NUGEX 2011 Election Ballot

Voting is open to fill open positions on the NERSC User Group (NUG) Executive Committee. There are 9 (nine) vacancies.

Voting Instructions

Vote for up to 9 (nine) candidates below. The candidates are grouped by DOE Office, but you may vote for any candidate and for any number of candidates from any office. The top vote-getters from each office will fill the open positions for that office. The top vote-getter among all remaining candidates will serve on the committee as an at-large representative.

Vote for up to 9 Candidates

The candidates' statements are included on the ballot below. The ballot is organized alphabetically by DOE Office and last name.

- Advanced Scientific Computing Research (ASCR): 0 openings, 0 candidates
- Biological and Environmental Research (BER): 1 opening, 4 candidates
- Basic Energy Sciences (BES): 0 openings, 1 candidate
- Fusion Energy (FES): 2 openings, 5 candidates
- High Energy Physics (HEP): 3 openings, 5 candidates
- Nuclear Physics (NP): 2 openings, 3 candidate
- At Large: 1 opening

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DOE Office: Advanced Scientific Computing Research (ASCR)

Zero (0) open positions; all candidates are eligible for at-large positions.

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DOE Office: Biological and Environmental Research (BER)

One (1) open position; all candidates are eligible for at-large positions.

Check Box to Vote	
☐	**Barbara Collignon** Oak Ridge National Laboratory & University of Tennessee, Knoxville BER

Project: Molecular Dynamics Simulations of Protein Dynamics and Virtual High-throughput Screening of Estrogenic Compounds

Candidate Statement: Dr. Barbara Collignon is a computational molecular biophysicist, with an appointment at the University of Tennessee, Knoxville and in the UT/ORNL Center for Molecular Biophysics, Oak Ridge. Her primary research focus is developing and implementing state-of-the-art ligand-protein docking simulations for leadership class computing facilities. To date, she has successfully developed the task-parallel (MPI) automated docking program "Autodock4.lga.MPI" on the Franklin XT4 machine. As a result, Autodock4 is now capable of quickly testing very large databases of compounds. Scanning such large databases of molecular shapes, known as Virtual High-Throughput Screening (VHTS), is commonly used to select compounds as potential candidates that have a desired interaction with DNA, proteins, etc. Improving efficiency, scaling and at-scale performance has direct benefits to drug discovery, (e.g.,http://www.ornl.gov/info/press_releases /get_press_release.cfm?ReleaseNumber=mr20101209-00), functional proteomics, molecular biology and environmental toxicology. In 2009/2010 Dr. Collignon used ~3 million CPU hours on Franklin and the corresponding research was published in the Journal of Computational Chemistry [1]. More recent research involves removing the I/O bottleneck that presents in Autodock4.lga.MPI above 32K processors [2]. By utilizing the parallel I/O HDF5 libraries, linear scaling is being extended to 65K processors on the Hopper2 XE6 machine.

Dr. Collignon routinely uses the Valgrind, Totalview and DDT suites for at-scale debugging and profiling, while I/O and MPI overheads are assessed using the CRAYPAT analysis tool. In addition, an MPI+CUDA implementation of AutoDock4 is under development using the experimental CPU/GPU Dirac machine.

Dr. Collignon is most willing to represent NERSC users at NUGEX and believes she is well qualified to discuss the various issues users face when developing and implementing massively parallel applications.

[1] Collignon B. et al.: Task-parallel message passing interface implementation of Autodock4 for docking of very large databases of compounds using high-performance super-computers. J. Comput. Chem. 2010 Dec 7. [Epub ahead of print] [2] Collignon B. et al.: Research poster presentation, Supercomputing Conferences 2010 (SC10), New Orleans, LA.

