Partnership Center for High-fidelity Boundary Plasma Simulation

Princeton Plasma Physics Laboratory (PPPL)

Street Address	Postal Address
100 Stellarator Rd.	P.O. Box 451, MS-27
Princeton, NJ 08540	Princeton, NJ 08543-0451

Administrative Contact: Marie Iseicz, (609) 243-2456, miseicz@pppl.gov

Lead PI: Choong-Seock Chang, (609) 243-2127, cschang@pppl.gov

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DOE Program Office: Fusion Energy Sciences

DOE Program Office Technical Contact: Dr. John Mandrekas and Dr. Randall Laviolette

PAMS Preproposal Number: PRE-0000011802

Research Area: Boundary Physics

To be performed in collaboration with the following institutional PIs and Co-PIs:

L. Chacon (LANL), M. Adams (LBNL), J. Hittinger (LLNL),

S. Klasky and E. D'Azevedo (ORNL), B. Hoffman (Kitware),

J. Myra (Lodestar), M. Greenwald (MIT), P. Worley (PHWorley Consulting)

M. Shephard (RPI), G. Tynan (UCSD), S. Parker (U. Colorado Boulder),

V. Carey (U. Colorado Denver) D. Curreli (U Illinois UC),

R. Moser and D. Hatch (U. Texas Austin)

This proposal is targeted at providing a verified and validated high-fidelity, kinetic understanding of critically important boundary physics in existing tokamaks, enabling prediction of those phenomena in future magnetic fusion reactors, including ITER. The project's exascale-aware codes are and will be able to attain maximal concurrency on the largest leadership class DOE computers, today and in the near future, via a close collaboration with ASCR's applied mathematicians and computer scientists. The project codes will be ready for coupling with plasma-wall interaction models, whole device models, and others.

The critical need for high-fidelity boundary physics simulation run on the largest computers has been well documented in the recent DOE workshop reports on Plasma Materials Interaction (chaired by R. Maingi), Integrated Simulation (chaired by P. Bonoli), and FES/ASCR Exascale Requirement Review (chaired by C.S. Chang, the PI of this proposal)

Collaboration Details

Institutions & Principal/Co-Principal Investigators

Princeton Plasma Physics Laboratory: C. S. Chang, Lead PI, coordinator and contact point,
Oak Ridge National Laboratory: S. A. Klasky / E. D'Azevedo,
Los Alamos National Laboratory: L. Chacon,
Lawrence Livermore National Laboratory: J. A. F. Hittinger,
Lawrence Berkeley National Laboratory: M. F. Adams,
University of Colorado, Boulder: S. E. Parker,
University of Texas at Austin: R. D. Moser / D. R. Hatch,
Rensselaer Polytechnic Institute: M. S. Shephard,
University of Illinois at Urbana-Champaign: D. Curreli,
Lodestar Research Corporation: J. R. Myra,
PHWorley Consulting: P. H. Worley,
Kitware: B. Hoffman,
University of California, San Diego: G. Tynan,
University of Colorado, Denver: V. Carey,
Massachusetts Institute of Technology: M. Greenwald.

Leadership Structure

- C.S. Chang will have overall responsibility for ensuring that proper collaborative activities are arranged and executed and that the scientific and software development goals are successfully executed.

- C.S. Chang will make final decisions on project prioritization and personnel in conjunction with the Executive Management Team and Group Leaders.

- Key decisions made by the Executive Management Team on plans and priorities will be guided by input from an external Program Advisory Committee.

- The Executive Management Teams consists of:

  Project Leader: C. S. Chang
  Physics: S. E. Parker
  Applied Math: L. Chacon
  Computer Science: S. A. Klasky

- The Group Leaders reporting to the Executive Management Team are:

  Kinetic Physics: S. Ku / G. W. Hammett
  MHD: N. M. Ferraro
  Neutral Physics: D. P. Stotler
  Validation: M. Greenwald
  Algorithms: M. F. Adams / C. D. Hauck
  UQ: R. D. Moser
  Verification: J. A. F. Hittinger
  Meshing: M. S. Shephard
  Code Performance: E. D'Azevedo / P. H. Worley
  Data Management: S. Klasky / J. Choi
  Software Engineering: B. Hoffman

- See also Sec. 5 and Appendix 0

Facilities

The principal "facilities" used by this collaboration are the DOE Office of Science high performance computers.

Oak Ridge Leadership Computing Facility (OLCF): operating 27PF Titan and 200PF Summit (in 2018). XGC is in their pre-exascale program CAAR.

National Energy Research Computing Center (NERSC): operating 28PF Cori. XGC is in their pre-exascale program NESAP.

Argonne Leadership Computing Facility (ALCF): operating 10PF Mira, 10PF Theta and 200PF Aurora (in 2019), XGC is in their Early Science Program.

Each institutions will use local clusters for subroutine and algorithm development.

Our validation team will utilize data from the three U.S. tokamak facilities and the worldwide tokamak facilities.

Collaborative Application Information

These are the budgets for each of the institutions submitting a collaborative proposal, labeled by PI and institution. FES fund/ASCR fund in each row. Units: $1,000.

Partnership	Year 1	Year 2	Year 3	Year 4	Year 5	Total
Chang, PPPL*	1150/ 430	1150/ 430	1150/ 430	1150/ 430	1150/ 430	5750/ 2150
Klasky & D'Azevedo, ORNL	0/545	0/545	0/545	0/545	0/545	0/2725
Parker, U. Colo. Boulder	330/0	330/0	330/0	330/0	330/0	1650/0
Chacon, LANL	0/245	0/245	0/245	0/245	0/245	1225/0
Hittinger, LLNL	0/195	0/195	0/195	0/195	0/195	0/975
Moser & Hatch, U. Texas, IFS	160/135	160/135	160/135	160/135	160/135	800/675
Adams, LBNL	0/150	0/150	0/150	0/150	0/150	0/750
Shephard, RPI	0/150	0/150	0/150	0/150	0/150	0/750
Myra, Lodestar	100/0	100/0	100/0	100/0	100/0	500/0
Tynan, UCSD	70/0	70/0	70/0	70/0	70/0	350/0
Greenwald, MIT	40/0	40/0	40/0	40/0	40/0	200/0
Totals	1850/ 1850	1850/ 1850	1850/ 1850	1850/ 1850	1850/ 1850	9250/ 9250

*The PPPL annual budget includes subcontracts and pass-through overheads for the following subcontractors:

University of Illinois, Urbana-Champaign (D. Curreli, PI): PMI Interface
University of Colorado, Denver (V. Carey, PI): UQ
PHWorley Consulting (P. H. Worley, PI): Performance Engineering
Kitware (B. Hoffman, PI): Software Engineering

Task Breakdown Information

The project budget is here broken down further by task. Note that the level of discretization is somewhat finer than that used in Appendix 0. FES funds/ASCR funds in units of $1,000.

