

# Rick Archibald

Computer Science and Mathematics Division  
Oak Ridge National Laboratory  
PO BOX 2008 MS 6211  
Oak Ridge, TN  
**Telephone:** (865) 576- 5761   **Fax:** (865) 241-0381  
**Electronic Mail:** archibaldrk@ornl.gov

---

## Education

### Arizona State University

Tempe, AZ.

Thesis Advisor: Anne Gelb. Thesis title: *Boundary Detection and Reconstruction in Magnetic Resonance Imaging*. Focus of study: spectral methods, partial differential equations, statistics, computational biology, and medical image analysis.

*Ph.D. in Mathematics*

**August 1998– May 2002**

### University Of Alberta

Edmonton, AB.

Thesis Advisor: Abel Cadenillas. Focus of study: mathematical finance, stochastic partial differential equations, and numerical computation.

*M.Sc. in Applied Mathematics*

**September 1996– April 1998**

### University Of Alberta

Edmonton, AB.

Focus of study: partial differential equations, computer programming, and biological physics.

*B.Sc. in Honors Physics*

**September 1992– April 1996**

## Professional Experience

### Computer Science and Mathematics Division

Oak Ridge National Laboratory

Supervisor: Clayton Webster. Focus of study: Climate science, experimental facilities data analysis, high performance computing, and uncertainty quantification.

*Staff Scientist*

**August 2007–Present**

### Computer Science and Mathematics Division

Oak Ridge National Laboratory

Supervisor: Ed D’Azevedo. Focus of study: hyperspectral imaging, nano-technology, parallel computing, and partial differential equations.

*Householder Fellow*

**August 2005–August 2007**

### Department of Neuroscience

Brown University

Supervisor: Jerome Sanes. Focus of study: Data fusion and beamforming in Electroencephalography (EEG), Magnetoencephalography (MEG) and functional Magnetic Resonance Imaging (fMRI).

*Post Doctorate*

**August 2004–July 2005**

### Center for System Science and Engineering Research

Arizona State University

Supervisor: Frank Hoppensteadt. Focus of study: Dynamical nano-systems and image analysis.

*Post Doctorate*

**May 2002–August 2004**

### Alzheimer Disease Research Center

Good Samaritan Hospital, AZ.

Studied under the guidance of Kewei Chen in the areas of medical imaging methods and analysis.

*Research Assistant*

**January 1999– May 2002**

## Publications

I have over 100 reviewed publication (see [Google Scholar](#)) and over 70 invited presentation.

Feng, Archibald, and Maksymovych, “Lvy Backward SDE Filter for Jump Diffusion Processes and Its Applications in Material Sciences”, *Communications in Computational Physics*, **27**(2), 589–618, 2019.