Brian Hingerty
Tennessee Wesleyan College
BER

Project: Owner Knox Computer Consultants

Brian Hingerty is retired from the Biosciences Division at Oak Ridge National Laboratory, an Adjunct Professor at Tennessee Wesleyan College, and owner of Knox Computer Consultants.
Research Interests: Research in computer model building studies of the binding of carcinogenic and mutagenic metals and organic compounds (poly-nuclear aromatics - PNAs) with DNA. Computational Biology. NMR structures of chemically modified DNA. Computer graphics. Supercomputer applications. X-ray and neutron crystallography. Protein Crystallography. Neutron diffraction of biologically important molecules using the High Flux Isotope Reactor (HFIR) and Spallation Neutron Source (SNS) at ORNL. Small molecule crystallography. Energy minimization and structure prediction. Structural Genomics. Discovery of "Flip- Flop" hydrogen bond networks in cyclodextrin carbohydrates using neutron diffraction. Planned study of the Photosystem II Mn complex using the SNS MANDI device when available in 2012.

Candidate Statement: I have served on NUGEX and its predecessors since the mid 1980's. I served as vice chair from 1992-1993 and as chair from 1994-1995. I also served as vice-chair again from 2003-2005. I am willing to continue doing this in retirement.

Ned Patton
National Center for Atmospheric Research, Boulder, Colorado
BER

Project: Impact of vegetation on turbulence over complex terrain: a wind energy perspective

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Bio
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Education:
   1991 B.Sc. Atmospheric Science, University of California, Davis
   1997 Ph.D. Atmospheric Science, University of California, Davis

Employment:
   2007-present Project Scientist II, Mesoscale and Microscale
   Meteorology Division, National Center for Atmospheric Research,
   Boulder, CO.
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2005-2007 Project Scientist I, Mesoscale and Microscale Meteorology
Division and The Instituted for Integrative Multidisciplinary
Earth Studies, NCAR, Boulder, CO.

2002-2005 Long-Term Visitor (Project Scientist I), Mesoscale and
Microscale Meteorology Division, NCAR, Boulder, CO (visiting
from The Pennsylvania State University).

2000-2002 Research Associate, Department of Meteorology, The
Pennsylvania State University, University Park, PA.

1997-2000 Supercomputing Fellow, Minnesota Supercomputing
Institute, University of Minnesota, Minneapolis, MN, and
Post-Doctoral Researcher, Department of Soil, Water and Climate,
University of Minnesota, St.  Paul, MN.

1992-1997 Research Assistant, Department of LAWR, University of
California, Davis, CA
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Candidate Statement: I use turbulence-resolving simulations to investigate interactions between the planetary boundary layer and complex land-surfaces (vegetation, orography, wind turbines, etc). Our code is developed in-house. It solves the time-dependent three-dimensional incompressible Boussinesq equations and is a pure MPI application parsing out the work using a two-dimensional domain decomposition strategy. I perform a wide range of computations on the NERSC facilities, i.e. small computations using 10^6 grid points on four processors extending up to about 10^{10} gridpoints on 65536 CPUs. I also have experience performing visualizations and data analysis on datasets with sizes ranging from a megabyte to terabytes.

I have been a NERSC PI on two distinct projects spanning the most recent eight years. Over that time, I've worked on six different NERSC machines. I therefore have experience working with, debugging and running code on the machines that NERSC users currently utilize. I also compute at four other centers, which provides a relatively wide view of how other centers operate. I can therefore speak from a broad perspective while advocating for the hardware/software and data management/transfer needs or concerns of NERSC's complex user base.

During my eight years working on the NERSC machines, I have frequently interacted with the NERSC consulting group and therefore sincerely appreciate the ability return the favor by serving as a member of NUGEX helping to guide the management and maintenance of the compute systems from a user perspective. I recently served one term as a member of NUGEX.