Task	Leader	Year 1	Year 2	Year 3	Year 4	Year 5	Total
(Management & Subcontract OH)	Chang	170/170	170/170	170/170	170/170	170/170	850/850
XGC development	Ku/Parker	280/0	280/0	280/0	280/0	280/0	1,400/0
MHD coupling	Ferraro	120/0	120/0	120/0	120/0	120/0	600/0
Physics study	Parker/Chang	300/0	300/0	300/0	300/0	300/0	1,500/0
PMI Interface	Davide	150/0	150/0	150/0	150/0	150/0	750/0
(Neutrals & Atomic Physics)	Stotler	130/0	130/0	130/0	130/0	130/0	650/0
Develop Gkeyll	Hammett/Hauck	200/0	200/0	200/0	200/0	200/0	1,000/0
Validation	Greenwald	110/0	110/0	110/0	110/0	110/0	550/0
(Phys. Scouting & Cross-benchmark w/ GEM&GENE)	Parker/Hatch	290/0	290/0	290/0	290/0	290/0	1,450/0
Math. verification	Hittinger	0/195	0/195	0/195	0/195	0/195	0/975
Algorithms	Chacon/Hauck	0/270	0/270	0/270	0/270	0/270	0/1,350
Solver	Adams/Chacon	0/275	0/275	0/275	0/275	0/275	0/1,375
UQ	Moser/Hauck	0/230	0/230	0/230	0/230	0/230	0/1,150
Meshing	Shephard	0/150	0/150	0/150	0/150	0/150	0/750
Data Management	Klasky/Choi	0/280	0/280	0/280	0/280	0/280	0/1,400
Code Performance	D'Azevedo/Worley	0/280	0/280	0/280	0/280	0/280	0/1,400
Software Eng.	Hoffman	100/0	100/0	100/0	100/0	100/0	500/0
Totals		1,850/ 1850	1,850/ 1,850	1,850/ 1,850	1,850/ 1,850	1,850/ 1,850	9,250/ 9,250

Contents

1 Background

1.1 Science Driver The turbulent boundary of fusion plasmas is critical since the physics therein determines the performance of the reactor core and the characteristics of the power exhausted to the divertor plates. This region is defined as extending from the top of the pedestal, $\sim 10\%$ of the outer minor radius in from the magnetic separatrix, through the open-field-line scrape-off layer (SOL), and out to the material walls (Fig. 1, 2). The "pedestal" in the density and temperature profiles develops after the transition from low- (L) to high- (H) confinement mode [187] once the heating power is raised above a threshold value. A deep well in the radial electric field E_r forms within the pedestal layer, bringing with it a significant reduction in turbulence intensity. The ion temperature in the core then increases rapidly by a factor proportional to the temperature at the top of the pedestal; ITER requires the latter to be $4-6$ keV to achieve its targeted fusion power.

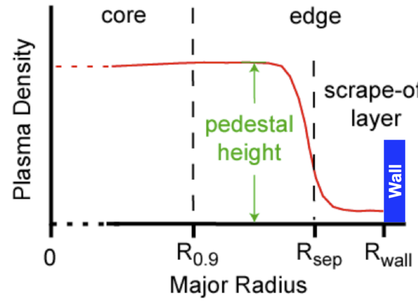


Figure 1: *Boundary region, showing major radii at 90% flux surface, separatrix (right dashed vertical line), and material wall*

The power exhausted by the plasma across the separatrix is, by design, directed along open field lines to the "divertor" or "target" plates (see Fig. 2). Present experiments find that the width of the heat flux striking these surfaces is extremely narrow. An extrapolation of the existing experimental widths to ITER parameters yields values so narrow ($\leq$1 cm at the divertor target, $\leq$1 mm if mapped to midplane) that the associated steady state heat loads would be too severe to be withstood by any known solid material, complicating ITER operation.

The sharp pedestal gradients also serve as a source of free energy that can be tapped by MHD edge-localized modes (ELMs) that can "crash" the pedestal. The resulting transient heat and particle fluxes can also rapidly erode the divertor target materials, another serious concern for ITER. Ongoing primary ELM-control research is to generate stochastic magnetic fields in the pedestal region to gain control over the pressure gradient there and, thus, over the ELMs. The predicted critical gradient required for ELM instability represents yet another extrapolation of existing tokamak data.

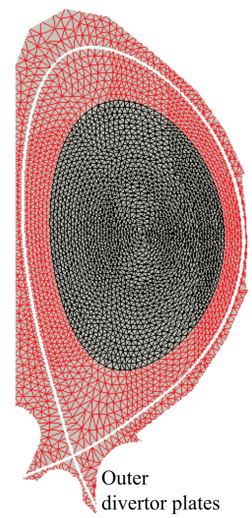


Figure 2: *Edge region (red) to be studied in the proposed research using unstructured triangular mesh.*

The fundamental understanding of edge turbulence, pedestal structure, L-H transition, and ELM stability and control that would permit extrapolation beyond the existing database remains elusive, despite decades of research, due to the multiscale kinetic nature of the boundary plasma and the complexity of its geometry. The non-Maxwellian and non-equilibrium character of the boundary plasma results from orbit loss and nonlocal orbit mixing, plasma wall interactions, and neutral recycling; impurities created at the wall further complicate the problem. The tremendous drop in temperature and density from the top of the pedestal to the SOL results in a collisionality that varies rapidly with radius from almost collisionless to highly collisional. These characteristics violate the near-Maxwellian assumptions required for fluid and even reduced-δf kinetic models. Instead, comprehensive, first-principles-based, at least 5D gryokinetic (GK), simulations that consistently incorporate all of the important, multiscale physics are required. The principal assumption of the GK approach is that the interesting turbulence and transport physics is on time scales much slower than gyro-motion of the particles in a strong magnetic field so that one can average over this motion to analytically reduce the full 6D kinetic equations to 5D. The resulting system remains complex, in terms of both the algorithms and the extreme scale computation needed, requiring a strong collaboration with ASCR scientists, as well as maximal concurrency on the new hardware and software architectures anticipated from upcoming leadership class computers.

1.2 Enabling Technologies The ambitious science program envisioned under this proposal is underpinned by an equally ambitious applied mathematics and computer science *enabling tech-*

nologies agenda. The focus of the majority of these efforts will be the XGC PIC code, although attention will also be given to the development of the Discontinuous Galerkin continuum Gkeyll code for cross-verification and technology synthesis between particle and continuum methods.

Since its inception, XGC has targeted extreme-scale computing of the boundary plasma. ASCR's enabling technologies have been an integral part of XGC's development since its inception, starting with DOE's Prototype Fusion Simulation Project a decade ago and continued with two SciDAC projects. The modern XGC code is highly modularized, with state-of-the-art algorithms, unstructured triangular mesh, scalable solvers (PETSc), and adaptive data management capabilities (ADIOS). Modern programming practices ensure portability and optimal performance on different HPC architectures. The XGC team has paid strong attention to solver technology and performance engineering from the beginning. PETSc solver execution time in large-scale production XGC runs is kept to less than a few percent of the total time, resulting in excellent weak and strong scalability from large number of marker particles at full scale on all DOE open science HPCs (Titan, Mira, Edison), which have been providing the computational resources demanded by XGC (see Sec. 3.2.5). Efficient I/O is ensured by the ADIOS library and the associated in-memory data-management techniques. ADIOS was originally developed within the XGC partnership, and reduced XGC's I/O time from over 50% to less than 6% of the total time. Other high-performance computing projects rapidly recognized its value, contributing to ADIOS' 2013 R&D award.

Aggressive improvements in our enabling technologies are planned in preparation for electromagnetic studies of ITER-scale plasmas on the new pre-exascale computers (both GPU-dominant and CPU-dominant architectures) and to increase XGC's accuracy, efficiency, performance and portability. XGC being in all three Pre-Exascale Programs (the only such fusion code, and among only a few from the entire science and engineering areas) –NESAP at NERSC for Cori, CAAR at OLCF for Summit, and Early Science Program at Argonne for Aurora, such improvements are already well underway. Present status and proposed plans for enabling technology are in Sec.3.

