, et al., N.G. Hatsopoulos

Conf Proc IEEE Eng Med Biol Soc;2012:4587-90.PMID:23366949

On docking, scoring and assessing protein-DNA complexes in a rigid-body framework

M. Parisien, K.F. Freed, T.R. Sosnick

PloS ;7(2):e32647.PMCID:PMC3290582

Growing Point-to-Set Length Scale Correlates with Growing Relaxation Times in Model Supercooled Liquids

G. Hocky, T. Markland, D. Reichman

Physical Review Letters ;108(22)

***Elucidating the molecular details of phosphatidylserine membrane recognition in immune response**

G. T. Tietjen, C.H. Chen, J. Crooks, et al. K.Y. Lee

Biophysical Journal ;104(2),p363a.

De novo prediction of protein folding pathways and structure using the principle of sequential stabilization

A.N. Adhikari, K.F. Freed, T.R. Sosnick

PNAS USA ;109(43):17442-7.PMCID:PMC3491489

Dynamic mechanisms of cell rigidity sensing: insights from a computational model of actomyosin networks

C. Borau, T. Kim, T. Bidone, J.M. García-Aznar, R.D. Kamm

PloS ;7(11):e49174.PMCID:PMC3489786

***Mechanisms of contractility and coarsening of active cytoskeletal networks**

T. Kim, M. L. Gardel, E. Munroe
Biophysical Journal ;102(3)p693a.

Determination of membrane-insertion free energies by molecular dynamics simulations

J. Gumbart, B. Roux
Biophysical Journal ;102(4):795-801.PMCID:PMC3283816

Conference proceedings and abstracts 2012

Ion conduction and selectivity in an open pore sodium channel

K.M. Callahan, B. Roux
XSEDE12 Conference, Extreme Science and *Engineering Discovery Environment* (2012)

A network of subpopulation of neurons in primary motor cortex and beta oscillation waves exhibit similar spatiotemporal patterns

K. Takahashi, K. Brown, S. Kim, T. Coleman, N.G. Hatsopoulos
Nanosymposium on Signal Propagation, The annual meeting, Society for Neuroscience (2012)

Structural reorganization of active actin networks via competition between force generation and dissipation

T. Kim, E. Munro, M.L. Gardel
BMES annual meeting (2012)

Evaluating Communication Performance in IBM BG/Q and Cray XE6 Supercomputing Systems

H. Bui, V. Vishwanath, J. Leigh, M. E. Papka
Proceedings of the IEEE/ACM International Conference for High Performance Computing, Networking, Storage and Analysis (SC 2012)

FLASH simulations of 120MJ target explosions in LIFE reactor chamber

R. Sacks, G. Moses, M. Fatenejad
54th Annual Meeting of the APS Division of Plasma Physics (2012)

Computer-aided image analysis and detection of prostate cancer using immunostaining for alpha-methylacyl-CoA racemase, p63, and high-molecular-weight cytokeratin

Y. Peng, Y. Jiang, X.J. Yang

Machine Learning in Computer-Aided Diagnosis: Medical Imaging Intelligence and Analysis. IGI Global, 2012

****Context and Force Field Dependence of the Loss of Protein Backbone Entropy upon Folding Using Realistic Denatured and Native State Ensembles**

M.C. Baxa, E.J. Haddadian, A.K. Jha, K.F. Freed, T.R. Sosnick

Journal of the American Chemical Society;134(38),15929–15936.PMCID:PMC3464005

****Sensory-like Responses in Motor Cortex Enhance the Performance of a Brain-Machine Interface**

A.J. Suminski, D. Tkack, A.H. Fagg, K. Takahashi, N.G. Hatsopoulos

22nd Annual Meeting of the Society for the Neural Control of Movement

Conference proceedings and abstracts 2011

Ab initio protein structure prediction aided by sequential stabilization of tertiary structure

A.N. Adhikari, J. DeBartolo, K. F. Freed, T.R. Sosnick

Protein Folding Symposium. Berkeley, California, USA, June, 2011

Mini-conference on Understanding Astrophysical Dynamos

F. Cattaneo, "Magneto-Rotational Turbulence and Dynamo Action

53rd Annual Meeting of the APS Division of Plasma Physics, Salt Lake City, Utah, USA, November, 2011

Scaling Behavior Of Computational Model of Neocortex

H. C. Lee, M. Hereld, S. Visser, L. Pesce, and W. van Drongelen

4th International Meeting on Epilepsy Research, Chicago, IL, May 2011

PanSystematic prediction and validation of RNA-protein interactome

M. Parisien, T. R. Sosnick

RNA Society, Kyoto, June 2011

**Use of Data Reduction Techniques for the Visualization of Computer-
Extracted Lesion Features in the Diagnostic Interpretation of Breast Cancer**

R. Jamieson, K. Drukker, M. L. Giger,

Radiological Society of North America, 2011

**Numerical Simulations of Strong Incompressible Magnetohydrodynamics
Turbulence, Physics of Plasmas**

J. Mason, J.C. Perez, S. Boldyrev, F. Cattaneo

53rd Annual Meeting of the APS Division of Plasma Physics, Vol. 56, No. 16