Michael M. McKerns

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Research Interests

My research interests include the development of software infrastructure for optimization and machine learning, and the application of this infrastructure to the modeling, simulation, and automated design of materials. I am particularly interested in design of experiments under uncertainty, the discovery of structure-property relationships, and the development of robust predictive analytics for nonlinear dynamical systems with missing or limited information.

Education

University of Notre Dame	Applied Physics	BS, 1994
University of Alabama at Birmingham	Physics	MS, 1997
University of Alabama at Birmingham	Physics	PhD, 2002
California Institute of Technology	Materials Science	Post-Doc, 2002-2004

Employment

2018- Scientist III, Information Sciences (CCS-3), LANL
2017-2019 Instructor and Scientific Software Developer, Enthought, Inc.
2017-2020 Research Professor, Institute for Advanced Computational Science, Stony Brook
2014-2017 Guest Scientist, Theoretical Physics and Chemistry of Materials (T-1), LANL
2014-2016 Senior Scientist, Computing and Mathematical Science, Caltech
2011-2014 Senior Scientist, Center for Advanced Computing Research, Caltech
2011-2012 Software Architect: Investment Banking Technology, J.P. Morgan; Enthought, Inc.
2006-2011 Senior Scientist and Project Manager, Materials Science, Caltech
2004-2006 Technical Staff, Materials Science, Caltech
2002-2004 Postdoctoral Scholar, Materials Science, Caltech
1998 Associate Research Engineer, Imaging and Spectrometry Technology Division, JPL
1995 Research Assistant, Polymer Branch, US Air Force Wright Laboratory
1994-2002 Research Assistant, Physics, University of Alabama Birmingham

Consulting

2023- Consultant: Vybe Energy; the UQ Foundation.
2023- Consultant: Advanced Materials, Lockheed Martin Corporation; the UQ Foundation.
2019-2020 Consultant: Space Systems, Lockheed Martin Corporation; the UQ Foundation.
2019-2020 Software Engineering Lead: Roche Sequencing Solutions; the UQ Foundation.
2019-2020 Consultant: Vybe Energy; the UQ Foundation.
2017-2019 Software Developer: Roche Sequencing Solutions; Enthought, Inc.
11/2013-01/2014 Software Developer: Large Data Visualization; Shell Canada; Enthought, Inc.
2013- Software Architect: the UQ Foundation.
2013-2020 Instructor: Enthought Inc; the UQ Foundation; Python Academy; Logit Academy.
2012-2015 Software Architect: Investment Banking Technology, J.P. Morgan; Enthought, Inc.
10/2009 Review Panelist: Academic Research Infrastructure review panel, Division of Materials Research, Mathematical & Physical Sciences Directorate, National Science Foundation.
07/2006 Workshop Participant: e-Research for the Structural Sciences Workshop, Molecular and Materials Structure Network, Australian Research Council.

Professional Service & Honors

2015-2016 Reviewed publications for *Nature Scientific Instruments*
2013- Board Chairman and Vice President, the UQ Foundation

2009-2016 Reviewed publications for *Python in Science Conference*, *Optics Express*, and *Journal of Computational Science*

03/2011 NIST American Recovery and Reinvestment Act (NIST-ARRA) Senior Fellowship proposal selected for funding; I did not accept the position and funding

2008-2011 Reviewed proposals for Spallation Neutron Source (SNS) ARCS, SEQUOIA, CNCS, BASIS, POWGEN, and NPD beamlines

06/2008 Oak Ridge Institute for Science and Education (ORISE) Instrument Development Fellowship selected for funding; Department of Energy (DoE) did not release the funding

06/2006 Finalist for Oak Ridge National Laboratory (ORNL) Clifford G. Shull Fellowship

2005-2010 Reviewed software engineering design and implementation for DANSE project; monthly formal and weekly informal reviews of software work products from Caltech, Columbia, Michigan State, Maryland, Tennessee, and Iowa State development teams

08/2003, 03/2014 Reviewed grant proposals for the U.S. Civilian Research and Development Foundation

2002-2003 Reviewed publications for *Canadian Journal of Chemistry* and *Optics Express*

06/2002 National Research Council (NRC) fellowship proposal selected for funding; NASA reorganization deleted the position and funding

1999-2002 Awarded National Science Foundation (NSF) GK-12 graduate teaching fellowship; taught kindergarten through graduate students

07/2000 Attended Caltech Summer School for Planetary Sciences, an introduction to NASA proposal and mission planning for young investigators

Grants & Contracts

* LMCO, “Efficient Optimal Engineering Design of Alloys for Additive Manufacturing”, $100k, 2024 (PI).
* LANL, “Fast Realization of a Robust Quantum Sensor using Adaptive Learning”, $50k, 2024.
* LANL, “Quantum Computing for High Energy Density Science”, $3.0M, 2024-2026 (CoPI).
* LANL, “Predictive Response Model of Dual-Axis Radiographic Hydrodynamic Test (DARHT) End Targets”, $232k, 2024.
* Vybe, “Development and Testing Environment to Test Vybe Energy’s Cloud-based Demand Optimization Application”, $30k, 2023-2024 (PI).
* LMCO, “Closed Loop Artificial Intelligence Machine to Fabricate Additive Materials Effectively”, $24k, 2023 (PI).
* LANL, “Machine-Learning Optimal Flux Limiters for Hydrodynamic Calculations”, $60k, 2023 (CoPI).
* LANL, “Enabling robust, real-time, automated Rietveld refinement”, $250k, 2022-2023 (PI).
* LANL, “Unwrapping radiograph target disassembly measurements using robust predictive surrogate models”, $250k, 2022-2023.
* LANL, “Enabling Real-time Scattering Data Analysis with Scalable Optimization”, $150k, 2022-2023 (PI).
* LANL, “Accelerating Scientific Discovery by Advancing Data Analysis for Diffraction Experiments”, $15k, 2022.
* LANL, “Flattening the Rietveld Learning Curve”, $100k, 2021-2022 (PI).
* LANL, “Flattening the Rietveld Learning Curve”, $60k, 2021-2022 (CoPI).
* LANL, “Unwrapping Radiograph Target Disassembly using Adaptive Machine Learning”, $60k, 2021-2022.

* LANL, “Charged Particle Beam Control and Diagnostics using Adaptive Machine Learning”, $5.0M, 2022-2025 (CoPI).
* LANL, “Adaptive Machine Learning for Closely Spaced Ultra-Short Intense Accelerator Beams”, $630k, 2020-2021 (CoPI).
* LANL, “Machine Learning for Realizing Next-Generation Quantum Hardware”, $5.0M, 2020-2023 (CoPI).
* LANL, “Real-time Production of Accurate and Optimal Surrogates of Molecular Dynamics Simulations via Active Learning”, $50k, 2020 (CoPI).
* LANL, “Demonstration of surrogate guided learning of chemical reaction surfaces”, $40k, 2020 (PI).
* LANL, “Adaptive Machine Learning for Advanced Diagnostics and Autonomous Control of Particle Accelerators”, $300k, 2019-2020.
* LMCO, “Validation and Verification framework for model and process optimization”, $40k, 2019-2020 (PI).
* Roche, “Model Unification, Multidimensional HMM, and Automation of the Simulation-Experiment Calibration Pipeline”, $450k, 2019-2020 (PI).
* Vybe, “Integrate Mystic into Hybrid Energy Grid Optimization”, $6k, 2019 (PI).
* LANL, “Enabling Predictive Scale-Bridging Simulations through Active Learning”, $4.7M, 2019-2021.
* LANL, “Compare Optimal Uncertainty Quantification and Sampling Methods in the Context of Materials Strength Models with Limited or Missing Information”, $60k, 2016.
* LANL, “Develop and Implement a Comprehensive Rigorous and Algorithmic Uncertainty Quantification Framework in the Context of Materials Simulations”, $450k, 2014-2016.
* BNL, “Solving the Nanostructure Problem”, $100k, 2013-2014 (PI).
* AFOSR, “Scientific Computation of Optimal Statistical Estimators”, $900k, 2012-2015.
* LANL, “UQ and V&V for the Exascale Co-design Center for Materials in Extreme Environments”, $150k, 2012-2013.
* DOE BES, “Measuring the Dynamics of Excited Materials and Molecules”, $300k, 2007.
* NSF IMR-MIP, “DANSE: Distributed Data Analysis for Neutron Scattering Experiments”, $12M, 2006-2012.

Books & Book Chapters

* M. McKerns, F. Alexander, K. Hickmann, T. J. Sullivan, D. Vaughn, “Optimal Bounds on Nonlinear Partial Differential Equations in Model Certification, Validation, and Experiment Design”, in: K. Kleese van Dam, et al. (Eds.), Advanced Analysis Solutions for Leading Experimental Techniques 978-981-120-444-9 (World Scientific, 2020).
* M. McKerns, “Is Automated Materials Design and Discovery Possible?”, in: T. Lookman, et al. (Eds.), Materials Discovery and Design: By Means of Data Science and Optimal Learning 978-3-319-99465-9 (Springer, 2018).
* M. McKerns (Ed.), “Introduction to Software for Uncertainty Quantification” in: R. Ghanem, et al, (Eds.), Handbook of Uncertainty Quantification, 978-3-319-12385-1 (Springer, 2017).
* C. Scovel, H. Owhadi, T. Sullivan, M. McKerns, M. Ortiz, “What is UQ?”, Los Alamos National Laboratory Associate Directorate for Theory, Simulation, and Computation (ADTSC) Science Highlights LA-UR 12-20429 (2012).
* B. Fultz, T. Kelley, M. McKerns, J. Lin, J. Lee, O. Delaire, M. Kresch, M. Aivazis, Experimental Inelastic Neutron Scattering (California Institute of Technology, 2004).

* M. McKerns, Characterization of Molecular Structure, Excited-state Absorption, and Nonlinear Optical Response of Metallotexaphyrin Complexes, Doctoral Dissertation (University of Alabama at Birmingham, 2002).

Journal Articles

* C. Uzun, M. McKerns, M. Boshier, "Machine learning optimization of a guided atom interferometer", (in preparation).
* P. Czarnik, M. McKerns, A. Sornborger, L. Cincio, "Efficient optimal learning of quantum landscapes", (in preparation).
* T. Bersano, M. McKerns, C. Uzun, M. Boshier, "Online learning of accurate surrogates for the efficient optimization of complex systems", (in preparation).
* L.H. Nguyen, T.J. Sullivan, M. McKerns, H. Owhadi, "Automated dimensional reduction as optimization constraints", (in preparation).
* R. Chiodi, N. Nguyen-Fotiadis, M. McKerns, A. Sornborger, D. Livescu, "Deriving a B-spline slope limiter for the Euler equations using machine learning", (in preparation).
* M. McKerns, L. Roth, N. Iyengar, D. Lamm, "Rigorous bounds on the failure of shielding due to helium-ion radiation", (in preparation).
* N. Nguyen-Fotiadis, R. Chiodi, M. McKerns, D. Livescu, A. Sornborger, "Probabilistic flux limiters", (in preparation).
* C.M. Biwer, Z. Feng, D. Finstad, M. McDonnell, M. McKerns, D.J. Savage, M. Knezevic, S.C. Vogel, "Spotlight: efficient automated global optimization in Rietveld analysis of diffraction data", (under review).
* P. Czarnik, M. McKerns, A. Sornborger, L. Cincio, "Robust design under uncertainty in quantum error mitigation", https://arxiv.org/abs/2307.05302 (under review).
* P. Czarnik, M. McKerns, A. Sornborger, L. Cincio, "Improving the efficiency of learning-based error mitigation", https://arxiv.org/abs/2204.07109 (under review).
* A. Diaw, M. McKerns, I. Sagert, L. G. Stanton, M. S. Murillo, "Efficient learning of accurate surrogates for simulations of complex systems", https://arxiv.org/abs/2207.12855 (to be published in *Nature Machine Intelligence*).
* D.J. Savage, L. Lutterotti, C.M. Biwer, M. McKerns, C. Bolme, M. Knezevic, S.C. Vogel, "MILK: a Python scripting interface to MAUD for automation of Rietveld analyses", *Journal of Applied Crystallography* 56(4), 1277, (2023).
* S. Karra, M. Mehana, N. Lubbers, Y. Chen, A. Diaw, J.E. Santos, A. Pachalieva, R.S. Pavel, J.R. Haack, M. McKerns, C. Junghans, Q. Kang, D. Livescu, T.C. Germann, H.S. Viswanathan, "Predictive scale-bridging simulations through active learning", https://arxiv.org/abs/2209.09811, *Scientific Reports* 13, 16262, (2023).
* N. Nguyen-Fotiadis, M. McKerns, A. Sornborger, "Machine learning changes the rules for flux limiters", *Physics of Fluids* 34, 085136, (2022).
* A. Diaw, K. Barros, J. Haack, C. Junghans, B. Keenan, Y.W. Li, D. Livescu, N. Lubbers, M. McKerns, R.S. Pavel, D. Rosenberger, I. Sagert, T.C. Germann, "Multiscale simulation of plasma flows using active learning", *Physical Review E* 102(2), 023310, (2020).
* D.C. Price, S. Celles, P.T. Eendebak, M.M. McKerns, E.M. Olson, C. Raffel, B. Yi, "Hickle: A HDF5-based python pickle replacement", *Journal of Open Source Software*, 3(32), 1115, https://doi.org/10.21105/joss.01115 (2018).
* F. Khoshnoud, I.I. Esat, C.W. de Silva, M.M. McKerns, H. Owhadi, "Self-powered dynamic systems in the framework of optimal uncertainty quantification", *ASME Journal of Dynamic Systems, Measurement, and Control* 139(9), 091005-1 (2017).