2 Present Science Capabilities and Proposed Plans

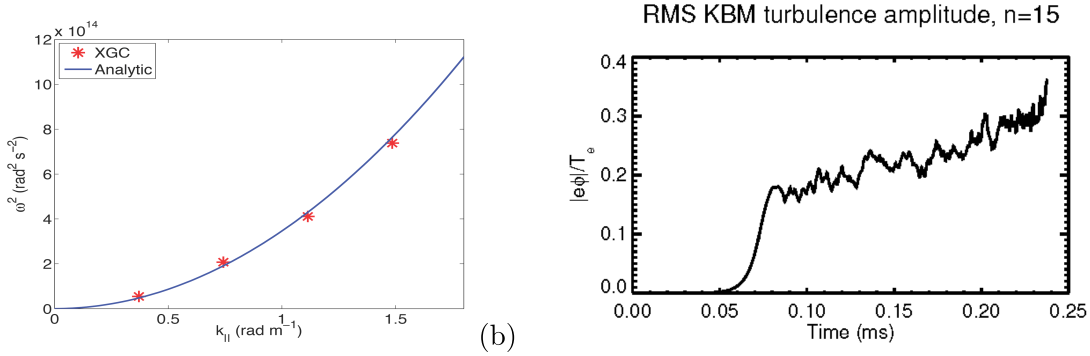
Here, we introduce the main code XGC and the ITER critical physics issues that require high-fidelity kinetic simulations on the largest leadership class computers. Plans for development of a complementary kinetic code Gkeyll, cross-verification of turbulence in the difficult steep pedestal region, interfacing with material models and others, and experimental validation are also described.

2.1 XGC and Its Global Boundary Plasma Simulation Capabilities

2.1.1 The XGC Gyrokinetic Edge Code (Ku, Hager, Chen, Parker, and others):

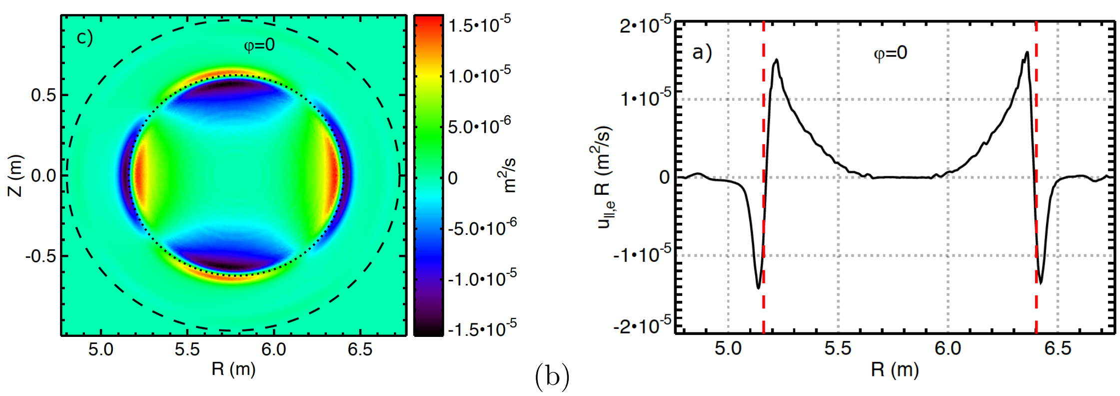
XGC is a particle-in-cell (PIC) gyrokinetic code treating diverted tokamak plasmas, including the core plasma, X-point and scrape-off layer (SOL), and is presently the only production kinetic code that simulates multiscale edge tokamak plasma physics (turbulence, neoclassical physics and neutral particle dynamics) in such realistic geometries. XGC is distinguished from conventional GK codes by: (1) having total-f simulation capabilities to handle the non-Maxwellian distribution functions arising in the edge plasma via a 5D phase space continuum grid in addition to the particles-in-cell technology [119, 116]; (2) simulating edge neoclassical (e.g., orbit loss), neutral particles, and nonlocal turbulent transport consistently without assuming scale separation between them; (3) treating the scrape-off-layer plasma using a simplified plasma-wall interaction, with a logical sheath model at their interface (a Debye sheath model is being implemented), enabling divertor heat-load calculations; and (4) optimizing for extreme-scale HPCs to render the computational requirements of these features tractable; again, XGC has demonstrated efficient scaling at maximal concurrency on Titan (Cray XK at ORNL), Edison (Cray XC at NERSC), and Mira (Blue Gene/Q at ALCF) (see Sec. 3.2.5). We have already ported XGC to Cori at scale. The parallelization uses MPI, OpenMP, OpenACC, CUDA Fortran, and SIMD vectorization for Intel MIC. XGC has been well-verified; its continued verification will be a high priority activity (see Secs. 2.2 & 3.1.6).

XGC previously had three electron models in conjunction with its gyrokinetic ions: (i) a conventional drift-kinetic (or gyrokinetic) model for multiscale electrostatic physics [116], (ii) a parallel canonical-momentum model for electromagnetic microturbulence utilizing a split-weight scheme [33, 34], and (iii) a fluid model for long-intermediate wavelength MHD/fluid type electromagnetic perturbations [78, 35]. The second method has been effective in removing the so-called "cancellation" problem [48, 33, 87, 105, 135, 136] for short wave length modes, but problematic for the



(a) (b)

Figure 3: *(a) Verification of shear Alfven waves from the fully implicit kinetic electron version of XGC in a circular cross-section torus with $R_0/a = 3.5$ and β_e=0.3%. Red dots are from XGC and blue line is analytic solution [118]. (b) Fluid-electron XGC simulation of nonlinear kinetic ballooning mode (KBM) behavior in time, without the neoclassical driver, for the n=20 mode in the same torus at β_e=2% [113]. At such a high β_e well above the instability threshold ($\beta_e \sim$ 1.2%), nonlinear KBM turbulence saturation is difficult as well known. We will perform higher-resolution global simulations including the neoclassical drive term to study profile relaxation and saturation,*



(a) (b)

Figure 4: *(m=2,n=1) tearing mode from XGC[78] has been verified against M3D-K[18] in the fluid limit in a circular cross sectional torus. The mode structures are virtually indistinguishable between two codes, and the linear growth rate agrees within 6% even though they use highly different discretization. (a) 2D plot of perturbed parallel current $u_{\|}R = -j_{\|}R/e$ at toroidal angle $\varphi = 0$, where R is the major radius. (b) 1D plot of $u_{\|}R$ across the midplane.*

long wave length modes. Due to the importance of the long wavelength MHD-type modes in the edge pedestal, the second method will not be discussed here. Recently, a fully implicit scheme with kinetic electrons for gyrokinetic electromagnetic simulation, based on the Vlasov-Darwin PIC algorithm[28], was implemented in XGC [118], which is valid for all wave-length modes and insensitive to the magnetic geometry. Verification tests demonstrate that the cancellation problem, is eliminated by this scheme (see Fig. 3(a)) [118]. Example electromagnetic verifications from both fully implicit kinetic electrons and hybrid fluid electron model are shown in Figs. 3 and 4. Verification of other essential electromagnetic modes can be found in [117, 78, 113]. Cross-verification with BOUT++ in the intermediate wavelength regime also shows excellent agreement (Fig. 5 of [26]). Electromagnetic XGC has already been used to study NSTX and DIII-D edge plasma [117, 113, 121], and found that the NSTX edge plasma is not usually subject to the Kinetic Ballooning Mode instabilities while DIII-D edge plasma is (benchmarked with GYRO); and that the gyrokinetic Peeling-Ballooning Modes can be unstable in both devices (benchmarked with GEM). Both kinetic and fluid electron models will be used depending upon the science. The recent pullback approach in [87, 105, 135, 136] also looks promising. Even though the fully implicit method will be XGC's primary method and our applied mathematical team will focus on its improvement, the physics team will also investigate the pullback approach as an alternative.

