ACMD Postdoctoral Opportunities

This document describes National Research Council Postdoctoral Research Associateships tenable within the Applied and Computational Mathematics Division (ACMD) of the NIST Information Technology Laboratory. Research areas of interest include combinatorial and discrete algorithms, computational materials science, computational fluid dynamics, computational electromagnetics, mathematical modeling of magnetic systems, computational biology, orthogonal polynomials and special functions, applied optimization and simulation, combinatorial software testing, data mining, immersive visualization, parallel and distributed algorithms, quantum information science, and statistics for quantum systems. See below for more details on these opportunities and the research advisors associated with them. Candidates are urged to contact potential advisors in advance of formal application. Candidates and their research proposals are evaluated in a competitive process managed by the National Research Council (NRC) Associateship Programs. For further details on the application process, see the link below. For further information on the program within ACMD, contact Ronald Boisvert (boisvert@nist.gov).

NIST NRC Research Associateship Program

- NIST Postdoctoral Research Associateships Program details
- Application Deadline: February 1 or August 1
- U.S. Citizenship Required

ACMD Research Topics and Advisors

Gaithersburg, MD

- Mathematical Modeling
- Dynamical Systems and Computational Biology
- Orthogonal Polynomials, Special Functions, and Digital Repositories
- Computational Fluid Dynamics and Mathematical Modeling
- Combinatorial and Discrete Algorithms
- Mathematical Modeling of Magnetic Systems
- Applied Optimization and Simulation

- Finite Element Analysis of Material Microstructure
- Virtual Measurements from Quantum Chemistry
- Stochastic Modeling, Verification, Validation, and Calibration of Computer Simulations
- Complex Systems and Networks: Performance, Control, and Security
- Cloud Computing and Combinatorial Software Testing
- Quantum Algorithms and Complexity
- Quantum Information and Cryptography
- Quantum Frequency Conversion for Hybrid Quantum Networks
- Computational Methods for the Solution of the Time Dependent Schroedinger Equation
- Scientific Datamining
- Real-time Quantitative Visualization
- Parallel and Distributed Computing Algorithms and Environments

Boulder, CO

- Quantum Information Science
- Statistics for Quantum Systems
- Uncertainty Quantification and Computational Materials Science
- Computational Electromagnetics

Gaithersburg, MD

Mathematical Modeling

Contact: Geoffrey B. McFadden

Working closely with scientists in other NIST laboratories, we formulate large-scale but computationally feasible models, develop efficient computer programs, and validate our simulations by comparison with experimental results. This position requires knowledge of analytical and numerical methods and application areas. It is suitable for candidates whose interest is more in mathematical modeling than in the specific application. Candidates with backgrounds in applied mathematics, engineering, physics, and materials science are encouraged to suggest a specific project.

Opportunity Number: 50.77.11.B2044

Dynamical Systems and Computational Biology

Contact: Fern Hunt

Our research projects are concerned with the application of stochastic processes in nonlinear dynamical systems and computational biology. Data from complex physical and biological systems present challenges to conventional modeling and statistical techniques. The goal is to apply recent theoretical advances in probability and dynamical systems to areas relevant to NIST's mission. We are currently studying dynamical systems that arise from the control of computer networks, as well as the emergence of patterned behavior and aggregation in complex networks.

Opportunity Number: 50.77.11.B6285

Orthogonal Polynomials, Special Functions, and Digital Repositories

Contact: Howard Cohl

This opening in Special Functions is connected with a multidisciplinary program of research and development that focuses on functions that have recognized or potential importance in scientific applications. Research proposals relating to mathematical analysis and computer science in the area of orthogonal polynomials and special functions will be considered. Contact Howard Cohl for further information.

Opportunity Number: 50.77.11.B8087

Computational Fluid Dynamics and Mathematical Modeling

Contact: Geoffrey McFadden

Numerical and analytical methods are used to study problems that involve convection or diffusion in physics and chemistry. Of particular interest is the formulation and implementation of methods that are suitable for large-scale computations. Analysis of model problems is also pursued when appropriate.

One application is the description of convection occurring during the solidification of binary alloys. Interesting features of this problem include the existence of significantly different time scales associated with diffusion of temperature and concentration, and the behavior of the interface between the liquid and solid phases of the material.

Opportunity Number: 50.77.11.B2054

Combinatorial and Discrete Algorithms

Contact: Isabel Beichl

We combine prababilistic methods with combinatorics to solve problems in the physical sciences, which can be formulated as combinatorial counting questions on graphs. We have devised novel formulations of statistical techniques such as importance sampling and Monte Carlo time that can be applied to these graph problems. We plan to extend these techniques to other fundamental problems related to measurement science and optimization of communications.