- Brendan, Archibald, Azadmanesh, Vandavasi, Langan, Coates, Lynch, and Langan, “BraggNet: integrating Bragg peaks using neural networks”, *Journal of Applied Crystallography*, **52**(4), 854–863, 2019.
- Xian, Archibald, Mayer, Liu and Li, “An effective online data monitoring and saving strategy for large-scale climate simulations”, *Quality Technology & Quantitative Management*, **16**(3), 330–346, 2019.
- Evans, Archibald, Gardner, Norman, Taylor, Woodward, and Worley, “Performance analysis of fully explicit and fully implicit solvers within a spectral element shallow-water atmosphere model”, *The International Journal of High Performance Computing Applications*, **33**(2), 268–284, 2019.
- Sullivan, Archibald, Vandavasi, Langan, Coates and Lynch, “Volumetric Segmentation via Neural Networks Improves Neutron Crystallography Data Analysis”, *2019 19th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGRID)*, **10.1109/CCGRID.2019.00070**, 2019.
- Shang, Archibald, Gelb and Luke, “Sparsity-based photoacoustic image reconstruction with a linear array transducer and direct measurement of the forward model”, *Journal of Biomedical Optics*, **24**(3), 1 – 9, 2018.
- Sullivan, Archibald, Langan, Dobbek, Bommer, McFeeters, Coates, Wang, Gallmeier, Carpenter, Lynch, and Langan, Paul, “Improving the accuracy and resolution of neutron crystallographic data by three-dimensional profile fitting of Bragg peaks in reciprocal space”, *Acta Crystallographica Section D*, **74**(11), 1085–1095, 2018.
- Archibald, Krogel, and Kent, “Gaussian process based optimization of molecular geometries using statistically sampled energy surfaces from quantum Monte Carlo”, *The Journal of Chemical Physics*, **149**(16), 164116, 2018.
- Barnard, Bilheux, Toops, Nafziger, Finney, Splitter, and Archibald, “Total variation-based neutron computed tomography”, *Review of Scientific Instruments*, **89**(5), 053704, 2018.
- Dyck, Bao, Ziatdinov, Nobakht, Shin, Law, Maksov, Sumpter, Archibald, Jesse, and Kalinin, “Leveraging Single Atom Dynamics to Measure the Electron-Beam-Induced Force and Atomic Potentials”, *Microscopy and Microanalysis*, **24**(S1), 96-97 2018.
- Shang, Archibald, Gelb and Luke, “Computational Photoacoustic Imaging with Sparsity-Based Optimization of the Initial Pressure Distribution”, *Proc. SPIE*, **10494**, 7, 2018.
- Somnath, Law, Morozovska, Maksymovych, Kim, Lu, Alexe, Archibald, Kalinin, Jesse, Vasudevan, “Ultrafast Current Imaging by Bayesian Inversion”, *Nature Communications*, **9**(1), 513, 2018.
- Brugiapaglia, Adcock, and Archibald, “Recovery Guarantees for Compressed Sensing with Unknown Errors”, *2017 International Conference on Sampling Theory and Applications (SampTA)*, 533–537, 7, 2017.
- Lingerfelt, Belianinov, Endeve, Ovchinnikov, Somnath, Borreguero, Grodowitz, Park, Archibald, Symons, Kalinin, Messer, Shankar, and Jesse, “BEAM: A Computational Workflow System for Managing and Modeling Material Characterization Data in HPC Environments”, *Procedia Computer Science*, **80**, 2276–2280, 2016.
- Bao, Archibald, Niedziela, Bansal, and Delaire, “Complex Optimization for Big Computational and Experimental Neutron Datasets”, *Nanotechnology*, **27**(48), 484002, 2016.
- Kalinin, Strelcov, Belianinov, Somnath, Vasudevan, Lingerfelt, Archibald, Chen, Proksch, Laanait, and Jesse, “Big, Deep, and Smart Data in Scanning Probe Microscopy”, *ACS Nano*, **10**(10), 9068–9086, 2016.

- Belianinov, Gobeljic, Shvartsman, Endeve, Lingerfelt, Archibald, Kalinin, and Jesse, “High Performance Computing Tools for Cross Correlation of Multi-Dimensional Data Sets Across Instrument Platforms”, *Microscopy and Microanalysis*, **22**(S3), 288, 2016.
- Sang, Lupini, Unocic, Meyer, Ward, Lee, Endeve, Archibald, Borisevich, and Kalinin, “Distortion Correction in Scanning Transmission Electron Microscopy with Controllable Scanning Pathways”, *Microscopy and Microanalysis*, **22**(S3), 900, 2016.
- Jesse, Chi, Borisevich, Belianinov, Kalinin, Sergei Endeve, Archibald, Symons, and Lupini, “Using Multivariate Analysis of Scanning-Rochigram Data to Reveal Material Functionality”, *Microscopy and Microanalysis*, **22**(S3), 292, 2016.
- Bao, Archibald, Niedziela, Bansal, and Delaire, “Hierarchical Optimization for Neutron Scattering Problems”, *Journal of Computational Physics*, **315**, 39–51, 2016.
- Sang, Lupini, Unocic, Chi, Borisevich, Kalinin, Endeve, Archibald, and Jesse, “Dynamic Scan Control in STEM: Spiral Scans”, *Advanced Structural and Chemical Imaging*, **2**(1), 6, 2016.
- Langan, Archibald, and Lamberti, “Nuclear Forensics Attribution with Missing and Uncertain Data”, *Journal of Radioanalytical and Nuclear Chemistry*, **308**(2), 687–692, 2016.
- Archibald, Gelb, and Platte, “Image Reconstruction from Undersampled Fourier Data Using the Polynomial Annihilation Transform”, *Journal of Scientific Computing*, **67**(2), 432–452, 2016.
- Bracco, Archibald, Dvovrolis, Foundalis, Luo and Neelin, “The parameter optimization problem in state-of-the-art climate models and network analysis for systematic data mining in model intercomparison projects”, *The Fluid Dynamics of Climate, Courses and Lectures Vol. 564*, Edited by A. Provenzale, E. Palazzi and K. Fraedrich pp 121–141, Springer, 2016.
- Kalinin, Sumpter, and Archibald, “Big, Deep, and Smart Data: Guiding Materials Design through Imaging”, *Nature Materials*, **14**, 973–980, 2015.
- Fu, Allen, and Archibald, “Evaluating the Relationship between the Population Trends, Prices, Heat Waves, and the Demands of Energy Consumption in Cities”, *Sustainability*, **7**(11), 15284–15301, 2015.
- Belianinov, Vasudevan, Strelcov, Steed, Yang, Tselev, Jesse, Biegalski, Shipman, Symons, Borisevich, Archibald, and Kalinin, “Big Data and Deep Data in Scanning and Electron Microscopies: Functionality from Multidimensional Data Sets”, *Advanced Structural and Chemical Imaging*, **1**(1), 1–25, 2015.
- Archibald, Evans, Salanger, “Accelerating Time Integration for Climate Modeling Using GPUs”, *Journal of Computational Science*, **51**, 2046–2055, 2015.
- Joubert, Archibald, Berrill, Brown, Eisenbach, Grout, Larkin, Levesque, Messer, Norman, Philip, Sankaran, Tharrington, and Turner, “Accelerated Application Development: The ORNL Titan Experience”, *Computers & Electrical Engineering*, **46**, 123–138, 2015.
- Wasserman, Archibald, and Gelb, “Image Reconstruction from Fourier Data Using Sparsity of Edges Polynomial Annihilation Sparsifying Transform”, *Journal of Scientific Computing*, **65**(2), 533–552, 2015.
- Denker, Archibald, and Gelb, “An Adaptive Fourier Filter for Relaxing Time Stepping Constraints for Explicit Solvers”, *Spectral and High Order Methods for Partial Differential Equations ICOSAHOM 2014*, 157–166, 2015.
- Langan, Archibald, Plumlee, Mahajan, Ricciuto, Yang, Mei, Mao, and Shi, “Stochastic Parameterization to Represent Variability and Extremes in Climate Modeling”, *Journal of Computational Science: Procedia*, **29**, 1146–1155, 2014.