Several versions of global electromagnetic gyrokinetic equations have been derived and used in various formulations, orderings, and levels of accuracy ([14, 34, 86, 19, 185, 182, 16, 146, 147, 80, 55, 165, 130] and references therein). We currently use equations that are used in most gyrokinetic codes, and will improve them as the project progresses. We will use our 6D fully kinetic code development to ultimately verify and improve the 5D gyrokinetic equations (see Sec. 2.2.2). Improving the efficiency of the scalable implicit electromagnetic algorithms in the edge geometry, together with portability and performance optimization, will be a significant part of the proposed joint research among physicists, applied mathematicians, and computer scientists.

The planned studies listed below require large amount of computational resources. With XGC exascale-aware and in all three Pre-Exascale Programs, enabling ∼20X more number of simulations than today for the same problem, it is expected that the proposed studies listed below will have adequate computing resources. However, the total number of full-scale XGC simulations will still not be extremely large, and a well coordinated and centralized simulation plan will be exercised. We note here that many of the listed studies below do not need independent simulations, and will be done in conjunction with other simulations (piggy-backing on each other).

2.1.2 Nonlinear Intermittent Turbulence (Ku, Churchill, Myra, Parker, Chang, Maingi):

Intermittent, nonlinear coherent structures in the plasma turbulence (simply referred to as "blobs" here, even though its original definition might be different [56, 109]) have been observed to dominate the experimental boundary plasma; understanding them is critical for predicting ITER's boundary plasma. XGC uniquely produces gyrokinetic blobs [116, 40] across magnetic separatrix, consistently with other physics such as kinetic orbit (loss) dynamics and global neoclassical physics. Understanding the basic blobby turbulence generation mechanisms, scaling of fluctuation levels, blob propagation to the near and far SOL, and the associated transport [139, 83, 111] are critical to ITER high priority physics, such as projecting the survivability of ITER's plasma facing materials at both the divertor plate and main chamber walls, the low-to-high mode transition, and the pedestal structure. Contributions to our knowledge of these topics have been made by others in the fusion community using simple analytic theory [133, 158, 42, 126, 62, 12, 110, 193, 70, 154], mostly in model geometries. Consequently, significant gaps in our understanding of these phenomena remain; XGC is uniquely capable of filling them, given its ability to perform fully kinetic simulations in realistic divertor geometries. Figure 5 depicts a snapshot from an XGC simulation showing the normalized density fluctuations, $\delta n/n$, in the edge turbulence of a DIII-D H-mode like plasma. ExB-flow sheared structure of ITG-TEM turbulence can be seen in the inner radial region, while coherent, "blobby" turbulent structures can be seen on and outside of the magnetic separatrix. Preliminary analysis of XGC results along these lines suggests an important role for extensive theory-based [140] post-processing analyses of edge and SOL phenomena [100]. Recent research, described in Sec. 2.1.4, has shown that "blobby" turbulence plays an important role in setting the divertor heat-flux width in ITER. Given the code's large computing demands, extracting information, understanding, and experimentally validating as much as possible from FES/ASCR group activity is imperative. Thus far, only electrostatic edge turbulence has been studied; electromagnetic edge turbulence will be studied in multiple tokamaks as part of the proposed research. The properties and roles of "blobs" in ITER-critical physics phenomena, as discussed in the subsequent subsections, will be studied.

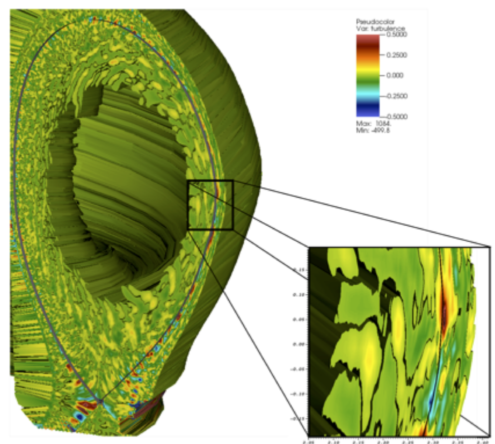


Figure 5: *Density fluctuations $\delta n/n$ from an XGC simulation in the edge turbulence of a DIII-D H-mode like plasma[116]. Coherent, "blobby" turbulent structures are seen on and outside of the magnetic separatrix. (The mean density has been subtracted out to make the small amplitude fluctuations visible, they are less than 1% in the core plasma, but greater in edge.)*

2.1.3 L-H Transition in Burning Plasmas (Chang, Ku, Parker, Tynan, Churchill, J. Hughes, Maingi):

H-mode operation and, thus, the L-H transition [187], is essential for ITER to achieve its ultimate goal of a ten-fold fusion energy gain. However, thirty years of work has yet to deliver a comprehensive model for the L-H transition. We *do* know that it hinges on multiple kinetic phenomena: ion orbit dynamics, on both sides of the separatrix, X-point orbit loss [25, 114], kinetic turbulence, including the trapped electron mode, and a self-consistent $E \times B$ shearing dynamics. Further complicating the picture, recent ITER-like tungsten divertor experiments on JET and ASDEX-U yielded a *lower* L-H threshold power, relative to carbon divertor operation, yet with significantly poorer H-mode confinement [124].

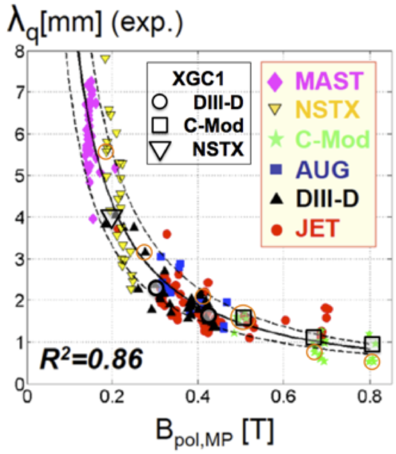
A fully kinetic XGC simulation of a C-Mod model plasma, in a global edge geometry with a separatrix and neutral recycling and using 90% of Titan's capacity, has, for the first time, revealed a fast L-H transition dynamics under strong heating [24]. The simulation results agree with some of the assumptions underlying the popular predator-prey model [102], but with one important modification: neoclassical ion orbit loss physics plays a key role in the bifurcation process. We observe that an edge turbulence and transport bifurcation event occur when the microscale turbulence-driven Reynolds force and the macroscale neoclassical orbit loss force reinforce each other, and when the resulting $E \times B$ shearing rate in the edge layer reaches a critical level (in this case, matching the growth rate of the collisional trapped electron mode). Thus, the experimental explanation based upon the orbit loss mechanism in Ref. [107] and the conventional Reynolds stress argument [50] work together.