Opportunity Number: 50.77.11.B5288

Mathematical Modeling of Magnetic Systems

Contact: Mike Donahue

We work with scientists in other NIST laboratories to develop tools for computer simulation and analysis of magnetic systems at the nanometer scale. Model verification is achieved by comparison against experiment and by development of reference problems. Important issues include controlling round-off and truncation error to obtain high accuracy solutions in complex, large scale simulations, and the development towards this end of efficient, highly parallel software running on commodity hardware. Novel methods to compute the stray field from magnetized material with attention to interface and boundary effects are of particular interest. Applications include MRAM, field sensors, and magnetic logic devices.

Opportunity Number: 50.77.11.B4449

Applied Optimization and Simulation

Contact: Anthony Kearsley

Applied Optimization and simulation form an area of engineering that sits between mathematics and computer science. They include computational tools used to solve important problems in engineering, economics, and all branches of science. Current concerns include the development and analysis of algorithms for the solution of problems of estimation, simulation and control of complex systems, and their implementations on computers. We are particularly interested in nonlinear optimization problems, which involve computationally intensive function evaluations. Such problems are ubiquitous; they arise in simulations with finite elements, in making statistical estimates, or simply in dealing with functions that are very difficult to handle. The comparability among the various techniques for numerical approximation through optimization algorithms is very important. What makes one formulation for the solution of a problem more desirable than another? This work requires the study and understanding of the delicate balance between the choices of mathematical approximation, computer architecture, data structures, and other factors - a balance crucial to the solution of many application-driven problems.

Opportunity Number: 50.77.11.B4450

Finite Element Analysis of Material Microstructure

Contact: Stephen Langer

We are developing object-oriented computational tools for the analysis of material microstructure. The goal is to predict the macroscopic behavior of a material from knowledge of its microscopic geometry. Starting from a digitized micrograph, the program identifies features in the image, assigns material properties to them, generates a finite element mesh, and performs virtual measurements to determine the effect of the microstructure on the macroscopic properties of the system. More information is available at http://www.ctcms.nist.gov/oof/. Opportunities exist in image analysis, materials science, physics, and computer science.

Opportunity Number: 50.77.11.B4451

Virtual Measurements from Quantum Chemistry

Contact: Raghu Kacker

A measurement is the estimated value of a quantity plus a quantitative estimate of its uncertainty. A "virtual measurement" is a measurement produced by computation or simulation. Thus, the goal of this project is to determine the uncertainties associated with predictions from quantum chemistry calculations. Current work focuses on scaling factors, with associated uncertainties, for vibrational frequencies from ab initio and density-functional calculations. For fundamental vibrational frequencies and zero-point energies this has been completed. Scaling factors for anharmonic fundamental frequencies are now being developed. Future work will address predictions of thermochemical quantities such as entropies and heat capacities, which depend on the vibrational partition function. Alternatives to traditional frequency scaling will also be investigated.

Opportunity Number: 50.63.21.B6751

Stochastic Modeling, Verification, Validation, and Calibration of Computer Simulations

Contact: Jeffrey Fong

Simulations of high-consequence engineering, physical, chemical, and biological systems depend on complex mathematical models. Such models may include large number of variables, parameters with uncertainties, incomplete physical principles, and imperfect methods of numerical solution. To ensure the public that decisions made on the basis of such models are well founded, rigorous techniques for verification and validation of computer simulations must be developed. Techniques under investigation include stochastic modeling, metrology-based error analysis, standard reference benchmarks and protocols, design of physical and numerical experiments, and uncertainty analysis. We are also interested in applications to specific engineering, physical, chemical, and biological systems of technological importance; and basic research in continuum physics, irreversible non-equilibrium thermodynamics, nonlinear viscoplasticity theory, fatigue, fracture, and damage mechanics; fire-structure dynamics; nanoscale contact mechanics; cochlear mechanics of human inner ear; and stability of stochastic elastic, viscoelastic, and viscoplastic systems.

Opportunity Number: 50.77.11.B6328

Complex Systems and Networks: Performance, Control, and Security

Contact: Vladimir Marbukh

We are developing novel methodologies and approaches to modeling complex systems consisting of a large number of interacting elements. The models should not only have predictive power, but should also provide guidance for controlling complex systems. Since performance of complex systems is characterized by multiple competing criteria, which include economic efficiency, resilience, and security, the purpose of control is optimization of the corresponding trade-offs. In a situation of complex systems comprised of selfish elements, control should take advantage of market mechanisms, which elicit desirable behavior through incentives. Resilience, robustness, and security should be modeled against malicious agents attempting to cause deterioration in the system performance.