Rao, Archibald, and Evans, “Emulation to simulate low resolution atmospheric data”, *International Journal of Computer Mathematics*, **91**(4), 770–780, 2014.

Surace, Archibald, and Saxena, “On the Use of the Polynomial Annihilation Edge Detection for Locating Cracks in Beam-Like Structures”, *Computers & Structures*, **114**, 72–83, 2013.

Archibald, Constantinescu, Evans, Finkel, Haut, Norris, Norman, Sandu, Stonyanov, Tokman, Wingate, and Xing, “Resilient, Communication-Reducing, and Adaptive Time Stepping to Accelerate Exascale Scientific Applications”, *DOE Workshop on Applied Mathematics Research for Exascale Computing*, 2013.

Archibald, “Error Estimation in High Dimensional Space for Stochastic Collocation Methods on Arbitrary Sparse Samples”, *AIP Conference Proceedings*, **1558**, 906–909, 2013.

Archibald, Deiterding, Hauck, Jakeman, and Xiu, “Approximation and Error Estimation in High Dimensional Space for Stochastic Collocation Methods on Arbitrary Sparse Samples”, *Exascale Research Conference*, Portland, OR, USA, 2012.

Norman, Larkin, Archibald, Carpenter, and Anamtharaj, “The Path to Accelerating the Community Atmospheric Model Spectral Element Dynamical Core on Hybrid Multi-Core Systems”, *KIAPS International Symposium on Global NWP System Modeling*, 2012.

Archibald, Chakoumakos, and Zhuang, “Characterizing the Elements of Earth’s Radiative Budget: Applying Uncertainty Quantification to the CESM”, Special issue Empowering Science: ICCS 2012, *Journal of Computational Science: Procedia*, **5**(2), 85 – 89, 2012.

Liu, Martha, Nelson, Archibald, Pannala, Andrews and Nanda, “TXM-XANES Studies on High Voltage Lithium Rich Composite Cathodes: 3D Morphology and Phase at Nanoscale”, *MRS abstract*, 2012.

Surace, Yan, Archibald, Saxena, and Feng, “Structural Damage Detection using the Polynomial Annihilation Edge Detection Method”, *Australian Journal of Structural Engineering*, 2012.

Rao, Evans, and Archibald, “Emulation to Simulate Low Resolution Atmospheric Data”, *ORNL/TM-2012/317* ([www.osti.gov/servlets/purl/1051448/](http://www.osti.gov/servlets/purl/1051448/)), 2012.

Nanda, Bilheux, Voisin, Veith, Archibald, Walker, Allu, Dudney, and Pannala, “Anomalous Discharge Product Distribution in Lithium-Air Cathodes”, *The Journal of Physical Chemistry*, **116**(15), 8401 – 8408, 2012.