* P.H.T. Kamga, B. Li, M. McKerns, J. Mihaly, L.H. Nguyen, M. Ortiz, H. Owhadi, A.J. Rosakis, T.J. Sullivan, "Optimal uncertainty quantification with model uncertainty and legacy data", *Journal of the Mechanics and Physics of Solids* 72, 1 (2014).
* P. Juhas, M. McKerns, S. Billinge, "Nanostructure studies using complex modeling method", *Acta Crystallographica* A70, 1435 (2014).
* T.J. Sullivan, M. McKerns, D. Meyer, F. Theil, H. Owhadi, M. Ortiz, "Uncertainty quantification for legacy data observations of Lipschitz functions", *Mathematical Modeling and Numerical Analysis* 47, 1657 (2013).
* H. Owhadi, T.J. Sullivan, M. McKerns, M. Ortiz, C. Scovel, "Optimal uncertainty quantification", *SIAM Review* 55(2), 271 (2013).
* M. Adams, A. Lashgari, B. Li, M. McKerns, J. Mihaly, M. Ortiz, H. Owhadi, A.J. Rosakis, M. Stalzer, T.J. Sullivan, "Rigorous model-based uncertainty quantification with application to terminal ballistics. Part II: systems with uncontrollable inputs and large scatter", *Journal of Mechanics and Physics of Solids*, 60(5), 1002 (2012).
* A.A. Kidane, A. Lashgari, B. Li, M. McKerns, M. Ortiz, H. Owhadi, G. Ravichandran, M. Stalzer, T.J. Sullivan, "Rigorous model-based uncertainty quantification with application to terminal ballistics. Part I: systems with controllable inputs and small scatter", *Journal of Mechanics and Physics of Solids*, 60(5), 983 (2012).
* T.J. Sullivan, U. Topcu, M. McKerns, H. Owhadi, "Uncertainty quantification via codimension-one partitioning", *International Journal for Numerical Methods in Engineering*, 85, 1499 (2011).
* C.W. Li, M.M. McKerns, B. Fultz, "A Raman spectroscopy study of phonon anharmonicity of zirconia at elevated temperatures", *Journal of the American Ceramic Society*, 94(1), 224 (2011).
* J.B. Keith, J.R. Fennick, D.R. Nelson, C.E. Junkermeier, J.Y.Y. Lin, C.W. Li, M.M. McKerns, J.P. Lewis, B. Fultz, "AtomSim: web-deployed atomistic dynamics simulator", *Journal of Applied Crystallography*, 43, 1553 (2010).
* C.W. Li, M.M. McKerns, B. Fultz, "A Raman spectroscopy study of phonon anharmonicity of hafnia at elevated temperatures", *Physical Review B* 80, 054304 (2009).
* A. Spivey, V. Fedorov, M. McKerns, C. Lawson, S. Mirov, "Amplification of narrow line LiF:F_2^{+**} color center laser oscillation", *Optics Communications*, 254, 290 (2005).
* M. McKerns, W. Sun, C. Lawson, G. Gray, "Higher-order triplet interaction in energy-level modeling of excited-state absorption for an expanded porphyrin cadmium complex", *Journal of the Optical Society of America B*, 22(4), 852 (2005).
* C. Byeon, M. McKerns, W. Sun, T. Nordlund, C. Lawson, G. Gray, "Excited state lifetime and intersystem crossing rate of asymmetric pentaazadentate porphyrin-like metal complexes", *Applied Physics Letters*, 84(25), 5174 (2004).
* P. Mouroulis, M. McKerns, "Pushbroom imaging spectrometer with high spectroscopic data fidelity: experimental demonstration", *Optical Engineering*, 39, 808 (2000).
* W. Sun, C. Byeon, M. McKerns, C. Lawson, G. Gray, D. Wang, "Optical limiting performances of asymmetric pentaazadentate porphyrin-like cadmium complexes", *Applied Physics Letters*, 73(9), 1167 (1998).
* W. Sun, C. Byeon, M. McKerns, C. Lawson, J. Dunn, M. Hariharasarma, G. Gray, "Oxidative enhancement of the $\chi^{(3)}$ values of solutions of *cis*-$Mo(CO)_4L_2$ (L = PPh_3, $AsPh_3$, PPh_2Np) complexes as measured by DFWM", *Optical Materials*, 11, 87 (1998).

Proceedings

* J.E. Koglin, J.E. Coleman, M. McKerns, D. Ronquillo, A. Scheinker, "Progress toward improving accelerator performance and automating operations with advanced analysis

software", *Proceedings of the North American Particle Accelerator Conference,* NAPAC2022, TUPA55, (2022).

* A. Paleyes, M. Mahsereci, M. McKerns, M. Naslidnyk, G. Pleiss, J. Wenger, "Scientific Software Development", in *Probabilistic Numerical Methods - From Theory to Implementation*, Dagstuhl Seminar 21432, *Dagstuhl Reports,* 11(9) (2022).
* A. Mohan, Z. Cao, M. Anghel, M. Maltrud, C. Sweeney, M. McKerns, X. Davis, "Multiscale reduced order modeling and parameter estimation for climate sciences", in *Artificial Intelligence for Earth System Predictability,* AI4ESP2021, 10.2172/1769752, (2021).
* B.T. Nadiga, M. McKerns, M.A. Taylor, "Co-evolving climate models under uncertainty to improve predictive skill", in *Artificial Intelligence for Earth System Predictability,* AI4ESP2021, 10.2172/1769688, (2021).
* F. Khoshnoud, M. McKerns, C. de Silva, H. Owhadi, I. Esat, R. Bosner, "Self-powered and bio-inspired dynamic systems: research and education", *Proceedings of ASME,* 50541, V04AT05A046 (2016).
* T.J. Sullivan, M. McKerns, M. Ortiz, H. Owhadi, C. Scovel, "Optimal uncertainty quantification: distributional robustness versus Bayesian brittleness" *ASME Journal of Medical Devices*, 7(4), 040920 (2013).
* M. Ortiz, M. McKerns, H. Owhadi, T. J. Sullivan, C. Scovel, "Optimal uncertainty quantification" in *Advanced Computational Engineering*, 12-18 February 2012. *Olberwolfach Reports*, 9(1), (2012).
* M.M. McKerns, L. Strand, T. Sullivan, A. Fang, M.A.G. Aivazis, "Building a framework for predictive science", *Proceedings of the 10th Python in Science Conference*, 67 (2011).
* T.J. Sullivan, M. McKerns, U. Topcu, H. Owhadi, "Uncertainty quantification via codimension-one domain partitioning and a new concentration inequality" *Procedia – Social and Behavioral Sciences*, 2(6), 7751 (2010).
* P.A. Kienzle, N. Patel, M. McKerns, "Parallel kernels: an architecture for distributed parallel computing", *Proceedings of the 8th Python in Science Conference*, 36 (2009).
* M. McKerns, Q. Wei, C. Lawson, S.B. Mirov, G.M. Gray, "Studies of metal organic complexes with a powerful tunable laser", *Frontiers in Optics*, OSA Technical Digest MT19 (2003).
* W. Sun, M. McKerns, C. Lawson, G. Gray, C. Zahn, D. Wang, "Solvent effect on third-order nonlinearity and optical limiting ability of a stilbazolium-like dye", *Proceedings of SPIE*, 4106, 280 (2000).
* W. Sun, C. Byeon, M. McKerns, C. Lawson, S. Dong, D. Wang, G. Gray, "Characterization of third-order nonlinearity of [(CH_3-TXP)Cd]Cl", *Proceedings of SPIE*, 3798, 107 (1999).
* W. Sun, C. Byeon, M. McKerns, C. Lawson, G. Gray, D. Wang, "Relationship between chemical structure and optical limiting properties of asymmetric pentaazadentate porphyrin-like metal complexes", *Proceedings of SPIE*, 3472, 127 (1998).
* W. Sun, C. Byeon, M. McKerns, C. Lawson, J. Dunn, M. Hariharasarma, G. Gray, "Enhancement of the third-order susceptibilities of *cis*-$Mo(CO)_4(PPh_3)_2$ solution by oxygen in different solvents", *Proceedings of SPIE*, 3472, 108 (1998).

Released Software

* D.J. Savage, et al, "MILK: MAUD interface language kit", *https://github.com/lanl/MILK* (2022-present).
* N. Nguyen-Fotiadis, et al, "fluxlimiter: machine learning for flux limiters", *https://github.com/lanl/fluxlimiter* (2022-present).

* C.W. Biwer, et al, “spotlight: distributed-computing for Rietveld analyses using an ensemble of local optimizers”, *http:/github.com/lanl/spotlight* (2019-present).
* M. McKerns, “multiprocess: better multiprocessing and multithreading in python”, *http://pypi.org/project/multiprocess* (2015-present).
* M. McKerns, “ppft: distributed and parallel python”, *http://pypi.org/project/ppft* (2014-present).
* M. McKerns, “klepto: persistent caching to memory, disk, or database”, *http://pypi.org/project/klepto* (2014-present).
* S.J.L. Billinge, et al, “diffpy-cmi: python libraries for complex modeling initiative”, *http://diffpy.org* (2014-2015).
* M. McKerns, “dill: serialize all of python”, *http://pypi.org/project/dill* (2010-present).
* M. McKerns, M.A.G. Aivazis, “pox: filesystem exploration and automated builds”, *http://pypi.org/project/pox* (2010-present).
* M. McKerns, M.A.G. Aivazis, “pyina: MPI parallel map and cluster scheduling”, *http://pypi.org/project/pyina* (2010-present).
* M. McKerns, M.A.G. Aivazis, “pathos: parallel graph management and execution in heterogeneous computing”, *http://pypi.org/project/pathos* (2010-present).
* J.Y.Y. Lin, J.B. Keith, A. Dementsov, N. Markovskiy, X. Tang, M. McKerns, M. Aivazis, B. Fultz, “VNF: a facility for computational neutron scattering science”, *http://vnf.caltech.edu* (2010-2012).
* M. McKerns, P. Hung, M.A.G. Aivazis, “mystic: highly-constrained non-convex optimization and uncertainty quantification”, *http://pypi.org/project/mystic* (2009-present).
* B. Fultz, et al., “DANSE: distributed data analysis for neutron scattering experiments”, *http://danse.us* (2006-2011).
* M. McKerns, “pyIDL: python bindings to IDL”, *http://pypi.org/project/pyIDL* (2005-present).
* M. McKerns, “pygrace: python bindings to Grace 2-D plotting”, *http://pypi.org/project/pygrace* (2005-present).
* T. Kelley, M. McKerns, J. Lin, J. Lee, O. Delaire, M. Kresch, M. Aivazis, B. Fultz, “ARCS: software for a wide angular-range chopper spectrometer at the SNS”, *http://www.cacr.caltech.edu/projects/ARCS/Software.html* (2004-2007).
* M.A.G. Aivazis, et al., “pyre: an integration framework for high-performance computing”, *http://danse.us/trac/pyre* (2003-2011).