☐ **Jeff Wereszczynski**
University of California, San Diego
BER

Project: Simulations of Enzymatic Functions in Energy and Oxygen Transport and Regulation

Candidate Statement: As a postdoctoral fellow in the McCammon group, my research focuses on using large scale molecular dynamics simulations to examine the function and energetics of biomolecular complexes. I have extensive experience compiling and using the MD packages NAMD, CHARMM, Desmond, and Amber on numerous HPC platforms at both DOE and Teragrid sites. Two areas I am particularly excited about are introduction of the new XE series of Crays and the experimentation with GPU computing, both of which should significantly enhance NERSC computing power.

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DOE Office: Basic Energy Sciences (BES)

Zero (0) open positions; all candidates are eligible for at-large positions.

Check Box to Vote

☐ **Gregory Newman**
Lawrence Berkeley National Laboratory
BES

Project: Large Scale 3D Geophsycial Inversion & Imaging

Candidate Statement: Over the last seven years I have been running on the NERSC systems on Large Scale 3D Geophysical Inversion & Imaging of the subsurface; Repository m372. My current allocation is now at 2 million hours per year and is expected to double within the next year. The computations are big, typically using resources of several thousand to tens of thousands of processor cores per job. As the biggest user in the Basic Energy Sciences Geosciences program, I bring important insight into the computation needs for Earth Sciences on the NERSC systems. I am most interested in system queues and data storage on the NERSC platforms, as well as system access.

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DOE Office: Fusion Energy Sciences (FES)

Two (2) open positions; all candidates are eligible for at-large positions.

Check Box to Vote	
☐	**James Colgan** Los Alamos National Laboratory FES
	Project: Computational Atomic Physics for Fusion Energy **Candidate Statement:** I have been a NERSC user for over 10 years on a variety of platforms. I am a member of a team which studies electron, ion, and photon collisions with atomic and molecular systems, in order to provide data for use in magnetic fusion modeling and other plasma applications. Our calculations also explore fundamental few-body systems in collaboration with experimental groups worldwide. Many of our codes that make use of NERSC resources have taken advantage of the large-scale parallelism available, and can routinely make use of 1000s or even 10000s of cores. I regularly use the NERSC facilities and have been a test (early) user on several platforms as they are brought online. I wish to be a NUGEX representative for several reasons. The atomic data requirements for magnetic fusion modeling are set to vastly increase as attention increasingly focuses on the modeling requirements for the planned ITER machine. Thus, it is important that the computational needs of atomic data providers are recognized at the leading national computer centers, and also that the latest developments in new computing architectures and software are communicated to the physicists who provide such data. I am willing to act as a liaison between the atomic data providers and national computer centers in a role as a member of the NUG executive committee. Also, I believe that my considerable experience with developing and running code on NERSC platforms, as well as at other national supercomputing centers, enables me to be a strong voice on the NUGEX committee which can adequately represent any concerns or issues that NERSC users face. I look forward to the opportunity to serve on the NUGEX committee.
☐	**Stephane Ethier** Princeton Plasma Physics Laboratory FES
	Project: Turbulent Transport and Multiscale Gyrokinetic Simulation Stephane Ethier is a senior computational scientist at the Princeton Plasma Physics Laboratory (PPPL). He holds a Ph.D. in plasma physics from the INRS-Energie et Materiaux in Canada and an M.Sc. in condensed matter physics from the University of Montreal. His work involves the development and optimization of large-scale particle-in-cell codes for the study of microturbulence in tokamak fusion devices. He is involved in several projects related to exascale, working in close collaboration with computer scientists and applied mathematicians. Stephane has been very active in the NERSC User's Group for over ten years now. He has been representing the office of Fusion Energy Sciences on the NUGEX since 2004 and is currently serving as the chair of NUGEX. **Candidate Statement:** The success and popularity of NERSC is due to its user-centric approach. The NERSC staff continues to help the users maximize their scientific output by providing support in the form of solutions to problems, training on the new systems, maintaining a stable and diverse set of computing resources, and much more. This, however, requires a good communication channel between NERSC and its large body of users in order for the work to be useful and relevant. This is the role and duty of the NUGEX. The representatives communicate to NERSC the current and future needs of the users in their field. This is a most important task as it helps NERSC plan their activities and stay ahead of the curve. With the move to heterogeneous computing and the exascale looming at the horizon, NERSC needs more than ever the users' participation in order to anticipate their computing needs. As a member of NUGEX, I will continue to keep that communication channel alive and healthy.