Opportunity Number: 50.77.11.B7430

Cloud Computing and Combinatorial Software Testing

Contact: Raghu Kacker

Investigations of actual faults have shown that software failures can be triggered from certain combinations of the values of up to six variables. We have developed publicly available tools to generate test suites which assure that all t-way combinations for up to six are tested, have few test runs, and accommodate complex constraints inherent in the software under test. We are developing tools to identify faulty combinations from output of combinatorial test suites without assuming statistical models for the faults. Application domains include security, assurance of access control of health records, interoperability of systems, and assurance of modeling and simulation systems. We are investigating development of test infrastructures for cloud computing systems. It could target testing services running in the cloud or testing the cloud infrastructure or both.

Opportunity Number: 50.77.11.B7496

Quantum Algorithms and Complexity

Contact: Stephen Jordan

Quantum computers promise to solve certain computational problems faster than is possible using conventional classical algorithms. Although large-scale quantum computers do not yet exist, it is possible to mathematically analyze the computational power that quantum computers will have, if built. One branch of such analysis is the construction of quantum algorithms for specific computational problems. A second branch of such analysis uses the tools of computational complexity theory, which classify computational problems into complexity classes. We are involved in the design and analysis of quantum algorithms and in proving theorems about quantum complexity classes. We are particularly interested in quantum algorithms for simulating physical systems; alternative models of quantum computation, such as the adiabatic model; and quantum algorithms applied to cryptanalysis.

Opportunity Number: 50.77.11.B7891

Quantum Information and Cryptography

Contact: Yi-Kai Liu

Quantum mechanical devices can perform certain information processing tasks that are impossible using only classical physics. However, the construction of such devices requires new ideas from computer science, mathematics, and physics. We are interested in a broad range of topics in this area, including quantum devices that implement novel cryptographic functionalities, methods for testing and characterizing experimental quantum information processors, and classical cryptosystems that are secure against quantum adversaries. We are also interested in related areas such as quantum algorithms, complexity theory, and machine learning.

Opportunity Number: 50.77.11.B7913

Quantum Frequency Conversion for Hybrid Quantum Networks

Contact: Paulina Kuo

Future quantum networks will consist of a mixture of different technologies that operate at different wavelengths. Our research focuses on photonic devices that can bridge these different wavelengths while maintaining the quantum properties. We study quantum frequency conversion (QFC) using high efficiency, nonlinear optical frequency conversion (sum- and difference-frequency generation). We are interested in properties of QFC devices, such as efficiency, noise, and bandwidth, and potential integration of QFC devices with qubit technologies.

Opportunity Number: 50.77.11.B8345

Computational Methods for the Solution of the Time Dependent Schroedinger Equation

Contact: Barry Schneider

The solution of the time dependent Schroedinger equation for many-electron atoms and molecules exposed to electromagnetic radiation presents a formidable problem both conceptually and computationally. A group of researchers at Drake University, the Technical University of Vienna, the Louisiana State University, and NIST have been developing quite sophisticated computational approaches to treating "small" atomic and molecular systems exposed to short, intense laser radiation.

Extracting quantitative results has necessitated large-scale calculations on supercomputers. The methods developed are state-of-the-art and the codes have been algorithmically designed to scale efficiently to many thousands of processors. They have been applied to a number of one, two, and many electron atoms and molecules to extract single and double ionization probabilities. To date, the calculations have revealed numerous interesting and unexpected features, and double ionization processes that are among the first of their kind.

We are interested in expanding the scope of our work in several ways. In order to treat larger molecular systems, new approaches are required. These include things such as developing more efficient hybrid basis sets adapted to treat large molecules, new time propagation algorithms and density-functional-based methods that are needed to quantitatively model dynamical processes in very large molecular systems. Of particular interest are reformulations DFT to explicitly remove self-interaction errors and extending these functionals to the strong-field, time-dependent domain. Dynamical processes of specific interest include spin-dependent electronic rearrangements and their impact on technologically interesting collective phenomena, such as magnetic behaviors, in these systems.

The group currently has a number of NSF and DOE awards and has successfully competed for computational resources on the eXtreme Science and Engineering Discovery Environment project. An Associate joining the project will have access to the most sophisticated and powerful computers in the world and will also get to collaborate with a world class group of theoretical and computational physicists.