Technical Reports & White Papers

* M. McKerns, “Machine learning for optimal ccuracy and robustness under uncertainty”, *UQF Technical Report* (in preparation).
* M. McKerns, “Rigorous model validation”, *UQF Technical Report* (in preparation).
* S. Batha, et al., “Fuel dopants in ICF: using ML to optimize performance burn”, *LANL Technical Report* (April, 2024).
* M. McKerns, et al., “Design of novel artificial intelligence workflows for accelerated time-to-discovery”, *LANL Technical Report* (March, 2024).
* M. McKerns, et al., “Robust surrogate-accelerated design of complex engineering systems”, *LANL Technical Report* (March, 2024).
* M. Cerezo, et al., “A new paradigm for hybrid quantum computation”, *DOE ASCR Technical Report* (February, 2024).
* C. Uzun, et al., “Transforming quantum sensors through adaptive learning”, *LANL Technical Report* (February, 2024).

* D. Savage, et al., “Enabling component scale microstructure diagnostics using Bragg-edge radiography”, *LANL Technical Report* (February, 2024).
* N. Nguyen-Fotiadis, et al., “Statistically-robust generative learning of flux limiters for multifluid plasma flow simulations”, *LANL Technical Report* (February, 2024).
* M. Aguilo, et al., “Nuclear full system optimization”, *DOE ASCR Technical Report* (January, 2024).
* M. Aguilo, et al., “Accelerating the design cycle for space additive manufacturing”, *DARPA DSO Technical Report* (November, 2023).
* C. Uzun, et al., “Fast realization of a robust quantum sensor using adaptive learning”, *LANL Technical Report* (October, 2023).
* M. McKerns, et al., “Capability demonstrations of high-impact science enabled by real-time Rietveld analysis”, *LANL Technical Report* (October, 2023).
* M. McKerns, et al., “Real-time multimodal Rietveld refinement of materials parameters”, *LANL Technical Report* (October, 2023).
* M. McKerns, et al., “Automated real-time discovery and mapping of multi-dimensional phase boundaries”, *LANL Technical Report* (October, 2023).
* C. Uzun, et al., “Efficient adaptive learning-based optimization to realize a robust quantum sensor”, *LANL Technical Report* (October, 2023).
* T. Bersano, et al., “Enhancing efficiency of sampling for optimizer-directed machine learning”, *LANL Technical Report* (October, 2023).
* D. Savage, et al., “Accelerating diffraction analysis with the diffraction vocabulary”, *LANL Technical Report* (October, 2023).
* M. Aguilo, et al., “A performance portable photovoltaic simulator with automatic differentiation targeting performance, reliability, and scalability of photovoltaic modules in solar energy markets”, *DOE ASCR Technical Report* (October, 2023).
* Y. Rosen, et al., “Quantum computing for high energy density science”, *LANL Technical Report* (September, 2023).
* J. Koglin, et al., “Predictive response model of dual-axis radiographic hydrodynamic test (DARHT) end targets”, *LANL Technical Report* (July, 2023).
* M. McKerns, et al., “AIBL: a scalable artificial intelligence framework for beamline science”, *DOE OSC Technical Report* (June, 2023).
* F. Alexander, et al., “Foundations for optimal operations of complex uncertain systems (FO^{2}CUS)”, *DOE OSC Technical Report* (June, 2023).
* A. Marino, et al., “Accelerating the path toward networked quantum systems”, *DOE OSC Technical Report* (June, 2023).
* R. Chiodi, et al., “Discovering optimal flux-limiter algorithms”, *LANL Technical Report* (May, 2023).
* C. Sweeney, et al., “Reinforcement learning for building accurate surrogates for plasma hydrodynamics”, *LANL Technical Report* (May, 2023).
* M. McKerns, et al., “Realtime design of diffraction experiments using active learning”, *LANL Technical Report* (May, 2023).
* C. Biwer, et al., “Adaptive learning of accurate surrogates for Rietveld-EVPSC-coupled models”, *LANL Technical Report* (May, 2023).
* M. Sangid, et al., “Combining material informatics and high throughput testing to enable material aware topology optimization”, *DARPA DSO Technical Report* (April, 2023).
* F. Alexander, et al., “AI for Science: Software Accelerating Progress Toward a Fusion Pilot Plant”, *DOE OSC Technical Report* (March, 2023).
* M. McKerns, et al., “Robust domain-aware online adaptive scientific machine learning”, *ASCR SciML Technical Report* (March, 2023).

* M. McKerns, et al., “Active machine learning optimization of quantum sensors”, *LANL Technical Report* (February, 2023).
* D. Savage, et al., “Machine learning of single crystal elastic properties of U-6Nb under experimental uncertainty”, *LANL Technical Report* (November, 2022).
* D. Savage, et al., “Determination of single crystal elastic properties of U-6Nb under experimental uncertainty using physics-informed learning”, *LANL Technical Report* (October, 2022).
* C. Biwer, et al., “Enabling Real-time Scattering Data Analysis with Scalable Optimization”, *LANL Technical Report* (September, 2022).
* C. Biwer, et al., “Accelerating Scientific Discovery by Advancing Data Analysis for Diffraction Experiments”, *LANL Technical Report* (February, 2022).
* A. Sornborger, et al., “AI for Efficient Quantum Machine Learning”, *LANL Technical Report* (February, 2022).
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* M. McKerns, “mystic: software for autonomous discovery and design under uncertainty”, *CAMERA Technical Report* (April, 2021).
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* E. Kober, et al., “Robust Unsupervised Learning for Understanding Reaction Processes of Energetic Materials”, *DOE ASC Technical Report* (April, 2020).
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* M. McKerns, E. Kober, “Optimal Design of Learned Models for Chemical Reaction Surfaces of Energetic Materials”, *LANL Technical Report* (October, 2019).
* M. McKerns, et al., “Optimal Bounds for Nonlinear Partial Differential Equations in Model Certification, Validation, and Experiment Design”, *LANL Technical Report* (May, 2019).
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* M. McKerns, “mystic: a Brief Introduction”, *LANL Technical Report* (March 2019).
* M. McKerns, et al., “Physics-Injected Optimal Learning for Beamline Science”, *LANL Technical Report* (February, 2019).
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* A. Scheinker, M. McKerns, et al., “Non-Evasive Diagnostics and Adaptive 6D Control of Particle Accelerator Beams”, *LANL Technical Report* (April, 2018).
* M. McKerns, et al., “Critical Feature Extraction and Anomaly Detection in High-Dimensional Data”, *LANL Technical Report* (March, 2018).
* M. McKerns, et al., “Active Learning in Optimal Management of Extreme-Scale Computing Resources”, *LANL Technical Report* (February, 2018).
* F. Khoshnoud, et al., “Nature-inspired Navigation Algorithms for Autonomous Maneuvering in the Framework of Optimal Uncertainty Quantification, and Efficient Experimental Validation Techniques”, *NASA Technical Report* (July, 2017).
* F. Khoshnoud, et al., “Solar Powered Airships: Toward Infinite Endurance Unmanned Vehicles”, *NASA Technical Report* (October, 2016).
* M. McKerns, et al., “Compare Optimal Uncertainty Quantification and Sampling Methods in the Context of Materials Strength Models with Limited or Missing Information”, *LANL Technical Report* (June, 2016).
* D. Morgan, et al., “Universal Structure Identification Toolkit”, *DOE BES Technical Report* (April, 2016).
* L. Dalton, et al., “Optimal Statistical Inference for Accelerated Materials Discovery”, *DARPA Technical Report* (June, 2015).
* M. McKerns, et al., “Adaptive Workflow Optimization of Extreme-Scale Computing Resources”, *DOE ASCR Technical Report* (May 2015).
* G. Jacobs, et al., “Machine Learning for Intelligent Multiscale Simulations of Flows with Stochasticity”, *DARPA Technical Report* (March, 2015).
* T. Sahai, et al., “System Certification for Rare Events and Model Error”, *DARPA Technical Report* (March, 2015).
* H. Owhadi, et al., “Hierarchical Information Games for Discovery in Materials Science”, *DARPA Technical Report* (January, 2015).
* M. McKerns, “Optimization and Uncertainty Quantification at Exascale”, *Caltech Technical Report* (July, 2014).
* S. Billinge, et al., “Towards Understanding and Control on Nano-scale Fluctuations in Strongly Correlated Electron Systems”, *BNL Technical Report* (July, 2014).
* M. McKerns, et al., “Optimal Statistical Inference and Error Estimation”, *DARPA Technical Report* (June, 2014).
* M. McKerns, T. Sullivan, “Critical Feature Extraction and Anomaly Detection in High-Dimensional Data”, *DARPA Technical Report* (May, 2014).
* H. Owhadi, M. McKerns, “Develop and Implement a Comprehensive Rigorous and Algorithmic Uncertainty Quantification Framework in the Context of Materials Simulations”, *LANL Technical Report* (March, 2014).
* M. McKerns, et al., “Uncertainty Quantification Methodologies for Enabling Extreme-Scale Science”, *DOE ASCR Technical Report* (February, 2014).
* R. James, et al., “Multiscale Methods for the Discovery of Robust Functional Materials ”, *DoD Technical Report* (December, 2013).
* B. Fultz, J.J. Rehr, S.J.L. Billinge, et al., “Workflows for Computational Scattering Science 2013”, *NSF Technical Report* (August, 2013).
* M. McKerns, “Solving the Nanostructure Problem”, *BNL Technical Report* (July, 2013).
* R. Harrison, et al., “Extreme Scale Modeling and Optimal Uncertainty Quantification”, *DOE SC Technical Report* (July, 2013).

* W. Lindquist, et al., “IMCSF – an Integrated Mathematics Center for Science Facilities”, *DOE SC Technical Report*, (April, 2012).
* H. Owhadi, M. McKerns, “Hierarchical Information Flow in the Simulation and Analysis of Diffraction and Scattering Experiments at Next-generation Scientific Facilities”, *DOE BES Technical Report* (April, 2012).
* H. Owhadi, et al., “UQ and V&V for the Exascale Co-design Center for Materials in Extreme Environments”, *LANL Technical Report*, (April, 2012).
* H. Owhadi, et al., “Scientific Computation of Optimal Statistical Estimators”, *AFOSR Technical Report* (March, 2012).
* H. Owhadi, et al., “Information Flow in Heterogeneous Multiscale Materials”, *DOD ONR Technical Report* (September, 2011).
* M. McKerns, M. Aivazis, M. Stalzer, “Exploring the CACR Scientific Engineering Pipeline”, *Caltech CACR Technical Report* (August, 2011).
* M. Stalzer, et al., “Rigorous Quantification of Uncertainty for Biological Reaction Networks”, *NSF Technical Report* (January, 2011).
* B. Fultz, G.G. Long, K.W. Herwig, et al., “Report from Workshop on Computational Scattering Science 2010”, *NSF / DOE BES Technical Report* (January, 2011).
* M. McKerns, H. Owhadi, C. Scovel, T.J. Sullivan, M. Ortiz, “The optimal uncertainty algorithm in the mystic framework”, *Caltech Technical Report* (August, 2010).
* M. McKerns, “Predictive Science for Biological Soft Condensed Matter”, *NIST Technical Report* (July, 2010).
* M. McKerns, “Time-resolved Measurements of the Electronic Excited State and the Rational Design of Energy Materials”, *Caltech Technical Report* (September, 2008).
* B.Fultz, et al., “Measuring the Dynamics of Excited Materials and Molecules”, *DOE BES Technical Report*, (December, 2007).
* B. Fultz, M. Aivazis, M. McKerns, S. Billinge, P. Butler, P. Kienzle, T. Swain, E. Ustundag, “DANSE diversity strategic plan”, *NSF Technical Report* (September, 2007).
* B. Fultz, et al., “DANSE: Distributed Data Analysis for Neutron Scattering Experiments”, *NSF Technical Report*, (March, 2006).
* B. Fultz, M. McKerns, “Accomplishments under the DANSE CED design effort”, *NSF Technical Report* (December, 2005).
* M. McKerns, J. McCorquodale, B. Fultz, “Distributed analysis of neutron scattering experiments on the TeraGrid”, *ORNL Technical Report* (May, 2005).