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DOE Office: High Energy Physics (HEP)

Three (3) open positions; all candidates are eligible for at-large positions.

Check Box to Vote	
☐	**Edward Baron** University of Oklahoma HEP
	Project: Synthetic Spectra of Astrophysical Objects Areas of expertise: astrophysics, numerical radiative transfer, supernovae. **Candidate Statement:** I have been using NERSC facilities for over thirty years. Because the radiative transfer problem differs in character from many other scientific problems (6 dimensional, non-local) my numerical requirements often stretch the computational resources in ways different from those of other users. I also do both relatively small scale computations (32 nodes) as well as very large scale computations (few x 10 K) nodes. I will work to ensure that NERSC facilities are responsive to a broad range of users with differing computational needs.
☐	**Julian Borrill** Lawrence Berkeley National Laboratory HEP
	Project: Cosmic Microwave Background Data Analysis For The Planck Satellite Mission; Cosmic Microwave Background Data Analysis For Suborbital Experiments; Simulations and analyses for CMBpol mission concept studies Julian Borrill is a Senior Staff Scientist in the Computational Cosmology Center at Lawrence Berkeley National Laboratory and a Senior Research Physicist in the Space Sciences Laboratory at UC Berkeley. He holds masters degrees in mathematics and political science (Cambridge), astrophysics (London) and information technology (London), and a doctorate in theoretical physics (Sussex). For the last 12 years he has been the Principal Investigator for NERSC's CMB data analysis repositories, supporting over 100 scientists from about 20 experiments to date. His research focuses on (i) applying high performance computing resources to the analysis of the largest CMB data sets, and (ii) using realistic scientific applications as holistic performance evaluation tools for HPC systems. He has led the development of the MADCAP suite of massively parallel CMB data analysis tools, his MADbench software has been used as part of the NERSC procurement code suite, and he has assisted with the acceptance-testing of almost all of the NERSC systems fielded in the last decade. **Candidate Statement:** For the last dozen years I have been closely involved with all facets of NERSC. As a significant individual user I have become very familiar with almost all of the NERSC HPC facilities; as the PI of a number of large community allocation I have worked with hundreds of users with widely varying HPC requirements and experience; as a long-standing early user of new NERSC systems and computational systems architect for the US Planck team I have developed strong relationships with the full range of NERSC staff; and as a community representative and contributor to, amongst others, the NERSC Green Book and the Large Scale Computing and Storage Requirements for High Energy Physics report, I have worked with DOE (as well as NSF and NASA) staff in Washington to support HPC initiatives in general and NERSC in particular. With this experience, I will continue to work through the NUGEX to represent the interests of the HEP user community to help NERSC best address the technical and political challenges in the era of peta- and exa-scale computing.
☐	**Cameron Geddes** Lawrence Berkeley National Laboratory HEP
	Project: Particle Simulation of Laser Wakefield Particle Acceleration Cameron G.R. Geddes is a staff scientist at LOASIS program of the Lawrence Berkeley National Laboratory. His current research centers on intense laser matter interaction applied to development of high gradient laser driven particle acceleration using plasma waves, and associated radiation sources. In addition to on NERSC and ATLAS computational grants on these topics, he is a collaborator on the SciDAC COMPASS accelerator modeling project, and also pursues experiments on laser accelerators. His work over the last decade has also included long pulse laser plasma interactions experiments in fusion plasmas at Lawrence Livermore National Laboratory and Polymath research, equilibria of spheromak plasmas and nonlinear optics at Swarthmore College, and small aspect Tokamaks

at Princeton/U. Wisconsin. He received the Ph.D. in 2005 from the University of California, Berkeley. His work has earned the American Physical Society John Dawson Award for Excellence in Plasma Physics Research, the American Physical Society Rosenbluth and Hertz foundation dissertation awards, and LBNL Outstanding Performance awards. He also received the American Physical Society Apker award for the outstanding undergraduate thesis, and the Swarthmore College Ellmore prize for outstanding work in physics (1997). He has been a recipient of the Hertz (2000-2004), DOD NDSEG(1999-2000), and DOE undergraduate plasma physics (1995) fellowships, and is a member of the American Physical Society.