Archibald, Chakoumakos, and Zhuang, “Characterizing the Elements of Earth’s Radiative Budget: Applying Uncertainty Quantification to the CESM”, *Procedia Computer Science*, **9**, 1014–1020, 2012.

Norman, Larkin, Archibald, Carpenter, Anantharaj, Micikevicius, and Evans, “Porting the Community Atmosphere Model - Spectral Element Code to Utilize GPU Accelerators” *Cray User Group, CUG*, 2012.

Carpenter, Archibald, Evans, Larkin, Micikevicius, Rosinski, Schwarzmeier, and Taylor, “Progress Towards Accelerating HOMME on Hybrid Multi-Core Systems”, *Int. J. High Perf. Comput. Appl.*, **27**, 335–347, 2012.

Jakeman, Archibald, and Xiu, “Characterization of Discontinuities in High-dimensional Stochastic Problems on Adaptive Sparse Grids”, *Journal of Computational Physics*, **230**(10), 3977–3997, 2011.

Archibald, Fann, and Shelton, “Adaptive Discontinuous Galerkin Methods in Multiwavelets Bases”, *Applied Numerical Mathematics*, **61**(7), 2011.

Archibald, Drake, Evans, and White III, “Multiwavelet Discontinuous Galerkin Accelerated

ELP Method for the Shallow Water Equations on the Cubed Sphere”, *Monthly Weather Review*, **139**(2), 457–473, 2011.

Filippi, Archibald, Bhaduri, and Bright “Hyperspectral Agricultural Mapping using Support Vector Machine-Based Endmember Extraction (SVM-BEE)”, *Optics Express*, **17**(26), 23823–23842, 2009.

Archibald, Drake, Evans, and White III, “Time acceleration methods for convection on the cubed sphere”, *Computational Science*, 253–262, 2009.

Archibald, Gelb, Saxena, and Xiu, “Discontinuity Detection in Multivariate Space for Stochastic Simulations”, *Journal of Computational Physics*, **228**(7), 2676–2689, 2009.

Filippi and Archibald, “Support Vector Machine-Based Endmember Extraction”, *IEEE Transaction on Geoscience and Remote Sensing*, **47**(3), 771–791, 2009.

Archibald, Gelb, and Yoon, “Determining the Locations of Discontinuities in the Derivatives of Functions”, *Applied Numerical Mathematics*, **58**(5), 577–592, 2008.

White III, Evans, Archibald, Drake, Worley, and Kothe, “Acceleration of Time Integration”, *Cray User Group, CUG, Helsinki, Finland, May 5-8*, 2008.

de Almeida, Birdwell Jr., Tsouris, DePaoli, and Archibald, “Developing a Predictive Model for Nuclear Fuel Reprocessing Separations”, *Nuclear Separation Science Conference Proceedings*, 2008.

Chapman, Long, Datskos, Archibald, and Sepaniak, “Differentially Ligand-Functionalized Microcantilever Arrays for Metal Ion Identification and Sensing”, *Analytical Chemistry*, **79**(18), 7062–7068, 2007.

Lavrik, Archibald, Grbovic, and Datskos, “Uncooled MEMS IR Imagers with Optical Readout and Image Processing”, *Proceedings of the SPIE*, **6542**, 2007.

Archibald and Fann, “Feature Selection and Classification of Hyperspectral Images with Support Vector Machines”, *IEEE Geoscience and Remote Sensing Letters*, **4**(4), 674–677, 2007.

Archibald, Datskos, Devault, Lamberti, Lavrik, Noid, Sepaniak, and Dutta, “Independent Component Analysis of Nanomechanical Responses of Cantilever Arrays”, *Analytica Chimica Acta*, **584**, 101–105, 2007.

Sanes, OKeefe, Archibald, and Bienenstock, “Single-Trial Prediction of Discrete Hand Movements with Electroencephalography”, *Human Brain Mapping*, 2006.

Archibald, Gelb, Gottlieb, and Ryan, “One-Sided Post-Processing for the Discontinuous Galerkin Method Using ENO Type Stencil Choosing and the Local Edge Detection Method”, *Journal of Scientific Computing*, **28**, 2-3, 167–190, 2006.

Archibald, Gelb, and Yoon, “Polynomial Fitting for Edge Detection in Irregularly Sampled Signals and Images”, *SIAM Journal on Numerical Analysis*, **43**, 259–279, 2005.