In our proposed research, we will extend the L-H transition dynamics study to multiple tokamaks and discharges that have well-diagnosed turbulence and mean-flow dynamics (DIII-D and ASDEX-U), and study how the varying plasma conditions impact the transition physics on pre-exascale computers. The resulting XGC-predicted L-H transition powers will be compared with the empirical formula derived from existing tokamak data. We will also study effects of high-Z impurities on the transition using JET and ASDEX-U discharges since this is of critical interest to ITER. Even though the edge plasma at the time of L-H transition is at low-β, we will investigate the possible effects of electromagnetic turbulence. We will also predict whether or not ITER's heating power will be sufficient to make the L-H transition. A well organized plan with the experimental validation team will be executed in order to minimize the number of simulations.

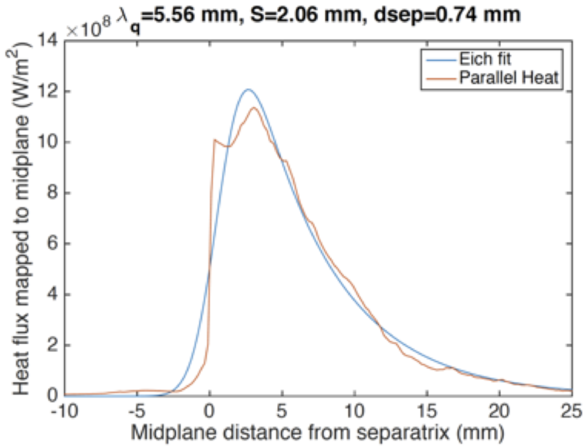
2.1.4 Divertor Heat-load Footprint (Ku, Churchill, Chang, Myra, Stotler, Maingi, Terry, Labombard, Hughes): A serious concern for ITER operation is the ability of its divertor to withstand the steady plasma exhaust heat that will be deposited on the divertor surface along a narrow toroidal strip. A regression analysis of experimental data from present devices shows that the heat-flux width follows a scaling $B_P^{-1.19}$ where B_P is the magnitude of the poloidal magnetic field on outboard midplane separatrix [64, 63]. For ITER operation at $I_P = 15$ MA with $q_{95} = 3$, this regression yields $\leq$ 1mm for the heat-flux width λ_q when mapped to outboard midplane (or $\leq$1 cm on the outer divertor plate). Such a narrow λ_q leads to very large local power fluxes in attached divertor conditions. The resulting heat fluxes exceed the divertor material's steady state design limits, forcing the use of the more complex and constraining detached divertor mode of operation.

However, since this heat flux width in ITER represents a significant data-extrapolation from present tokamaks, not based on fundamental understanding, it may not be valid. A high fidelity, nearly first principles calculation will allow us to extrapolate with much greater confidence; this was the purpose of the previous XGC studies [24]. Figure 6(a) shows excellent agreement of the XGC-produced λ_q values with the experimental DIII-D, C-Mod, and NSTX data from Fig. 3 of Ref. [63]. Open black inverted-triangle, circles, and squares represent the XGC-calculated λ_q values for NSTX, DIII-D, and C-Mod, respectively. All the XGC-produced λ_q values are within the experimental regression errors, thereby validating within the error bar the electrostatic gyrokinetic equations and boundary conditions used by XGC in predicting the heat flux width. JET experimental data might show some anomaly in Fig. 6(a). However, there are other experimental evidences that the experimental JET data may also follow the black curve [170]. The proposed research give a high priority to the XGC validation of these JET result. Whether or not these results will be affected by electromagnetic turbulence is to be determined as part of the proposed research. Neutral particle effects on λ_q have already been estimated as $< 10\%$ in the investigated low-recycling regime.

XGC predicts that ITER's λ_q is $\lesssim$ 5 mm (Fig. 6(b)), a significantly favorable result for its divertor. The XGC simulations of existing tokamaks show that the ion magnetic drift contribution



(a)



(b)

Figure 6: *(a) (from Ref. [23]) XGC1-produced $\lambda_q$results have been overlaid on Fig. 3 of Ref. [63]. Data points circled in orange represent experimental discharges that are used for simulation. (b) Parallel heat-flux footprint on the outer divertor plate, mapped to outboard midplane, in a model ITER plasma edge at 15MA. The "Eich fit" function describes well the XGC-produced footprint.*

to the heat flux width is dominant over that due to electron contribution from turbulence; in ITER the situation is reversed; Both the width and magnitude are dominated by electrons. The highest current C-Mod discharge studied so far is found to be in a mixed regime in that the turbulent electron width is narrower than the ion width, like DIII-D and NSTX cases, but the *magnitude* of the electron heat-flux is greater than that of the ions.

Our proposed λ_q investigation will be performed in three stages. First, we will test the ITER result using data from JET (UK), the largest tokamak and half the linear size of ITER. The XGC version used to generate the data in Figs.6 will be applied to a high current JET discharge, and the result will be tested against experimental data. The simulation geometry will then be numerically enlarged by a factor of 1.5, halving the extrapolation to ITER's size. Our primary focus will be on whether or not the contribution made by "blobby" turbulence to the heat flux width increases with increasing size while the neoclassical magnetic-drift contribution decreases, i.e., trying to identify how along the way the behaviors shift to those seen in the ITER simulation. Second, the possible corrections to λ_q by electromagnetic turbulence will be studied. Third, the effects of the high-Z impurity particles on λ_q will be investigated. Not only attached divertor plasmas, but also detached plasmas will be studied after the upgrade to the neutral particle routine (see Sec. 2.1.8).

2.1.5 Pedestal Structure (Hager, Ku, Chang, Parker, Chen, Maingi, Greenwald, Tynan, Stotler, Hammett): Saying that the pedestal structure, especially the height, determines core fusion performance is not an exaggeration. In a typical large-scale (type-I) ELMy H-mode model such as EPED [173], the edge profiles evolve with the pressure gradient determined by the kinetic ballooning mode (KBM) instability until a peeling ballooning mode (PBM, ideal MHD) stability limit is met, triggering an ELM crash. Such models have provided a valuable conceptual framework and have been quite successful for many standard operating regimes in present-day experiments.

However, the most important problems lie outside, either partially or fully, the scope of EPED-like models. For example, metal wall experiments (e.g., JET and ASDEX-U, with inability to match the pedestal temperature height to carbon wall) demonstrate the need to capture self-consistently the distinct dynamics of the density and temperature profiles, a difficult task for MHD codes [124]. Impurities also play a critical role in the ITER-like wall discharges and require kinetic treatment since their guiding center orbit width is comparable to the edge plasma scale length. Additionally, unlike the MHD-based physics, gyrokinetic KBM/PBM stability of conventional H-mode plasmas is found to be dependent on the ion and electron temperature profiles and density profiles [190]. Moreover, ELM-free regimes (e.g., I-mode, quiescent H-mode, ELM-suppressed RMP scenarios, etc.) by definition are not subject to an ELM-triggering MHD instability threshold; hence their pedestal structure cannot be understood from the MHD physics.