Invited Talks

* M. McKerns, “mystic and pathos: the summer project that evolved into a career of research in artificial intelligence, machine learning, and high-performance computing”, *Seattle Pacific University Engineering and Computer Science Seminar Series,* Seattle, WA (2024).
* M. McKerns, “mystic and the optimization accelerant”, *Enthought Executive Meeting*, Austin, TX (2024).
* M. McKerns, “time-series forecasting for power management”, *Morphorm Executive Meeting*, Albuquerque, NM (2024).
* M. McKerns, “introduction to mystic (and pathos)”, *Workshop on X-ray and Neutron Diffraction Data Analysis Automation,* Los Alamos, NM (2023).
* M. McKerns, “mystic: tools for AI, UQ, ML, model validation, and robust design under uncertainty”, *Lockheed Martin CLAIM2FAME Seminar,* Palo Alto, CA (2023).
* M. McKerns, “mystic and pathos: the summer project that evolved into a career of research in artificial intelligence, machine learning, and high-performance computing”,

FIU Knight Foundation School of Computing and Information Sciences Lecture Series, Miami, FL (2023).

* M. McKerns, "mystic: tools for AI, UQ, ML, model validation, and robust design under uncertainty", *CM4QC Group Seminar,* Virtual (2022).
* M. McKerns, "mystic: tools for AI and robust design under uncertainty", *UQ Tools Workshop,* Los Alamos, NM (2022).
* M. McKerns, "mystic: physics-informed learning and automated design/control under uncertainty", *JPL ITSD Open Developer Series,* Pasadena, CA (2021).
* M. McKerns, "mystic: physics-informed learning and automated design/control under uncertainty", *Applied Machine Learning Symposium*, Los Alamos, NM (2021).
* M. McKerns, "mystic: software for autonomous discovery and design under uncertainty", *Autonomous Discovery in Science and Engineering,* Berkeley, CA (2021).
* M. McKerns, A. Diaw, I. Sagert, L. Stanton, M. Murillo, "adaptive learning with directed sampling", *Nambe Meeting*, Los Alamos, NM (2020).
* M. McKerns, "mystic: machine learning for model validation and engineering design under uncertainty", *Lockheed Martin Feed Your Brain*, Denver, CO (2020).
* M. McKerns, "mystic: rigorous model validation and engineering design under uncertainty", *Roche Santa Clara Team Seminar*, Santa Clara, CA (2019).
* M. McKerns, "mystic: rigorous model validation and engineering design under uncertainty", *Computational Data Science Approaches for Materials Conference*, Los Alamos, NM (2019).
* M. McKerns, "mystic: rigorous model validation and engineering design under uncertainty", *Lockheed Martin Space Systems Materials Development Group Meeting*, Lawrence, KS (2019).
* M. McKerns, "mystic: rigorous model validation and engineering design under uncertainty", *Edwards Air Force Base Test Wing Seminar*, Edwards, CA (2018).
* M. McKerns, "mystic: rigorous model validation and engineering design under uncertainty", *Roche Santa Clara Team Seminar*, Santa Clara, CA (2018).
* M. McKerns, "mystic: rigorous model certification and engineering design under uncertainty", *LANL STR Workshop*, Los Alamos, NM (2018).
* M. McKerns, "Emerging trends in machine learning, risk analytics, and robust design", *Enthought Lunch & Learn Seminar Series*, Austin, TX (2018).
* M. McKerns, "mystic: rigorous model certification and engineering design under uncertainty", *LANL ANSI Seminar*, Los Alamos, NM (2018).
* M. McKerns, "Is rigorous automated materials design and discovery possible?", *Computational Neuroscience Group Meeting*, Princeton, NJ (2017).
* M. McKerns, "What is a trait and why should (or shouldn't) I use it?", *Roche Santa Clara Team Seminar*, Santa Clara, CA (2017).
* M. McKerns, "Is rigorous automated materials design and discovery possible?", *New York Scientific Data Summit*, New York, NY (2017).
* M. McKerns, "Is rigorous automated materials design and discovery possible?", *Data Analysis and Modeling Group Seminar*, Oak Ridge, TN (2017).
* M. McKerns, "Is rigorous automated materials design and discovery possible?", *Computational Science Initiative Seminar*, Upton, NY (2017).
* M. McKerns, "Is rigorous automated materials design and discovery possible?", *LIGO Group Seminar*, Pasadena, CA (2017).
* M. McKerns, "Is rigorous automated materials design and discovery possible?", *Information Sciences Group Seminar*, Los Alamos, NM (2017).
* M. McKerns, "Is rigorous automated materials design and discovery possible?", *Materials Genome Initiative Seminar*, Gaithersburg, MD (2016).

* M. McKerns, “Is rigorous automated materials design and discovery possible?”, *Data Science and Optimal Learning for Materials Discovery and Design Workshop*, Santa Fe, NM (2016).
* M. McKerns, “Are rigorous predictions in the stock market, battlefield scenarios, engineering design, and natural disasters possible?”, *Brunel University Department of Mechanical, Aerospace, and Civil Engineering Seminar*, Oxford, UK (2016).
* M. McKerns, “Statistical rigor versus statistical confidence in the optimal design of materials” [Keynote], *The Minerals, Metals, and Materials Society Meeting*, Nashville, TN (2016).
* M. McKerns, “Living with ‘dirty’ data while avoiding exascale ‘garbage in, garbage out’”, *Salishan Conference on High-Speed Computing*, Gleneden Beach, OR (2015).
* M. McKerns, “Redesigning optimization and UQ for exascale”, *ASCR Exascale Co-Design Program Meeting*, Livermore, CA (2015).
* M. McKerns, T. Sullivan, C. Scovel, H. Owhadi, “OUQ+mystic: a framework for uncertainty quantification and predictive science”, *Information Science for Materials Discovery and Design Workshop*, Santa Fe, NM (2014).
* M. McKerns, H. Owhadi, T. Sullivan, C. Scovel, A. Fang, M. Aivazis, “'mystic' and uncertainty quantification in materials design, analysis, and failure”, *T-1 Division Seminar*, Los Alamos, NM (2013).
* H. Owhadi, M. McKerns, J. Belak, “Uncertainty quantification”, *Exascale Co-Design Center for Materials in Extreme Environments All-Hands Meeting*, Santa Fe, NM (2013).
* H. Owhadi, C. Scovel, T. Sullivan, M. McKerns, M. Ortiz, D. Meyer, F. Theil, B. Li, S. Brunett, L. Nguyen, P. Kamga, “Optimal uncertainty quantification”, *PSAAP Tri-Lab Sponsor Team Visit Meeting*, Pasadena, CA (2012).
* M. McKerns, H. Owhadi, T. Sullivan, A. Fang, L. Nguyen, M. Aivazis, “mystic: the Caltech UQ pipeline’s optimization framework”, *PSAAP Tri-Lab Sponsor Team Visit Meeting*, Pasadena, CA (2012).
* M. McKerns, H. Owhadi, T. Sullivan, C. Scovel, M. Ortiz, “mystic: a software framework for predictive science”, *LLNL CASC Seminar*, Livermore, CA (2012).
* J. Belak, D. Orikowski, S. Applegate, H. Owhadi, M. McKerns, “Quantifying model uncertainty”, *DOE/ASCR Exascale Research Conference*, Arlington, VA (2012).
* T. Sullivan, B. Li, M. McKerns, D. Meyer, L.H. Nguyen, M. Ortiz, H. Owhadi, C. Scovel, F. Theil, “Optimal uncertainty quantification: towards a paradigm shift in predictive science”, *PSAAP V&V/UQ Workshop*, Ann Arbor, MI (2012).
* M. McKerns, H. Owhadi, T. Sullivan, C. Scovel, B. Li, S. Brunett, L. Strand, M. Aivazis, M. Ortiz, “Optimal uncertainty quantification as a driver for future large scale simulation”, *PSAAP V&V/UQ Workshop*, Ann Arbor, MI (2012).
* M. McKerns, “OUQ + mystic + pathos”, *Exascale Co-Design Center for Materials in Extreme Environments Working Meeting*, Pacific Grove, CA (2012).
* M. McKerns, “Building a framework for predictive science”, *BNL Scientific Computing Seminar*, Upton, NY (2012).
* H. Owhadi, C. Scovel, T. Sullivan, M. McKerns, M. Ortiz, “The optimal uncertainty quantification framework applied to the seismic safety assessment of a truss structure”, *SIAM Conference on Uncertainty Quantification*, Raleigh, NC (2012).
* H. Owhadi, C. Scovel, T. Sullivan, M. McKerns, M. Ortiz, “Optimal uncertainty quantification”, *PSAAP Site Visit Meeting*, Pasadena, CA (2011).
* H. Owhadi, C. Scovel, T. Sullivan, M. McKerns, M. Ortiz, “Optimal uncertainty quantification”, *PSAAP Tri-Lab Sponsor Team Visit Meeting*, Pasadena, CA (2011).
* M. McKerns, “A massively-parallel framework for optimization and parameter sensitivity analysis”, *DANSE Developer’s Workshop*, Pasadena, CA (2011).