Archibald, Hu, Gelb, and Farin, “Improving the Accuracy of Volumetric Segmentation Using Pre-Processing Boundary Detection and Image Reconstruction”, *IEEE Transactions on Image Processing*, **13**, No. 4, 2004.

Archibald, Chen, Gelb, and Renaut, “The Improvement of Human Brain Segmentation Through the use of the Gegenbauer Reconstruction Method as a Pre-Processing Step”, *NeuroImage*, **20**, 489–502, 2003.

Archibald and Gelb, “Reducing the Effects of Noise in MRI Reconstruction”, *Biomedical Imaging, Proceedings, 2002 IEEE International Symposium on*, 497–500, 2002.

Gelb and Archibald, “Reducing the Gibbs Ringing Artifact in MRI Scans While Maintaining Tissue Boundary Integrity”, *Biomedical Imaging, Proceedings, 2002 IEEE International Symposium on*, 923–926, 2002.

Archibald and Gelb, “A Method to Reduce the Gibbs Ringing Artifact in MRI Scans While Keeping Tissue Boundary Integrity”, *IEEE Transactions of Medical Imaging*, **21**, 305–319, 2002.

Archibald and Gelb, “Reducing The Effects of Noise in Boundary Detection”, *Journal of Scientific Computing*, **17**, 167–180, 2002.

**Funded Grants – Only PI and Co-PI**      **Frameworks, Algorithms and Scalable Technologies for Mathematics (FASTMath)**      *ASCR/DOE*

PI (Data Analytic Lead): Rick Archibald      **October 2017–September 2020**  
Develop data analytic and machine learning tools for high performance computing. Total award 18M.

**Accurate Quantified Mathematical Methods for Neutron Science**      *ASCR/DOE*

PI: Rick Archibald      **October 2014–September 2017**  
Solved mathematical challenges for Neutron sciences. Total award 2.4M.

**Sparse Recovery for Scientific Data**      *ASCR/DOE*

Co-PI: Rick Archibald      **October 2014–September 2017**  
Sparse recovery methods for HPC datasets. Total award 1.5M.

**A Mathematical Environment for Quantifying Uncertainty: Integrated and Optimized at the Extreme Scale**      *ASCR/DOE*

Co-PI: Rick Archibald      **October 2013–September 2016**  
Develop uncertainty quantification methods and theory at scale . Total award 4.2M.

**Advanced Dynamically Adaptive Algorithms for Stochastic Simulations on Extreme Scales**      *ASCR/DOE*

PI: Rick Archibald      **October 2010–September 2013**  
Advanced stochastic methods for computational simulation. Total award 1.3M.

**Service**      **Computational and Applied Mathematics Group**      *ORNL*

Group Deputy Leader      **October 2016– Present**  
Advisor to the Computational and Applied Mathematics group leader. Have the ability to help run all aspects of the group.

**Division Operational Committee**      *ORNL*

Member      **December 2012– February 2015**  
Scientific member of Computer and Applied Mathematics Division operational committee. Responsible for setting operation policy for the division.

**Advisory Board for KIAPS**      *Soul, South Korea*

Member      **December 2011–November 2012**  
Reviewed, provided guidance, and loaned expertise to the newly formed Korean Institute of Atmospheric Prediction Systems (KIAPS).

**Computer and Applied Mathematics Division Distinguish Seminar Series**      *ORNL*

Leader      **October 2008–September 2010**  
Directed distinguished seminar series for division, responsible for all aspects, from targeting speakers to facilitating interactions with staff.

## Affiliations

### **Institute of Functional Imaging of Materials**

*ORNL*

Mathematics Lead

**September 2014– Present**

One of three leads for the Institute of Functional Imaging of Materials, focusing on mathematical methods and theory for experimental data at ORNL. Coordinate a team of thirty members on the mathematical research directions of the institute.

### **Ugly Data Days**

*ORNL*

Lead

**September 2017**

Promote collaboration between experimental scientist and experts in data analytics at ORNL ([UDD](#)).

### **International Journal of Computer**

*Journal*

**Mathematics**

Associate Editor

**September 2012– 2018**

Editors for the International Journal of Computer Mathematics, focusing on computational mathematics and applications.

### **Climate Change Science Institute**

*ORNL*

Member

**September 2009– 2016**

Founding member of the Climate Change Science Institute, which consists of hundreds of scientist across ORNL. Part of interdisciplinary team that is delivering a new climate model to the Department of Energy, with a focus of national energy needs and predictions, and running at the highest possible resolution on world class computing facilities. Actively part of mathematical and computational work for this climate model.