First-principles gyrokinetic simulations are necessary to achieve a higher-fidelity predictive capability for pedestal structure that must be explored for ELM-free operation on ITER or other burning plasma devices. In fact, during the divertor heat-flux width studies described in Sec. 2.1.4, XGC found that even electrostatic turbulence yields a milder pedestal gradient in ITER than that predicted by the simple analytic KBM model. Whether or not ITER pedestals will be susceptible to ELMs is another high-priority topic in our project. Since its fully developed pedestals will most likely be subject to electromagnetic instabilities, we will try to predict ITER's pedestal structure using the new electromagnetic versions of XGC, as demonstrated in Ref [113]. These new XGC versions will also be able to study PBM and KBM type instabilities, including gyrokinetic ion effects. The pedestal structure study simulations will be performed in conjunction with other pedestal physics studies, such as those on divertor heat flux width and impurity effects. These studies may also shed light on the pedestal density limit physics that could lead to disruption event.

2.1.6 Transient Heat-Flux to Divertor from Nonlinear Edge Localized Modes (ELMs) and ELM control by external 3D magnetic perturbation (Ferraro, Hager, Maingi):

The transient heat and particle fluxes from large-scale type-I ELM crashes are expected to be sufficiently severe that they can rapidly erode or melt plasma facing components in ITER [67] even in the absence of the steady heat-flux discussed in the previous section. Consequently, understanding the fluxes associated with type-I ELM crashes and developing means of avoiding them are high priority research topics. Type-I ELMs are generally understood to be MHD type

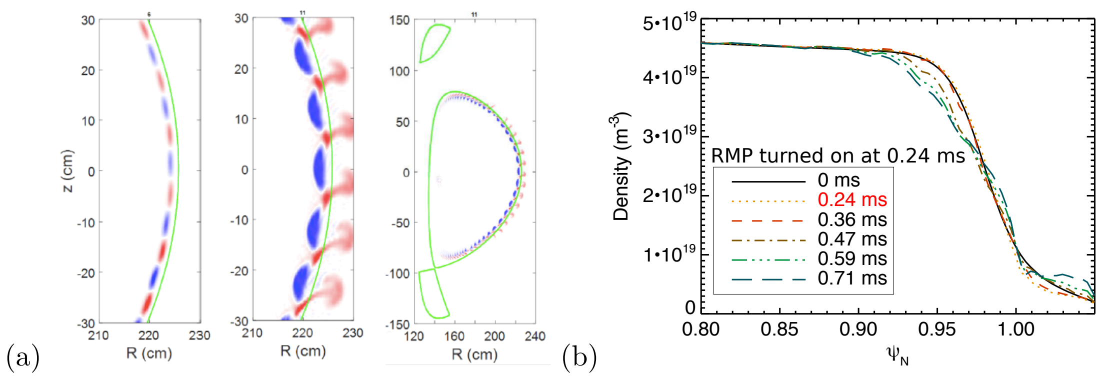


Figure 7: *(a) The perturbed pressure in a nonlinear M3D-C1 ELM simulation in KSTAR geometry [97]. Left and middle panels show the pressure perturbation on the outboard midplane at* $t = 13.8\,\mu$s *and* $t = 25.3\,\mu$s*, respectively. The green line represents the separatrix of the unperturbed (axisymmetric) equilibrium. The right panel shows the pressure perturbation over the full plasma cross-section at* $t = 25.3\,\mu$s*. (b) Evolution of the density profile in a DIII-D like H-mode plasma due to RMP induced neoclassical transport calculated with XGC. The non-axisymmetric perturbed field is switched on 0.24 ms into the simulation and rapid profile evolution ensues.*

instabilities driven by the steep pressure gradient and sharp current density (Peeling-ballooning modes, PBMs) in the H-mode pedestal, and ideal-MHD linear models generally provide a good understanding of the stability threshold in conventional discharges [174]. However, linear stability analysis does not provide an estimate of the heat flux delivered by an ELM To get that information, nonlinear calculations are required. Just such calculations have been performed with the extended-MHD code M3D-C1 in both ITER and KSTAR geometry (Fig. 7). While these simulations likely provide a reasonable description of the nonlinear evolution of the magnetic field and convective losses in the pedestal and SOL, the extended-MHD model does not accurately capture parallel fluxes, neoclassical transport, turbulent transport, radiation, neutrals, or sheath physics.

To quantify the impact of these non-MHD, kinetic effects on the divertor heat flux, we plan to extend the M3D-C1 calculations with a coupling to XGC. The gyrokinetic backbone in the XGC code will include a model of neutral transport, ionization, and radiation through an interface to DEGAS2 (Sec. 2.1.8), as well as a 6D kinetic sheath model (Sec. 2.3.1). The coupling between M3D-C1 and XGC will be mathematically loose: M3D-C1 will calculate the nonlinear evolution of the ELM, and XGC1 will use the MHD-produced non-axisymmetric electromagnetic field and plasma profile evolution to calculate the transient transport of particles and heat to the divertor plates as a function of time during the evolution of the ELM. The kinetic closure information from XGC will be continuously fed back into M3D-C1 for a higher fidelity MHD calculation. This will be done both in DIII-D geometry with experimental measurements of divertor heat load during ELMs, and in a $Q_{DT} = 10$, $I_P = 15$MA ITER scenario to provide an estimate of the expected transient flux amplitude and distribution. Advanced in-memory data transfer methods between the codes will be utilized, as described in Sec. 3.2.1. This coupling would represent important progress towards a multi-physics model capable of describing transient heat load physics.

ELM control by 3D magnetic perturbation: The application of non-axisymmetric 3D magnetic perturbations has been demonstrated as an effective means of suppressing ELMs and is planned for use in ITER. The mechanism by which this occurs is not fully understood, nor is their penetration into the tokamak edge plasma. The EPED model [173] predicts that ELMs can be stabilized by driving transport near the top of the pedestal, which would act to prevent the pedestal from growing to an unstable width. Therefore, the idea that non-axisymmetric fields stabilize ELMs by driving kinetic transport at the top of the pedestal, either though enhanced turbulent transport, neoclassical transport, or parallel transport by stochastic magnetic fields, is among the leading hypotheses for ELM suppression.

We plan to use M3D-C1 to model the plasma equilibrium in the presence of non-axisymmetric fields [68, 104], and XGC for a kinetic model of transport in the non-axisymmetric equilibrium. A successful example of including the perturbed equilibrium in a kinetic XGC transport code already exists [145, 144] and presented as an invited talk at the 2011 APS-DPP Conference. XGC will calculate the kinetic transport and the new plasma profile using the M3D-C1 computed 3D-perturbed MHD equilibrium, and M3D-C1 will then establish an updated 3D-perturbed MHD equilibrium, with the goal of exploring how a converged solution can be reached efficiently. The MHD ELM stability will be evaluated with the new XGC-calculated plasma profiles at every few coupling steps. A file-based interface for reading the M3D-C1 perturbed equilibrium has already been implemented in XGC and initial studies of RMP induced neoclassical transport, i.e., without turbulent fluctuations, have been successfully undertaken (see Fig. 7).

XGC also has its own electromagnetic solver within its gyrokinetic ion kinetic framework (Sec. 2.1.1); it includes the necessary MHD-type modes, kinetic ballooning modes, and other microturbulence (in an incompressible plasma limit). At a later phase of proposed research, the gyrokinetic RMP penetration dynamics, 3D perturbed kinetic equilibrium, and kinetic transport will be simulated in a fully consistent manner at each time step (as demonstrated in [144]), and the results will be compared with that obtained from XGC coupled to M3D-C1. RMP effect on the gyrokinetic edge-localized mode onset will also be studied consistently within XGC.