* M. McKerns, “A massively-parallel heterogeneous computing framework for optimization and parameter sensitivity analysis”, *IPAM Workshop on Optimization, Search and Graph-Theoretical Algorithms for Chemical Compound Space*, Los Angeles, CA (2011).
* H. Owhadi, C. Scovel, T. Sullivan, M. McKerns, M. Ortiz, “Bridging scales with incomplete information – optimal uncertainty quantification”, *BIRS Workshop*, Banff, Alberta, Canada (2011).
* M. McKerns, P. Butler, P. Kienzle, “SANS & reflectometry software in DANSE”, *Mantid / DANSE Collaboration Workshop*, Oak Ridge, TN (2011).
* M. McKerns, “Component-based distributed parallel optimization”, *Mantid / DANSE Collaboration Workshop*, Oak Ridge, TN (2011).
* M. McKerns, J. Lin, P. Juhas, “Analysis software available from DANSE”, *Mantid / DANSE Collaboration Workshop*, Oak Ridge, TN (2011).
* M. McKerns, P. Butler, P. Kienzle, “SANS & reflectometry software in DANSE”, *Mantid / DANSE Collaboration Workshop*, Didcot, England (2011).
* M. McKerns, “Component-based distributed parallel optimization”, *Mantid / DANSE Collaboration Workshop*, Didcot, England (2011).
* M. McKerns, J. Lin, P. Juhas, “Analysis software available from DANSE”, *Mantid / DANSE Collaboration Workshop*, Didcot, England (2011).
* H. Owhadi, M. Ortiz, M. McKerns, C. Scovel, A. Lashgari, B. Li, L. Lucas, T. Sullivan, U. Topcu, F. Theil, “UQ protocols with legacy data”, *PSAAP Site Visit Meeting*, Pasadena, CA (2010).
* M. McKerns, “Component-based distributed parallel optimization”, *DANSE Developer’s Workshop*, Pasadena, CA (2010).
* M. McKerns, “Mystic and pathos: what’s new?”, *DANSE Developer’s Workshop*, Pasadena, CA (2010).
* M. McKerns, “Status and future of: frameworks for optimization & high-performance computing”, *DANSE Developer’s Workshop*, Oak Ridge, TN (2010).
* M. McKerns, L. Strand, M. Aivazis, “The DANSE distributed service framework”, *DANSE Developer’s Workshop*, Pasadena, CA (2010).
* M. McKerns, J. Trater, S. Miller, “DANSE high-performance and distributed computing at the SNS”, *NSSD Cybersecurity Policy Meeting*, Oak Ridge, TN (2010).
* H. Owhadi, M. Ortiz, M. McKerns, C. Scovel, T. Sullivan, U. Topcu, A. Lashgari, B. Li, “Optimal uncertainty quantification”, *PSAAP Tri-Lab Sponsor Team Visit Meeting*, Pasadena, CA (2010).
* M. McKerns, “DANSE project plan & progress”, *DANSE Developer’s Workshop*, Pasadena, CA (2010).
* M. McKerns, “The mystic optimization framework”, *DANSE Developer’s Workshop*, Pasadena, CA (2010).
* H. Owhadi, M. McKerns, M. Ortiz, L. Lucas, A. Lashgari, B. Li, T. Sullivan, U. Topcu, M. Adams, L. Lambertson, J.M. Mihaly, A.J. Rosakis, “UQ: past, present, and future directions”, *PSAAP Site Visit Meeting*, Pasadena, CA (2009).
* M. McKerns, “DANSE project plan & progress”, *DANSE Developer’s Workshop*, Pasadena, CA (2009).
* M. McKerns, “Introduction to DANSE”, *DANSE Developer’s Workshop*, Pasadena, CA (2009).
* M. McKerns, “Optimization and parameter sensitivity”, *DANSE Developer’s Workshop*, Pasadena, CA (2009).
* M. McKerns, “Large-scale and high-impact computing”, *DANSE Developer’s Workshop*, Pasadena, CA (2009).

* M. McKerns, “DANSE distributed framework services”, *DANSE Developer’s Workshop*, Oak Ridge, TN (2009).
* M. McKerns, “DANSE project management”, *NSF IMR-MIP: DANSE CONST Annual Review*, Pasadena, CA (2009).
* M. McKerns, “DANSE project plan & progress”, *DANSE Developer’s Workshop*, Pasadena, CA (2009).
* M. McKerns, M.A.G. Aivazis, B. Fultz, “DANSE facility update”, *NOBUGS Conference*, Sydney, Australia (2008).
* M. McKerns, “Management of change”, *NSF IMR-MIP: DANSE CONST Annual Review*, Arlington, VA (2008).
* M. McKerns, “DANSE project infrastructure”, *DANSE Developer’s Workshop*, Pasadena, CA (2008).
* M. McKerns, “DANSE release planning”, *DANSE Developer’s Workshop*, Pasadena, CA (2007).
* M. McKerns, “DANSE project management”, *NSF IMR-MIP: DANSE CONST Annual Review*, Manassas, VA (2007).
* M. McKerns, M. Aivazis, K. Herwig, B. Fultz, “Extending the neutron scientist’s toolkit”, *NCNR Software Group Seminar*, Gaithersburg, MD (2007).
* M. McKerns, “DANSE project plan”, *DANSE Developer’s Workshop*, Oak Ridge, TN (2007).
* M. McKerns, “DANSE component design”, *DANSE Developer’s Workshop*, Oak Ridge, TN (2007).
* M. McKerns, “Data analysis and the (inelastic) instrument scientist's toolkit”, *SNS Inelastic Group Seminar*, Oak Ridge, TN (2006).
* M. McKerns, “A data analysis framework for the neutron community”, *XSD Scientific Software Workshop*, Argonne, IL (2006).
* M.M. McKerns, M.A.G. Aivazis, B. Fultz, “DANSE: extending the scientific toolkit for the neutron community”, *NOBUGS Conference*, Berkeley, CA (2006).
* M. McKerns, “The DANSE project plan”, *DANSE Project Kickoff Meeting*, Pasadena, CA (2006).
* M. McKerns, “A data analysis framework for the neutron community”, *Australian Research Council e-Research for the Structural Sciences Workshop*, Sydney, Australia (2006).
* M.M. McKerns, “DANSE: extending the scientific toolkit for the neutron community”, *American Conference on Neutron Scattering*, St. Charles, IL (2006).
* M. McKerns, “Measurement and design of electronic excited-state materials”, *CIT Neutron Group Seminar*, Pasadena, CA (2006).
* M. McKerns, “Techniques for the measurement and design of electronic excited-state materials”, *UAB Physics Dept. Seminar*, Birmingham, AL (2006).
* M. McKerns, “New techniques for the measurement and design of electronic excited-state materials”, *Clifford G. Shull Fellowship Presentation*, Oak Ridge, TN (2006).
* M. McKerns, “DANSE project management”, *NSF IMR-MIP: DANSE CONST Site Visit*, Oak Ridge, TN (2005).
* M. McKerns, “Vibrational study of electronic excited-states using pump-probe neutron scattering”, *USC CAM Group Seminar*, Los Angeles, CA (2005).
* M. McKerns, “Code integration and build procedure for pyre components”, *DANSE Project Workshop*, Pasadena, CA (2004).
* M. McKerns, “DANSE components”, *DANSE Project Workshop*, Pasadena, CA (2004).
* M. McKerns, “Grid services light”, *Neutron Scattering Software Workshop*, Pasadena, CA (2004).

* M. McKerns, M. Aivazis, B. Fultz, "DANSE -- distributed data analysis for neutron scattering experiments", *Neutron Scattering Software Initiative*, Oak Ridge, TN (2003).
* M. McKerns, "XML and distributed data analysis for neutron scattering experiments", *Neutron Scattering Software Workshop*, Pasadena, CA (2003).
* M. McKerns, "The DANSE client and server", *Neutron Scattering Software Workshop*, Pasadena, CA (2003).
* M. McKerns, "Designing a generic crystal structure container class", *Neutron Scattering Software Workshop*, Pasadena, CA (2003).
* M. McKerns, B. Fultz, "Proof of concept software: a demonstration of DANSE", *SNS Experimental Facilities Advisory Committee Meeting*, Oak Ridge, TN (2003).
* M. McKerns, "New directions in the characterization of organic NLO materials", *U.S. Air Force Academy Physics Dept. Seminar*, Colorado Springs, CO (2002).
* M. McKerns, "New technique for determining wavelength-dependent nonlinear optical response", *U.S. ARL Nonlinear Optics Division Seminar*, Adelphi, MD (2002).
* M. McKerns, "Correlating molecular structure and NLO response of metallotexaphyrin complexes", *UAB Physics Dept. Seminar*, Birmingham, AL (2001).
* M. McKerns, "Oxidative effect on nonlinear optical properties of metal-organics", *UAB Physics Dept. Seminar*, Birmingham, AL (1997).

Contributed Presentations

* J. Koglin, R. Chiodi, M. Woodward, D. Livescu, M. McKerns, N. Ramey, J. Waters, K. Perez, E. McDugald, "Predictive response model of dual-axis radiographic hydrodynamic test (DARHT) end targets", *LDRD 20240552MFR Phase 1 Review,* Los Alamos, NM (2024).
* M. McKerns, C. Biwer, D. Savage, S. Vogel, "Enabling real-time scattering data analysis with scalable optimization", *Pathfinder Review,* Los Alamos, NM (2023).
* Z. Feng, D.J. Savage, C.M. Biwer, M. McKerns, S.C. Vogel, "Developing fast optimization strategies for automated real-time Rietveld analysis", *MST Scattering Team Seminar,* Los Alamos, NM (2023).
* Z. Feng, D.J. Savage, C.M. Biwer, M. McKerns, "MILKing the HIPPO – automated approach to batch Rietveld refinement" [Poster], *LANL Student Symposium,* Los Alamos, NM (2023).
* M. Woodward, P. Chiodi, D. Livescu, M. McKerns, H. Morris, N. Ramey, J. Coleman, J. Koglin, "Physics informed reduced electron evolution models from rapid target heating based on measurements", *65th Annual Meeting of the APS Division of Plasma Physics,* Denver, CO (2023).
* J. Koglin, M. McKerns, A. Scheinker, D. Wakeford, "Machine learning for radiographic source optimization at linear induction accelerators" [Poster], *Digital Holography and Three Dimensional Imaging,* Boston, MA (2023).
* M. McKerns, "software infrastructure for adaptive learning", *LDRD 20220074DR Year 1 Review,* Los Alamos, NM (2023).
* C. Uzun, M. McKerns, K. Krzyzanowska, S. Panday, M. Martin, M. Boshier, "Optimizing a guided atom interferometer using machine learning" [Poster], *54th Annual Meeting of the APS Division of Atomic, Molecular, and Optical Physics,* Spokane, WA (2023).
* T. Bersano, C. Uzun, M. McKerns, M. Martin, M. Boshier, "Optimizing atom transfer in a double magneto-optical trap system with machine learning" [Poster], *54th Annual Meeting of the APS Division of Atomic, Molecular, and Optical Physics,* Spokane, WA (2023).

* M. Martin, M. McKerns, A. Sornborger, “Machine Learning for Realizing Next-Generation Quantum Hardware”, *LDRD 20210116DR Year 2 Review,* Los Alamos, NM (2023).
* D. Savage, C. Biwer, M. McKerns, C. Bolme, S. Vogel, “Scalable Rietveld refinements of diffraction”, *2023 TMS Annual Meeting & Exhibition,* San Diego, CA (2023).
* M. McKerns, “Flattening the Rietveld Learning Curve”, *Pathfinder Review,* Los Alamos, NM (2022).
* R. Chiodi, N. Nguyen-Fotiadis, M. McKerns, A. Sornborger, D. Livescu, “Machine Learning Flux-Limiters for Compressible Flow Simulations”, *75th Annual Meeting of the Division of Fluid Dynamics,* Indianapolis, IN (2022).
* P. Czarnik, M. McKerns, A. Sornborger, L. Cincio, “Improving the efficiency of learning-based error mitigation” [Poster], *Quantum Techniques in Machine Learning,* Naples, IT (2022).
* M. McKerns, “mystic: tools for AI, UQ, ML, model validation, and robust design under uncertainty”, *LDRD 20220074DR Group Meeting,* Los Alamos, NM (2022).
* M. McKerns, “the mystification of MAUD: an introduction to mystic”, *DMMSC ML Workshop,* Los Alamos, NM (2022).
* J. Koglin, J. Coleman, M. McKerns, H. Morris, N. Ramey, A. Scheinker, E. Toler, A. Williams, “Unwrapping radiographic target disassembly using adaptive machine learning”, *ISTI Project Seminar,* Albuquerque, NM (2022).
* E.H. Toler, J.E. Coleman, J.E. Koglin, M. McKerns, H.E. Morris, A. Scheinker, A.B. Williams, “Unwrapping Image Data Using Adaptive Machine Learning” [Poster], *North American Particle Accelerator Conference,* Albuquerque, NM (2022).
* J.E. Koglin, J.E. Coleman, M. McKerns, D. Ronquillo, A. Scheinker, K.L Van Buren, A.B. Williams, E.H. Toler, “Progress toward improving accelerator performance and automating operations with advanced analysis software” [Poster], *North American Particle Accelerator Conference,* Albuquerque, NM (2022).
* M. McKerns, “software infrastructure for active and optimal statistical learning”, *LDRD 20210116DR Midterm Review,* Los Alamos, NM (2022).
* M. McKerns, “efficient active learning of valid surrogates”, *LDRD 20190005DR Group Meeting* (2021).
* M. McKerns, “rigorous model validation and optimal design/control under uncertainty”, *LANL Information Sciences Group Meeting*, Los Alamos, NM (2021).
* J. Haack, A. Diaw, R. Pavel, I. Sagert, B. Keenan, D. Livescu, N. Lubbers, M. McKerns, C. Junghans, T. Germann, “Enabling Predictive Scale-bridging Simulations through Active Learning”, *APS Division of Plasma Physics Meeting*, Virtual (2021).
* J. Haack, A. Diaw, K. Barros, C. Junghans, B. Keenan, Y.W. Li, D. Livescu, N. Lubbers, M. McKerns, R.S. Pavel, D. Rosenberger, I. Sagert, T. Germann, “Multiscale Simulation of Plasma Flows Using Active Learning”, *APS Division of Plasma Physics Meeting*, Virtual (2020).
* M. McKerns, “adaptive learning with dynamic sampling”, *LDRD 20190005DR Group Meeting* (2020).
* M. McKerns, “mystic: a Brief Introduction”, *LDRD 20210160DR Group Meeting* (2020).
* M. McKerns, “mystic: a Brief Introduction”, *LDRD 20210116DR Group Meeting* (2020).
* M. McKerns, “model validity active learning”, *LDRD 20190005DR Midterm Review*, Los Alamos, NM (2020).
* A. Diaw, J. Haack, M. McKerns, R. Pavel, “Multiscale Simulation Method for Plasma Flows”, *APS March Meeting*, Virtual (2020).
* I. Sagert, J. R. Haack, A. Diaw, C. Junghans, B. Keenan, N. E. Lubbers, M. McKerns, R. S. Pavel, D. Livescu, “A 3D Multi-Species Kinetic-Fluid Coupling Technique for HEDP