Opportunity Number: 50.77.11.B8188

Scientific Datamining

Contact: Judith Terrill

NIST scientists are currently automating experiments resulting in increasing amounts of generated data in multidimensional spaces. The data come primarily from combinatorial experiments in materials science. This type of data consists of image data with additional measurements at each pixel. Other experiments result in spectra-like measurements taken over spatial domains. These datasets require techniques that can sift through large amounts of data for items of potential interest, as well as for discovery. We are collaborating with these scientists on ways to mine this data for scientific insight. Opportunities exist for the application of datamining techniques such as classification, rule finding, and automated model building to these datasets, as well as for the development of new techniques.

Opportunity Number: 50.77.11.B4825

Real-time Quantitative Visualization

Contact: Judith Terrill

We are working to create visualization systems that serve as precision measurement instruments, supporting interactive probing of "samples" to derive quantitative data to enable scientific discovery. We use virtual samples, built from data obtained from either physical measurement or computational simulation. Our ability to extend measurement science to the virtual world is enabled by advances in the speed and capability of graphics processing units (GPUs). In particular, visualization techniques that employ shaders have the potential to play a central role in measurement and analysis tools within a visualization system because these programs can perform substantial numeric processing within the visualization pipeline, where they have direct access to the geometric data describing the objects of study. Additionally, this allows access to the information needed to determine uncertainties, a prerequisite for precision measurement. This research opportunity focuses on all aspects of quantitative visualization, i.e., measurement and analysis applied to visualization objects directly in real time.

Opportunity Number: 50.77.11.B7763

Parallel and Distributed Computing Algorithms and Environments

Contact: William George

As the size and computational power of parallel and distributed computing systems increase, it is important to continually investigate the appropriateness of the algorithms we use for our scientific applications. Although we always strive to design and build scalable parallel applications, we must re-think these deigns when the available computational resources increase in power by even as small as a single order of magnitude with respect to the number of processors, main memory size, network speed, or other relevant parameters. This research opportunity focuses on (1) investigating and developing new parallel algorithms, especially for scientific applications, for the next generation of computing platforms; (2) characterizing the programming models presented by new parallel and distributed computing platforms; (3) investigating the design and performance of parallel programming languages and libraries; and (4) investigating the role of web services, fourth generation languages such as Matlab and Mathematica, computational grids, and other developing technologies in providing novel high-performance computing environments.

Opportunity Number: 507.77.11.B6377

Boulder, CO

Quantum Information Science

Contact: E. (Manny) Knill

Quantum information science covers the theoretical and experimental areas involving the use of quantum mechanics in communication and computation. We are particularly interested in benchmarking proposed physical system's performance on quantum information processing tasks, scalably realizing logical qubits, and developing algorithms that take advantage of quantum resources. The research is inspired by and will contribute to the technologies being developed at NIST.

Opportunity Number: 50.77.12.B5623

Statistics for Quantum Systems

Contact: S. Glancy or E. (Manny) Knill

Sophisticated, rigorous statistical tools are required to analyze data from experiments that manipulate and measure quantum systems with the goals of quantum computation, communication, and measurement. This project works to develop new methods for data analysis from quantum experiments. Particular applications of interest include quantum state and process tomography, certifying violation of local realism (e.g., in Bell tests), certification/quantification of randomness, and use of quantum resources to improve measurement precision. We work in close collaboration with experimental groups at NIST (trapped ions, superconducting qubits, photons) to assist experiment design and analysis and to inspire new theoretical research.

Opportunity Number: 50.77.12.B7973

Uncertainty Quantification and Computational Materials Science

Contact: A. Dienstfrey

We research and develop mathematical and statistical analysis and tools for uncertainty quantification in scientific computing, with particular emphasis on problems in computational material science. Application areas include, but are not limited to structural composites and electronic materials. This work, which is performed in collaboration with the NIST Material Measurement Laboratory, is in response to the multi-agency Materials Genome Initiative (http://www.whitehouse.gov/mgi/), which strives to reduce the time and costs for materials discovery, optimization, and deployment through the promotion of a new research and development paradigm in which computational modeling, simulation, and analysis will decrease the reliance on physical experimentation.

Opportunity Number: 50.77.12.B7897

Computational Electromagnetics

Contact: Zydrunas Gimbutas

We are developing high order integral equation methods and numerical tools for computational electromagnetics. This research focuses on the frequency domain electromagnetic field solvers that involve automatic geometry preprocessing/compressing in the presence of geometric singularities and coupling the obtained discretizations to the wideband fast multipole method based accelerators and direct solvers. Applications will include benchmarking, verification, and error analysis of magnetic resonance imaging simulators and electromagnetic scattering codes.

Opportunity Number: 50.77.12.B7912