2.1.7 Gyrokinetic Study of Impurity Particle Effects on Pedestal Properties (Hager, Chang, Koskela, Maingi, Stotler, Greenwald, Tynan): Recent experiments on JET and ASDEX-U have demonstrated that high-Z tungsten impurity particles from their ITER-like walls (ILW) can significantly degrade H-mode pedestal confinement and stability [124] relative to those seen with carbon walls, even though the L-H transition power is reduced. These findings are now a significant concern for the ITER program. With ILW, the electron temperature (T_e) pedestal height is reduced and the ELM stability limit is more restrictive in comparison with the conventional ideal-MHD peeling-ballooning mode boundary. JET and ASDEX-U have been able to partially recover the pedestal T_e by nitrogen gas puff, albeit without a fundamental understanding. They also find that the relative shift between the T_e and electron density n_e pedestal profiles is larger with the ILW than with carbon. The dependencies of pedestal confinement, structure and ELM stability on the collisionality also differ significantly between ILW and the experience with carbon walls. The observed phenomena may also be related to the $E \times B$ shearing and SOL layer physics.

MHD / fluid models have been unable to explain these observations well enough [124]. Most of the phenomena responsible are likely kinetic in nature and can only be understood in a comprehensive, nonlocal, multiscale kinetic code. XGC is capable of including high and low Z gyrokinetic impurity particles [103]. Each of our proposed research areas will include an examination of tungsten and nitrogen (or other low-Z impurity) effects to answer these questions.

2.1.8 Enhancement of the Neutral Particle capability for Detached Plasma (Stotler, Churchill, Hager, Maingi, Ku):

XGC contains either a simplified DEGAS2 type routine simulating atomic neutral particles or the full DEGAS2 routine as subroutine. Neutral particle effects in XGC simulations heretofore have been modest, although not negligible [179], as a result of low SOL densities, commonly referred to as low-recycling or "sheath limited" conditions. The SOL behavior of the code in this regime has been reasonably verified and validated [41]. Under the low-recycling condition, describing the neutrals as atoms is found to be reasonable enough.

Accurately simulating and validating against a broader spectrum of discharges will entail extending our investigations to lower SOL temperatures, e.g., via impurity radiation, and higher densities, reaching into the high recycling and detached regimes. Along the way, the rates of momentum and energy exchanged between neutral and plasma species will increase, leading to more stringent conservation requirements and the need for additional atomic physics processes.

We will first improve the momentum and energy conservation [178] in charge exchange reactions. Second, we will implement elastic scattering between ions and hydrogen molecules, a significant mechanism for momentum transport. The data and algorithms required for this step are already part of the DEGAS2 code. Enhancements to those data will then be made to account for the effects of vibrational excitation and other molecular processes via effective "collisional radiative" rates [108]. Finally, we will add volumetric recombination of hydrogen ions since this becomes a significant source of neutral atoms in the detached regime. Doing so is straightforward since it only entails expanding the existing impurity recombination routine [177] to include the main ions.

We will also incorporate radiation trapping effects into DEGAS2; the neutral densities typically encountered in detached divertors are sufficiently high to trap Lyman-α radiation [112]. A simple model for these effects, developed by Adams [2] and Scott [166], should suffice since the high opacities found in detached plasmas render the overall problem insensitive to the details of the radiation transport.

2.2 Scouting Simulation and Code Verification in Pedestal Using Core Codes

2.2.1 GEM and GENE (Parker, Hatch, Chen, Ku, Hager):

XGC includes much more physics than any other gyrokinetic code with its ability to handle non-thermal plasmas and complex separatrix geometries having both closed and open field lines. It pushes the absolute limits of parallel computing concurrency. To best utilize the limited number of large-scale XGC simulations, we propose to employ the existing, well-verified δf gyrokinetic turbulence codes GEM (PIC) and GENE (continuum) to execute physics "scouting" studies of the edge pedestal region, albeit on closed flux surfaces only. The scouting simulations will include the MHD/fluid type intermediate/long wavelength modes and all the microturbulence modes that may be important in the edge pedestal.

Also, the inherent complexity XGC drives a need for cross-verification against other well-verified gyrokinetic codes in an important region of common applicability: the pedestal. GEM and GENE have recently been among the leading core gyrokinetic codes to study electromagnetic instabilities in the steep edge pedestal region inside the sepratrix (e.g., [84, 85, 86] for GENE, [190, 189, 38] for GEM), and are well positioned for scouting turbulence studies and verification runs. They provide test beds from both particle and continuum technologies. Successful cross-verifications among these three codes already exist in various physics areas [117, 78, 121, 32]; including details of ITG modes (e.g., Fig. 8), ITG-KBM transition, kinetic peeling-ballooning modes, etc. Value of probing and verification of turbulence in the steep pedestal inside the separatrix can be recognized from the fact that the pedestal is a strong source of turbulence for the entire global edge. Besides the "direct" electromagnetic algorithm [33], GEM has an optional drift-fluid electron hybrid model that is efficient for studying low- to intermediate-n modes [35]; a technology transfer has provided XGC with the same option [78]. Fig. 9 shows gyrokinetic simulation of an ELM from GEM: XGC has been verified agaist

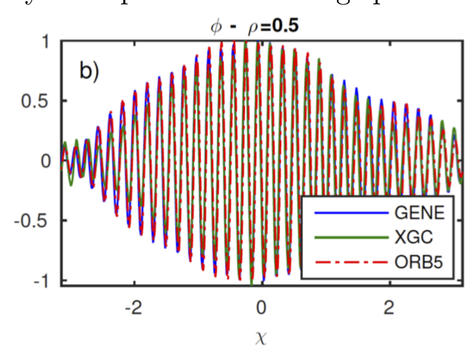


Figure 8: *Excellent agreement in the poloidal ITG mode structure between XGC and GENE. A similar agreement is obtained in the linear growth rate.*

this simulation. The drift-fluid electron model can utilize drift-kinetic electrons (enabling trapped electron modes) through perturbed pressure.

2.2.2 Multiscale Fully Kinetic 6D Ion Physics (Chen, Parker, Hager, Chacon, Ku): We propose to further develop an implicit, multiscale, electromagnetic, 6D ion (also called fully kinetic) model. Such a model is useful for verifying gyrokinetics in the situations where the gyrokinetic ordering parameters may not be so small, especially in the steep gradient edge pedestal region. We have already had recent success using an implicit orbit averaging, sub-cycling algorithm, accurately reproducing ion finite Larmor radius (FLR) effects for ion acoustic waves [181] and the toroidal ITG instability [180]. Such multiscale algorithms have been shown to be amenable to massively parallel hybrid architectures with GPUs or math co-processors [181]. We intend to further develop this electromagnetic model in tokamak geometry to verify and improve the gyrokinetic ion model in XGC. This is an especially useful tool for identifying second order terms in gyrokinetics that may be important in the steep edge region, thereby enhancing the fidelity of XGC edge simulations.