Simulations" [Poster], *International Conference on Numerical Simulations of Plasmas*, Santa Fe, NM (2019).

* M. McKerns, "mystic: rigorous model validation and engineering design under uncertainty", *Advanced Control Methods for Particle Accelerators*, Santa Fe, NM (2019).
* M. McKerns, "physics-injected optimal learning under uncertainty", *LANL Information Sciences Group Meeting*, Los Alamos, NM (2019).
* C.M. Biwer, S. Vogel, M. McKerns, J. Ahrens, "Developing automation and data exploration capabilities for diffraction analysis" [Poster], *the 2018 LANSE User Group Meeting*, Santa Fe, NM (2018).
* M. McKerns, "Dynamic optimization and machine learning using mystic", *the 17th Python in Science Conference*, Austin, TX (2018).
* M. McKerns, "mystic: rigorous model certification and engineering design under uncertainty", *LANL Python Workshop*, Los Alamos, NM (2018).
* M. McKerns, "mystic: rigorous model certification and engineering design under uncertainty", *SIAM Conference on Uncertainty Quantification*, Garden Grove, CA (2018).
* M. McKerns, "Modern optimization methods in python", *the 16th Python in Science Conference*, Austin, TX (2017).
* M. McKerns, "Scalable hierarchical parallel computing", *the 9th European Conference on Python in Science*, Erlangen, DE (2016).
* M. McKerns, "Efficient python for high-performance parallel computing", *EuroPython*, Bilbao, ES (2016).
* M. McKerns, "Scalable hierarchical parallel computing", *the 15th Python in Science Conference*, Austin, TX (2016).
* M. McKerns, "Efficient python for high-performance parallel computing", *PyCon*, Portland, OR (2016).
* M. McKerns, "mystic: Highly-constrained non-convex optimization and uncertainty quantification", *SIAM Conference on Parallel Processing for Scientific Computing*, Paris, FR (2016).
* M. McKerns, "mystic: Highly-constrained non-convex optimization and uncertainty quantification", *SIAM Conference on Uncertainty Quantification*, Lausanne, CH (2016).
* M. McKerns, "Modern optimization methods in python", *PyCon Ireland*, Dublin, IE (2015).
* M. McKerns, "klepto: Unified persistent storage to memory, disk, or database", *the 8th European Conference on Python in Science*, Cambridge, UK (2015).
* M. McKerns, "Modern optimization methods in python", *EuroPython*, Bilbao, ES (2015).
* M. McKerns, "klepto: Unified persistent storage to memory, disk, or database", *the 14th Python in Science Conference*, Austin, TX (2015).
* M. McKerns, "Modern optimization methods in python", *the 14th Python in Science Conference*, Austin, TX (2015).
* M. McKerns, "Efficient python for high-performance parallel computing", *the 14th Python in Science Conference*, Austin, TX (2015).
* M. McKerns, "Are rigorous predictions in the stock market, battlefield scenarios, engineering design, and natural disasters possible?", *ASME Verification & Validation Symposium*, Las Vegas, NV (2015).
* M. McKerns, H. Owhadi, T. Sullivan, C. Scovel, A. Fang, M. Aivazis, "'mystic' and uncertainty quantification in materials design, analysis, and failure" [Poster], *Opportunities in Materials Informatics*, Madison, WI (2015).
* M. McKerns, "The failure of python object serialization", *PyCon Ireland*, Dublin, IE (2014).

* M. McKerns, “The lack of reproducibility in statistical science, and how to fix it”, *PyCon Ireland*, Dublin, IE (2014).
* M. McKerns, “The failure of python object serialization”, *PyCon UK,* Coventry, UK (2014).
* M. McKerns, “The lack of reproducibility in statistical science, and how to fix it”, *PyCon UK*, Coventry, UK (2014).
* M. McKerns, “The failure of python object serialization”, *the 7th European Conference on Python in Science*, Cambridge, UK (2014).
* M. McKerns, T. Sullivan, C. Scovel, H. Owhadi, “mystic and rigorous validation in statistical science” [Poster], *the 7th European Conference on Python in Science*, Cambridge, UK (2014).
* M. McKerns, “The failure of python object serialization”, *the 13th Python in Science Conference*, Austin, TX (2014).
* M. McKerns, “Don’t be a lemming, statistically speaking”, *the 13th Python in Science Conference*, Austin, TX (2014).
* M. McKerns, T. Sullivan, C. Scovel, H. Owhadi, “mystic and the path to rigorous validation in statistical science” [Poster], *the 13th Python in Science Conference*, Austin, TX (2014).
* M. McKerns, “pathos: a framework for parallel graph management and execution in heterogeneous computing”, *the 25th International Conference for High Performance Computing, Networking, Storage and Analysis*, Denver, CO (2013).
* M. McKerns, T. Sullivan, C. Scovel, H. Owhadi, “Using mystic for optimal performance modeling and risk”, *the 25th International Conference for High Performance Computing, Networking, Storage and Analysis*, Denver, CO (2013).
* M. McKerns, T. Sullivan, C. Scovel, H. Owhadi, “mystic: a framework for optimal performance modeling” [Poster], *the 25th International Conference for High Performance Computing, Networking, Storage and Analysis*, Denver, CO (2013).
* M. McKerns, H. Owhadi, T. Sullivan, C. Scovel, A. Fang, M. Aivazis, “Predicting Black Swan Events”, *PyCon India*, Bangalore, India (2013).
* M. McKerns, H. Owhadi, T. Sullivan, C. Scovel, A. Fang, M. Aivazis, “mystic: a framework for predictive science” [Poster], *the 6th Annual Conference of Python in Science*, Brussels, Belgium (2013).
* M. McKerns, H. Owhadi, T. Sullivan, C. Scovel, A. Fang, M. Aivazis, “'mystic': a framework for predictive science”, *SIAM Annual Meeting*, San Diego, CA (2013).
* M. McKerns, H. Owhadi, T. Sullivan, C. Scovel, A. Fang, M. Aivazis, “'mystic': a framework for predictive science”, *the 12th Python in Science Conference*, Austin, TX (2013).
* D. Marsden, M. McKerns, H. Owhadi, T. Sullivan, C. Scovel, “Supporting the right scientific tools for reproducibility” [Poster], *the 12th Python in Science Conference*, Austin, TX (2013).
* M. McKerns, H. Owhadi, T. Sullivan, C. Scovel, A. Fang, M. Aivazis, “'mystic' and uncertainty quantification in materials design, analysis, and failure” [Poster], *SIAM Conference on Mathematical Aspects of Materials Science*, Philadelphia, PA (2013).
* M. McKerns, H. Owhadi, T. Sullivan, A. Fang, M. Aivazis, “OUQ+mystic: a framework for uncertainty quantification and predictive science”, *Mathematical Challenges of Molecular Dynamics Meeting*, Coventry, UK (2013).
* M. McKerns, H. Owhadi, T. Sullivan, A. Fang, M. Aivazis, “mystic: a framework for predictive science” [Poster], *the Python Conference*, Santa Clara, CA (2013).

* M. McKerns and H. Owhadi, "UQ and performance testing/optimization", *Exascale Co-Design Center for Materials in Extreme Environments All-Hands Meeting*, Santa Ana Pueblo, NM (2013).
* M. McKerns, H. Owhadi, T. Sullivan, A. Fang, L. Nguyen, M. Aivazis, "mystic: a framework for global optimization and uncertainty quantification", *SIAM Conference on Computational Science and Engineering*, Boston, MA (2013).
* M. McKerns, A. Fang, S. Brunett, T. Sullivan, M. Aivazis, "Software infrastructure of Caltech's uncertainty quantification pipeline" [Poster], *Scientific Workflows for Scattering Science Workshop*, Pasadena, CA (2013).
* M. McKerns, L. Strand, P. Kienzle, M.A.G. Aivazis, "Mystic: a framework for global optimization and heterogeneous computing" [Poster], *Scientific Workflows for Scattering Science Workshop*, Pasadena, CA (2013).
* J. Lin, B. Keith, A. Dementsov, M. McKerns, M. Aivazis, B. Fultz, "Virtual Neutron Facility" [Poster], *Scientific Workflows for Scattering Science Workshop*, Pasadena, CA (2013).
* T. Sullivan, M. McKerns, M. Ortiz, H. Owhadi, "Optimal uncertainty quantification using data-validated models" [Poster], *PSAAP V&V/UQ Workshop*, Ann Arbor, MI (2012).
* K. Smith, M. McKerns, S. Ross-Ross, "Efficient Parallel Python for High-Performance Computing", *the 11th Python in Science Conference*, Austin, TX (2012).
* M. McKerns, "Efficient Programming for Parallel Python", *PyGotham Conference*, Manhattan, NY (2012).
* M. McKerns, A. Fang, S. Brunett, T. Sullivan, M. Aivazis, "Software infrastructure of Caltech's uncertainty quantification pipeline" [Poster], *PSAAP Site Visit Meeting*, Pasadena, CA (2011).
* T. Sullivan, M. McKerns, D. Meyer, M. Ortiz, H. Owhadi, F. Theil, "Optimal uncertainty quantification using legacy data and validated models" [Poster], *PSAAP Site Visit Meeting*, Pasadena, CA (2011).
* M.M. McKerns, L. Strand, T. Sullivan, A. Fang, M.A.G. Aivazis, "Building a framework for predictive science", *the 10th Python in Science Conference*, Austin, TX (2011).
* M. McKerns, A. Fang, S. Brunett, T. Sullivan, M. Aivazis, "Software infrastructure of Caltech's uncertainty quantification pipeline" [Poster], *PSAAP Tri-Lab Sponsor Team Visit Meeting*, Pasadena, CA (2011).
* T. Sullivan, M. McKerns, D. Meyer, M. Ortiz, H. Owhadi, F. Theil, "Optimal uncertainty quantification using legacy data" [Poster], *PSAAP Tri-Lab Sponsor Team Visit Meeting*, Pasadena, CA (2011).
* T. Sullivan, D. Balzani, M. McKerns, M. Ortiz, H. Owhadi, C. Scovel, "Optimal uncertainty quantification and certification of material response", *Second Annual Caltech Solid Mechanics Symposium*, Pasadena, CA (2011).
* T. Sullivan, M. McKerns, M. Ortiz, H. Owhadi, C. Scovel, "Optimal uncertainty quantification", *ASME International Mechanical Engineering Congress & Exposition*, Vancouver, BC (2010).
* M. McKerns, A. Fang, S. Brunett, T. Sullivan, M. Aivazis, "Software infrastructure of Caltech's uncertainty quantification pipeline" [Poster], *PSAAP Site Visit Meeting*, Pasadena, CA (2010).
* L. Strand, M. Aivazis, M. McKerns, "Hydra" [Poster], *PSAAP Site Visit Meeting*, Pasadena, CA (2010).
* M. Aivazis, S. Brunett, B. Li, M. McKerns, "UQ pipeline operational performance considerations for OTM model" [Poster], *PSAAP Site Visit Meeting*, Pasadena, CA (2010).