Candidate Statement: I have conducted both simulations and experiments on plasma physics, ranging from spheromaks to advanced accelerators, for more than ten years. At NERSC I have been involved in simulations from mid-scale through use of more than half of the machines. This experience, together with contact with SciDAC collaborators working in other areas of accelerator physics and past service on NUGEX, gives me a view of a wide range of user needs in the HEP community. NERSC simulations have been crucial to developing understanding of our recent experiments. I would like to continue facilitating the development and usefulness of the facility for all users, including tailoring of cpu availability and job classes to user needs, accessibility of the new machines, data storage and visualization.

☐ **Steven Gottlieb**
Indiana University
HEP

Project: Quantum Chromodynamics with three and four flavors of dynamical quarks

Steven Gottlieb is currently Distinguished Professor of Physics at Indiana University. He received an A.B. from Cornell University with majors in Mathematics and Physics. He received Masters and Ph.D. degrees from Princeton in Physics. After postdoctoral appointments at Argonne National Lab, Fermilab and UC San Diego, he joined the faculty at Indiana. He is a Fellow of the American Physical Society, having been nominated through the Division of Computational Physics. He served on the NSF's Alliance Allocation Board and National Resource Allocation Committee for a number of years, as well as the Partnerships in Advanced Computational Infrastructure (PACI) review panel for two years. He also served on the Executive Committee of the Division of Computational Physics, several program committees, and is the current chair of the Metropolis Prize Committee (best thesis in computational physics). Gottlieb has been a Divisional Associate Editor of Physical Review Letters and is currently Associate Editor in Chief of Computing in Science & Engineering, which is jointly published by AIP and IEEE. He spent his most recent sabbatical at the National Center for Supercomputing Applications where he was helping to prepare the MILC code for the Blue Waters sustained petascale computer to be installed there.

Candidate Statement: My area of interest is lattice field theory which has led to sustained use of leading edge computing facilities for over 25 years. I have been a generally well satisfied user of NERSC and quite a few other NSF and DOE supercomputing facilities. I have also built local Beowulf clusters and am just getting started on a (small) new GPU cluster purchased with ARRA funds. In addition, I have attended a number of workshops on exascale computing, and am excited about the future of high performance computing. If elected to NUGEX, I hope to share my wide perspective as an active user of many centers with NERSC management to ensure a productive environment for all the scientists who use NERSC facilities. I would also welcome hearing about the concerns of other users and bringing them to the attention of management. Hopefully, NUGEX will have input on the future of computing at NERSC, and it will be possible to continue to increase the power of the computers there in an optimal way.

☐ **Frank Tsung**
UCLA
HEP

Project: Large scale particle-in-cell simulations of laser-plasma interactions relevant to Inertial Fusion Energy

Candidate Statement: My area of research is the simulation of laser plasma interactions (relevant to plasma based accelerators or inertial confinement fusion) using massively parallel particle-in-cell codes. For the past 20 years I have been a NERSC user and it has provided a user enviroment that is both world class and user friendly. As a NUGEX member since 2006, I have been trying to work with the NERSC staff to maintain this tradition and this is what I wish to provide in my next term if I was elected.

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DOE Office: Nuclear Physics (NP)

Two (2) open positions; all candidates are eligible for at-large positions.