* T. Sullivan, D. Meyer, M. McKerns, H. Owhadi, F. Theil, M. Ortiz, "Certification using legacy data McDiarmid diameter estimation and optimal bounds" [Poster], *PSAAP Site Visit Meeting*, Pasadena, CA (2010).
* J.B. Keith, J.Y. Lin, M. McKerns, A. Dementsov, N. Markovskiy, X. Tang, M. Aivazis, B. Fultz, "VNF: virtual neutron facility", *NOBUGS Conference*, Gatlinburg, TN (2010).
* T. Sullivan, U. Topcu, M. McKerns, H. Owhadi, "Uncertainty quantification via codimension one domain partitioning and a new concentration inequality", *the 6th International Conference on Sensitivity Analysis of Model Output*, Milano, Italy (2010).
* T. Sullivan, U. Topcu, M. McKerns, H. Owhadi, "Uncertainty quantification via codimension one domain partitioning and a new concentration inequality", *the 2010 SIAM Annual Meeting*, Pittsburgh, PA (2010).
* M. McKerns, "Mystic: a framework for optimization & uncertainty quantification", *the 9th Python in Science Conference*, Austin, TX (2010).
* M. McKerns, "Serialization of python objects with dill", *the 9th Python in Science Conference*, Austin, TX (2010).
* M. McKerns, M.A.G. Aivazis, K.W. Herwig, B. Fultz, "New analysis software available from DANSE", *American Conference on Neutron Scattering*, Ottawa, ON (2010).
* J.Y. Lin, J.B. Keith, M. Aivazis, M. McKerns, A. Dementsov, N. Markovskiy, X. Tang, B. Fultz, "Virtual neutron facility", *American Conference on Neutron Scattering*, Ottawa, ON (2010).
* M. McKerns, L. Strand, P. Kienzle, M.A.G. Aivazis, "Mystic: a framework for global optimization and heterogeneous computing" [Poster], *American Conference on Neutron Scattering*, Ottawa, ON (2010).
* M. McKerns, S. Brunett, M. Aivazis, "Caltech's uncertainty quantification pipeline" [Poster], *PSAAP Tri-Lab Sponsor Team Visit Meeting*, Pasadena, CA (2010).
* L. Strand, M. Aivazis, M. McKerns, "Hydra" [Poster], *PSAAP Tri-Lab Sponsor Team Visit Meeting*, Pasadena, CA (2010).
* A. Lashgari, B. Li, M. McKerns, M. Ortiz, H. Owhadi, T. Sullivan, U. Topcu, C. Scovel, "Optimal uncertainty quantification" [Poster], *PSAAP Tri-Lab Sponsor Team Visit Meeting*, Pasadena, CA (2010).
* M. McKerns, S. Brunett, M. Aivazis, "Caltech's uncertainty quantification pipeline" [Poster], *ASC Principal Investigators Meeting*, Las Vegas, NV (2010).
* M. McKerns, H. Owhadi, T. Sullivan, U. Topcu, "Adaptive subdivision in uncertainty quantification" [Poster], *ASC Principal Investigators Meeting*, Las Vegas, NV (2010).
* S. Brunett, J. Cummings, M. McKerns, "Virtual test facility scaling & performance" [Poster], *PSAAP Site Visit Meeting*, Pasadena, CA (2009).
* M. McKerns, T. Sullivan, U. Topcu, "Refinements of McDiarmid's inequality using partitioning: application to uncertainty quantification" [Poster], *PSAAP Site Visit Meeting*, Pasadena, CA (2009).
* M.M. McKerns, M.A.G. Aivazis, K.W. Herwig, B. Fultz, "DANSE: extending the scientific toolkit for the neutron community", *International Conference on Neutron Scattering*, Knoxville, TN (2009).
* J.Y.Y. Lin, J.B. Keith, M. McKerns, M. Aivazis, B. Fultz, "Virtual neutron facility" [Poster], *International Conference on Neutron Scattering*, Knoxville, TN (2009).
* M. McKerns, M.A.G. Aivazis, "A software framework for uncertainty quantification" [Poster], *PSAAP Tri-Lab Sponsor Team Visit Meeting*, Pasadena, CA (2009).
* N. Patel, M. McKerns, P. Kienzle, "Parallel kernels: an architecture for distributed parallel computing", *the 8th Python in Science Conference*, Pasadena, CA (2009).
* M. McKerns, "Pathos: core services for distributed computing", *the 8th Python in Science Conference*, Pasadena, CA (2009).

* M. McKerns, M.A.G. Aivazis, “A software framework for distributed services” [Poster], *NSF IMR-MIP: DANSE CONST Annual Review*, Pasadena, CA (2009).
* M. McKerns, M.A.G. Aivazis, “Engineering design for the UQ pipeline” [Poster], *International Conference for High Performance Computing, Networking, Storage and Analysis*, Austin, TX (2008).
* M. McKerns, M.A.G. Aivazis, “Engineering design for the UQ pipeline” [Poster], *PSAAP Site Visit Meeting*, Pasadena, CA (2008).
* M.M. McKerns, M.A.G. Aivazis, B. Fultz, “DANSE: extending the scientific toolkit for the neutron community” [Poster], *American Conference on Neutron Scattering*, Santa Fe, NM (2008).
* J.Y.Y. Lin, O. Delaire, M. Kresch, J.B. Keith, M. McKerns, M. Aivazis, B. Fultz, “Monte Carlo virtual neutron experiment” [Poster], *American Conference on Neutron Scattering*, Santa Fe, NM (2008).
* J.B. Keith, J. Purewal, C. An, J. Lin, M. McKerns, B. Fultz, “Hydrogen quantum states, dynamics, and nanoconfined melting in potassium intercalated graphite” [Poster], *American Conference on Neutron Scattering*, Santa Fe, NM (2008).
* J. Lin, M. Kresch, P. Hung, J. McCorquodale, O. Delaire, M. McKerns, M. Aivazis, B. Fultz, “Reduction package for neutron inelastic time-of-flight instruments in DANSE” [Poster], *NOBUGS Conference*, Berkeley, CA (2006).
* J. Lin, B. Fultz, M. Aivazis, O. Delaire, M. McKerns, “Instrument simulation under DANSE” [Poster], *American Conference on Neutron Scattering*, St. Charles, IL (2006).
* M.M. McKerns, M.A.G. Aivazis, B. Fultz, “DANSE: extending the scientific toolkit for the neutron community”, *The Minerals, Metals, and Materials Society Meeting*, San Francisco, CA (2005).
* T.L. Swan-Wood, M. Kresch, J. Lin, M. McKerns, B.T. Fultz, “Vibrational entropy of mixing and the phase stability of Al-Ag”, *The Minerals, Metals, and Materials Society Meeting*, San Francisco, CA (2005).
* M.M. McKerns, M.A.G. Aivazis, T.M. Kelley, S.J. Kim, B. Fultz, “DANSE – distributed data analysis for neutron scattering” [Poster], *American Conference on Neutron Scattering*, College Park, MD (2004).
* T. Swan-Wood, M. Kresch, J. Lin, M. McKerns, B. Fultz, “Vibrational entropy of dissolving Ag in Al” [Poster], *American Conference on Neutron Scattering*, College Park, MD (2004).
* T.M. Kelley, B.T. Fultz, M.M. McKerns, M.G. Aivazis, “Data reduction software for chopper spectrometers” [Poster], *American Conference on Neutron Scattering*, College Park, MD (2004).
* M. McKerns, W. Sun, C. Lawson, G. Gray, “New metal-organic nonlinear optical complexes” [Poster], *Alabama EPSCOR Conference*, Montgomery, AL (2000).

Websites & Web Content

* *http://mmckerns.github.io*
* *http://www.uqfoundation.org*
* *https://github.com/mmckerns*
* *http://stackoverflow.com/mmckerns*
* *https://uqfoundation.github.io/mystic*
* *https://uqfoundation.github.io/pathos*
* *https://pypi.org/project/mystic*
* *https://pypi.org/project/pathos*
* *https://pypi.org/project/dill*
* *https://pypi.org/project/pyina*

* *https://pypi.org/project/pox*
* *https://pypi.org/project/klepto*
* *https://pypi.org/project/ppft*
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* *https://pypi.org/project/pyIDL*
* *https://pypi.org/project/pygrace*
* *http://mystic.rtfd.io*
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* *http://ppft.rtfd.io*
* *http://multiprocess.rtfd.io*
* *http://pygrace.rtfd.io*

Trainings & Courses Authored

* M. McKerns, **Practical Data Science** (in preparation).
* M. McKerns, **Foundations of Data Science** (in preparation).
* M. McKerns, **Practical Machine Learning** (in preparation).
* M. McKerns, **Foundations of Machine Learning** (in preparation).
* M. McKerns, **Python for Science** (in preparation).
* M. McKerns, **Foundations of Machine Learning** (September 2019).
* M. McKerns, **Big Data and Scalable Computing** (August, 2018).
* M. McKerns, **Machine Learning** (August, 2018).
* M. McKerns, **Machine Learning** (June, 2018).
* M. McKerns, **Mystic** (April, 2018).
* M. McKerns, **Scalable Computing** (November, 2017).
* M. McKerns, **Modern Optimization Methods** (July, 2017).
* M. McKerns, **Big Data** (July, 2016).
* M. McKerns, **Time-series Analysis in Data Science** (July, 2016).
* M. McKerns, **Python for Data Scientists** (June, 2016).
* M. McKerns, **Parallel Computing in Python** (June, 2016).
* M. McKerns, **Persistent Storage in Python** (June, 2015).
* M. McKerns, **Astronomy of the Universe**, (March, 1999).
* M. McKerns, **Astronomy of the Universe**, (September, 1998).
* M. McKerns, **Astronomy of the Universe**, (March, 1998).
* M. McKerns, **Introductory Physics**, (December, 1997).
* M. McKerns, **Introductory Physics**, (September, 1997).

Teaching Experience

09/2019 Instructor, **Foundations of Machine Learning**, the UQ Foundation.
06/2019 Instructor, **Pandas Mastery Workshop**, Enthought, Inc.
01/2019, 07/2019 Instructor, **Python for Machine Learning**, Enthought, Inc.
08/2018 Instructor, **Big Data and Scalable Computing**, the UQ Foundation.
08/2018 Instructor, **Machine Learning**, the UQ Foundation.
04/2018, 05/2018, 07/2018, 09/2019 Instructor, **Machine Learning Mastery**, Enthought, Inc.
11/2017, 03/2018 Instructor, **Python for Data Analysis**, Enthought, Inc.
07/2016 Instructor, **Big Data**, Logit Academy
07/2016 Instructor, **Time-series Analysis in Data Science**, Logit Academy

06/2016 Instructor, **Data Analysis in Python**, Enthought, Inc.
06/2016 Instructor, **Python for Data Scientists**, Logit Academy
04/2016, 10/2016, 11/2016, 12/2016, 03/2017, 09/2017 Instructor, **Python Foundations**, Enthought, Inc.
08/2015, 11/2015, 12/2015, 03/2016, 05/2016, 03/2017, 04/2017, 05/2017, 06/2017, 07/2017, 10/2017, 12/2017, 02/2019 Instructor, **Python for Data Science**, Enthought, Inc
05/2015 Instructor, **Introduction to Python for Scientists**, Enthought, Inc
12/2014 Instructor, **Advanced Python**, Demonware
07/2012, 10/2012, 10/2013 Instructor, **Python for Acadian Asset Management**, Acadian Asset Management LCC
06/2012, 07/2012, 09/2012, 10/2012, 01/2013, 02/2013, 04/2013, 07/2013, 08/2013, 10/2013, 02/2014, 03/2014, 05/2014, 06/2014, 07/2014, 08/2014, 09/2014, 10/2014, 01/2015, 04/2015, 10/2015 Instructor, **Developing in Athena**, Investment Banking Technology, J.P. Morgan
05/2012, 09/2013, 11/2013, 12/2013, 03/2014, 04/2014, 05/2014, 12/2014, 03/215, 04/2015, 09/2015, 11/2015, 10/2016, 12/2016, 05/2017, 06/2017, 07/2017, 08/2017, 09/2017, 10/2017, 04/2018, 06/2018, 07/2018, 08/2018, 09/2018, 10/2018, 11/2018, 12/2018, 04/2019, 05/2019, 06/2019, 10/2019 Instructor, **Python for Scientists and Engineers**, Enthought, Inc.
02/2012, 05/2012, 06/2012, 08/2012, 11/2012, 08/2013, 01/2014, 09/2015, 01/2016 Instructor, **Python for Athena**, Investment Banking Technology, J.P. Morgan
1999-2003 Teaching Fellow, **NSF GK-12 Program**, Department of Physics, University of Alabama Birmingham
09/2000 Teaching Assistant, **Space Exploration**, Department of Physics, University of Alabama Birmingham
03/1998, 09/1998, 03/1999 Instructor, **Astronomy of the Universe**, Department of Physics, University of Alabama Birmingham
09/1997, 12/1997 Instructor, **Introductory Physics**, Department of Physics, University of Alabama Birmingham
06/1997 Instructor, **Preparatory Physics**, University of Alabama School of Medicine
1994-1997 Teaching Assistant, **General Physics I, II, III**, Department of Physics, University of Alabama Birmingham

Supervision & Mentoring

2022-2023 Robert Chiodi, "Advancements for Adaptive Multi-Physics Plasma Simulations on Next Generation Supercomputers", Postdoc, Computational Physics and Methods, Los Alamos National Laboratory
2021- Cinthia Aldereta, "Machine Learning for Realizing Next-Generation Quantum Hardware", Postdoc, Information Sciences, Los Alamos National Laboratory
07/2021 Nicholas Ezzell, "Neuromorphic Computing", Summer Research Intern, Beyond Moore's Law Project, Los Alamos National Laboratory
07/2011 Andrew Rodriguez, "Maximizing efficiency of parallel optimizers", Summer Undergraduate Research Fellow, PSAAP Project, California Institute of Technology
07/2010 Janet Chen, "Parameter sensitivity for a hypervelocity impact surrogate", Summer Undergraduate Research Fellow, PSAAP Project, California Institute of Technology
07/2010 Alta Fang, "Tools for solving constrained optimization problems", Summer Undergraduate Research Fellow, PSAAP Project, California Institute of Technology
07/2009 Alta Fang, "Optimization algorithms in mystic", Summer Undergraduate Research Fellow, DANSE Project, California Institute of Technology

07/2009 Cesar Cervantes, "Uncertainty in nonlinear optics experiments", Summer Undergraduate Research Fellow, PSAAP Project, California Institute of Technology
07/2009 Matthew Redmond, "Tensor decomposition toolbox", High-school student, Institute for Educational Advancement, DANSE Project, California Institute of Technology
07/2009 Nathan Tsai, "Installation of the virtual neutron facility", High-school student, Institute for Educational Advancement, DANSE Project, California Institute of Technology
07/2008 Nathan Tsai, "2d plotting on the web", High-school student, Institute for Educational Advancement, DANSE Project, California Institute of Technology
07/2008 Reed Molback, "2d plotting with flot", High-school student, Institute for Educational Advancement, DANSE Project, California Institute of Technology
07/2008 Joshua Hardenbrook, "Rendering of geometric shapes", High-school student, Institute for Educational Advancement, DANSE Project, California Institute of Technology
2008-2009 Lisa Mauger, "Raman spectroscopy of excited-state materials", Graduate Student, Materials Science, California Institute of Technology
2006-2012 Chen Li, "Raman spectroscopy of excited-state materials", Graduate Student, Materials Science, California Institute of Technology
2006-2007 Rebecca Stevens, "Neutron scattering of excited-state materials", Graduate Student, Materials Science, California Institute of Technology
07/2006 Daniel Beylkin, "Inverse modeling for phonon density of states", Summer Undergraduate Research Fellow, DANSE Project, California Institute of Technology
07/2005 Eliot Setzer, "Optimization in python", Summer Undergraduate Research Fellow, DANSE Project, California Institute of Technology
07/2005 Jeremy Ehrhardt, "Binding Java to python", Summer Undergraduate Research Fellow, DANSE Project, California Institute of Technology
2004-2006 June Kim, "Framework services for distributed computing", Technical Staff, Center for Advanced Computing Research, California Institute of Technology
07/2004 Victoria Winters, "Scientific plotting in python", Summer Undergraduate Research Fellow, DANSE Project, California Institute of Technology

Meetings & Workshops Organized

Workshop on X-ray and Neutron Diffraction Analysis Automation, Los Alamos, NM, Jun. 5-9, 2023
"Modeling the Near-Earth Environment" Symposium, *American Geophysical Union Fall Meeting,* San Francisco, CA, Dec. 9, 2019
NSF Scientific Software Innovation Institute for Advanced Analysis of X-Ray and Neutron Scattering Data (SIXNS) Workshop, Upton, NY, August 14-15, 2013
"Uncertainty Quantification" Symposium, *SIAM Annual Meeting,* San Diego, CA, July 12, 2013
Python in Science Conference, Austin, TX, June 24-29, 2013
"Emerging Trends In Uncertainty Quantification" Symposium, *SIAM Conference on Computational Science and Engineering,* Boston, MA, Feb. 27, 2013
Python in Science Conference, Austin, TX, July 16-21, 2012
DANSE Developer's Workshop, Pasadena, CA, May 4-6, 2011
DANSE Developer's Workshop, Oak Ridge, TN, May 19-20, 2010
DANSE Developer's Workshop, Pasadena, CA, Jan. 28-30, 2010
DANSE Developer's Workshop, Pasadena, CA, Sept. 24-26, 2009
DANSE Developer's Workshop, Pasadena, CA, May 27-29, 2009
DANSE Developer's Workshop, Pasadena, CA, Jan. 26-27, 2009
DANSE Developer's Workshop, Pasadena, CA, Aug. 25-26, 2008
DANSE Developer's Workshop, Pasadena, CA, Feb. 21-23, 2008
DANSE Project Kickoff Meeting, Pasadena, CA, Aug. 15-16, 2006

Synergistic Activities

Founded the Uncertainty Quantification Foundation, a non-profit for advancement of tools and knowledge supporting uncertainty quantification. Served as Vice President and on the Board of Directors since founding.

Lead developer and maintainer of the *mystic* optimization framework and the *pathos* framework for distributed and high-performance computing – providing key software for over 90$M of federally-funded projects. Primary author of over 10 scientific software packages, half of which are in the top 500 most-downloaded Python-language packages, with over 1.5G downloads of my publicly released software, and used in over 3k open-source packages and over 200k repositories. Educational materials regarding my software have been viewed by over 18M people.

Provided training and/or consulting in software design, HPC, machine learning, statistics, risk, and UQ for several industry and government institutions, including: LANL, SNL, EAFB, J.P. Morgan, Acadian Asset Management, Royal Dutch Shell, Lockheed Martin, and Roche Sequencing Solutions. 20 courses and workshops authored, and over 100 courses and workshops taught. Over 100 invited talks and over 100 contributed presentations.

Mentored over thirty software developers in the design, implementation, and integration of scientific software. Coordinated the development of all DANSE (*http://danse.us*) and UQ Foundation (*http://uqfoundation.org*) work products, including: a global optimization framework, a framework for heterogeneous parallel distributed computing, a neutron experiment simulation framework, and physics kernels for molecular and lattice dynamics, Rietveld refinement, and finite-element and self-consistent modeling.

Co-organized collaboration between DANSE and the Spallation Neutron Source (SNS) on software integration and specification, including distributed and high-performance computing applications. Organized the international DANSE kickoff meeting, and co-organized the semi-annual international meetings on neutron scattering software development. Organized and co-chaired DANSE weekly national virtual meetings.

Co-authored a successful DOE-BES proposal for construction of a time-resolved Raman facility. Coordinated the planning, design, and construction of the $300k time-resolved Raman facility. Served as lab manager of the Raman facility. Co-authored a successful $900k AFOSR proposal to construct a general framework for the calculation of optimal statistical estimators.

Authored three successful LANL subcontract proposals (totaling $660k) for applications of uncertainty quantification to materials simulations. Authored, and served as PI, for a $100k BNL subcontract proposal to build software to enable determination of nanostructures from neutron and x-ray diffraction data.

Played an integral role in planning, writing, and management of a funded 12 $M NSF Construction (CNST) proposal and a funded 3 $M NSF Conceptual and Engineering Design (CED) proposal. Served as Project Manager for the 12 $M NSF IMR-MIP: DANSE software project. Named in the IMR-MIP proposal to direct common scientific algorithm development and coordinate activities in education and outreach.

Guided vision, design, and architecture of prototype software for DANSE CED project, developed budget and work breakdown structure (WBS), and contributed to the project execution plan for IMR-MIP DANSE CNST effort.

Developed the earned value management infrastructure for the DANSE project. Developed project standards and software development practices, software testing and release plan, and coauthored the project's software quality guidelines. Planned and organized online project infrastructure for software versioning, issue tracking, and remote collaboration.

Designed and proposed the first experiment to measure the full phonon density of states for a material or molecule in an electronic excited state; additionally this technique allows for the determination of the variation of lattice parameters as the electronic excited state decays into the electronic ground state. Guided initial research on materials screening for time-resolved neutron measurements.

Devised design path for tailoring electronic properties of electronic excited-state materials. Determined vibrational ground-state structures for a series of metalloporphyrins; additionally a structure-property relationship was inferred through *ab initio* calculation of static hyperpolarizability and analysis of ground-state structure. Devised and performed first *ab initio* simulation to determine solvent effects on molecular structure, hyperploarizablity, and quinoid-aromatic character for a series of metalloporphyrins. Devised and performed first quantum chemical simulation to determine relationship between spectral response and molecular structure for a series of metalloporphyrins.

Developed first model capable of correctly describing nonlinear absorption and excited-state population dynamics in organic reverse-saturable absorbing materials at practical device energies; this technique allowed determination of relationships between phophysical parameters and nonlinear transmission for a series of metalloporphyrin complexes. Designed and built prototype 632 nm pumped LiF:F_2^+** color center laser, tunable in the 850-1050 nm range, capable of producing spectrally-narrow high-energy pulses required for wavelength-tunable nonlinear transmission measurements. Designed and built prototype wavelength-tunable spectrometer to determine singlet and triplet absorption cross-sections as a function of wavelength for electronic excited-state materials.

Additional Information

Reprints of selected publications can be obtained at http://mmckerns.github.io, while preprints of articles in preparation and professional references are available upon request.