Check Box to

Vote	
☐	**David Bruhwiler** Tech-X Corporation NP
	Project: Parallel Simulation of Electron Cooling Physics and Beam Transport David Bruhwiler received a B.A. from Carleton College in 1986 and a Ph.D from the University of Colorado at Boulder (CU) in 1990. Before he joined Tech-X Corp. in 1997, he was a staff scientist at Northrop Grumman Corp. David's research at CU included studies of deterministic chaos in Hamiltonian systems. While at Northrop Grumman, he designed electron beamlines for high-charge sub-picosecond pulses, and magnetic optics for high-current proton and deuterium beams with uniform irradiation. David co-developed the TOPKARK code for particle tracking and high-order map generation, including nonlinear self-fields, magnets and radio frequency cavities. David's work at Tech-X has focused on the collaborative development of cross-platform C++ codes for beam optics (MAPA), optimization (OptSolve++) and parallel particle-in-cell (PIC) simulation (OOPIC Pro and VORPAL). His current interests include direct simulation of the electron cooling of relativistic heavy ion beams via molecular dynamics, delta-f PIC, and Vlasov techniques. David is a fellow of the American Physical Society. **Candidate Statement:** As a graduate student, I used the facilities of the NSF-sponsored John von Neumann Supercomputer Center during its relatively brief existence in Princeton. Since 1999, I've been actively developing and using MPI-based C++ codes on NERSC computers. I have simulated charged particle acceleration of various types for 20 years, and look forward to new challenges in high-performance computing. I believe strongly in the importance of NERSC and the benefits it brings to the DOE Office of Science and the entire scientific community. I look forward to helping this enterprise in a small way by representing the NERSC Users Group as a member of the executive committee.
☐	**Daniel Kasen** Lawrence Berkeley National Laboratory and University of California, Berkeley NP
	Project: Radiation Transport of Astrophysical Explosions **Candidate Statement:** I am a scientist in the Nuclear Science Division at LBNL and an assistant professor in the physics department at UC Berkeley. My research focuses on computational astrophysics; in particular on using multi-dimensional simulations to study the nuclear physics of supernova explosions. Our nuclear theory group at LBNL aims more broadly to access and promote NERSC as a center for computational astrophysics, lattice QCD, and other applications in nuclear physics. Most of my time is spent developing and fielding scientific codes for high performance computing. I am the core author of the Sedona code (for astrophysical radiation transport) which was supported for development as part of the DOE Scientific Discovery through Advanced Computing (SciDAC) program and which has been tested and scaled on Franklin at NERSC. I have been a user of NERSC facilities for about 10 years, and have also worked extensively on the leading machines at other facilities, including those at ORNL, LLNL, and ANL. I am therefore familiar with the challenges facing scientists seeking to run efficiently on evolving architectures, and have a standard of comparison for the kind of support that could or should be available to NERSC users.
☐	**Martin Savage** University of Washington NP
	Project: Hadron-Hadron Interactions with Lattice QCD Martin Savage received his BSc (Physics and Math, 1983), and MSc in experimental nuclear physics (1984) from the University of Auckland, New Zealand. He received his PhD in theoretical particle physics from the California Institute of Technology in 1990. After postdoctoral positions at Rutgers University and the University of California at San Diego, and three years as an Assistant Professor at Carnegie Mellon University he became faculty at the University of Washington where he is a Professor. He has been the recipient of a SSC Fellowship (1992), and Outstanding Junior Investigator award from the Department of Energy (1995), and he is a Fellow of the American Physical Society (2002). Savage's research is focused on using high performance computing to perform calculations of sub-atomic processes. His work involves the direct numerical evaluation of the path-integral for quantum chromodynamics (QCD) with the goal of reliably calculating nuclear properties and interactions. He is a member of the NPLQCD (Nuclear Physics with lattice QCD) collaboration. **Candidate Statement:** NERSC has played an important role in providing the computational resources that have enabled nuclear physics and particle physics to perform calculations central to their fields. I will represent the nuclear physics and particle physics communities, and help guide NERSC during its evolution toward extreme-scale

	computing.

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