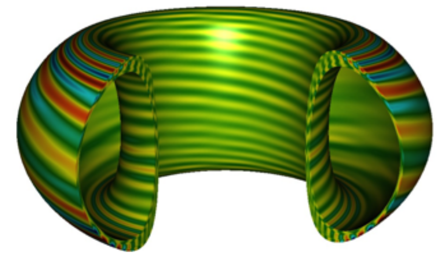


Figure 9: *Gyrokinetic structure of an ELM inside separatrix in GEM [189, 128] (and similarly in XGC). Nonlinear state reveals a fairly coherent dominant mode.*

2.3 Interface with other SciDAC projects

2.3.1 6D Sheath Modeling in XGC for Interface with Material Simulation (Curreli, Stotler, Chang, Churchill, Ku, Chacon, Shephard, Yoon):

A realistic plasma-material interaction simulation requires a proper ion energy distribution (IAD) for the ions bombarding the material surface across the plasma sheath. The outgoing neutral particle energy and angle distribution can then be used as a neutral source in XGC's Monte Carlo neutral calculation. Accurate simulation of all of the first surface layer physics requires IAD from a proper non-thermal kinetic code (like XGC) to handle the significant fraction of tail particles. Due to the short length scale of the Debye sheath, the charged plasma particles can no longer be treated as gyrokinetic particles and must be treated as fully kinetic. A proper accounting of the $E \times B$ and magnetic drift motions of the individual kinetic particles is also important.

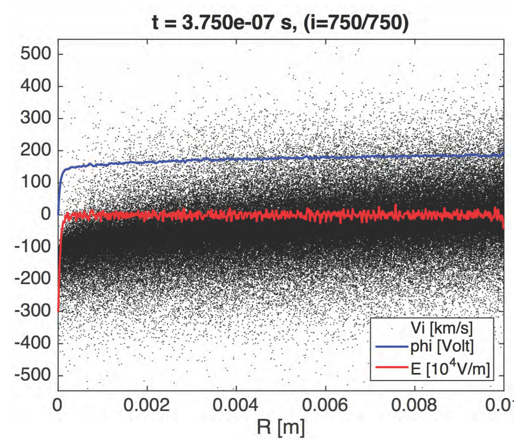


Figure 10: *Plasma sheath potential (blue line), electric field (red) and the ion particle speed (black dots) distributions from the coupled XGC-hPIC simulation.*

The gyrokinetic ion and electron particle distribution functions within several mm of the material surface in XGC will be converted into may more full 6D particles by using an up-sampling technique (a rejection sampling technique with multivariate normal distribution having covariance scale at its peak utilization) with the random gyro-angle distribution, with a grid refinement to resolve the Debye sheath scale. The Poisson equation will then be solved for the high-fidelity near-wall layer including the quasi-neutral region (collisional pre-sheath and magnetic pre-sheath), and the non-neutral Debye sheath. The established multi-species hPIC code [49] will be coupled into XGC as a subroutine by the U. of Illinois Co-PI (D. Curreli). The hPIC code has full-orbit electrons (Boris-Bunemann) and also tracking impurities. It has successfully been scaled up to 65,536 cores on the Blue Waters supercomputer [101], achieving weak scaling efficiency around 90-95% relative to single-node performance. This parallelization was for a single, local sheath calculation. The hPIC calculation needed here will be distributed over poloidal and toroidal angles. With the existing multi-dimensional particle domain decomposition in XGC, a massive parallelization of the sheath calculation will match well with XGC's parallelism. Further improvements to the speed of hPIC code will be achieved in the project through an implicit particle algorithm developed and already implemented in XGC by one of the co-authors of this proposal (L. Chacon)[27, 29].

Since both XGC and hPIC use the PETSc solver library, we will employ a unified XGC PETSc solver across the coarse-grained gyrokinetic and fine-grained Debye-sheath meshes with a smooth connection between them provided by RPI's meshing technology. The variable coefficient in the gyrokinetic Poisson solver will also be smoothly connected to the unity coefficient appearing in the full Poisson solver. The sheath solution not only enables XGC's interface with a material science code, but will also improve the "logical sheath model" currently used in XGC.

Preliminary attempts to this coupling have already been successful. For example, ion and electron particle distribution functions from an XGC simulation of a model DIII-D plasma [40] taken in front of the divertor plate, near the outer separatrix strike point, have been used as an input to the Debye sheath calculation. The XGC distribution functions are highly non-Maxwellian. Figure 10 shows the solution for the electrostatic potential (blue line) and the electric field along the magnetic field line. Black dots represent the ion $v_{parallel}/v_{i,thermal}$ distribution from XGC. Ions with positive speeds (away from the material surface) are due to scattering associated with neutral charge exchange and Coulomb collisions.

2.4 Development of the Continuum Code Gkeyll (Hammett, Hakim, Hauck): Particle and continuum models have mutually complementary advantages. PIC is amenable to complex modeling of geometry and multi-physics, e.g., neutral particle kinetics. Continuum models provide a low-noise alternative to standard PIC. It is desirable to have independent codes with different algorithms to cross-check each other, particularly for complex chaotic systems. Moreover, the cross-verifications described in Sec. 2.2 is only in the pedestal region inside the separatrix. Cross-checking the solutions across the separatrix will be important. For these reasons we will support the development of the continuum code Gkeyll, which uses certain versions of discontinuous Galerkin algorithms to explore how much they help with the challenges of the boundary region: a good complement to XGC's PIC algorithm. Gkeyll uses higher-order methods, which are attractive for massively-parallel computing because they extract more information per byte, thus lowering interprocessor communication costs. (If the resolution can be reduced by a factor of 2 in 5D, that reduces cost by a factor of 64.) Gkeyll is less developed in terms of comprehensive physics than XGC, but has recently carried out what we believe are the first 5D gyrokinetic continuum simulations of turbulence on open field lines including model sheath losses[169, 82]. Past attempts with continuum codes apparently had numerical or physical difficulties with the SOL. (The XGC PIC code has long done simulations like this, and furthermore is the only gyrokinetic turbulence code at present able to simulate open and closed field lines simultaneously.)

One could consider a hybrid of PIC ions with continuum electrons. While a full production continuum/particle hybrid model is quite futuristic, research in this area in the same cooperative team is prudent. We need to consider various options to take the best advantage of future HPCs. XGC1 in fact already has a 5D phase space grid for the nonlinear collision operator and non-Maxwellian distortion. Hence, XGC1 is within the continuum algorithm domain. Various continuum/PIC hybrid and forward Lagrangian schemes exist [52, 186, 47] and can be easily utilized within the XGC1 code framework. XGC and Gkeyll will learn from each other in this project.

Gkeyll implements a special combination [125] of DG for the distribution function F with a finite-element potential that conserves energy for Hamiltonian terms in the continuous time limit (or with certain time integrators) by restricting the potential to a continuous subspace of the space for F. This approach works even with upwinding or flux limiters.

Initial Gkeyll simulations[169, 82] have been done for the LAPD device at UCLA[73, 161] and show good qualitative agreement with the experiment and past fluid simulations. We have also done simulations of Torpex[153], which has a Simple Magnetized Torus geometry. Despite the geometrical simplicity, these simulations contain key elements of SOL turbulence in a fusion device (toroidal bad-curvature and strong gradients that drive large amplitude fluctuations, parallel losses with model sheath boundary conditions, localized sources to represent transport from the core) and demonstrate the basic feasibility of this approach.

We will pursue three main math/computational projects to upgrade Gkeyll that will be carried out in collaboration between the ASCR and FES sides of this partnership. The first is to upgrade to realistic tokamak geometry with a separatrix and X-points. It is important to use coordinates or grids that are at least approximately aligned with magnetic fields to reduce resolution requirements.

We introduced field-aligned coordinates to turbulence simulations[9] and will consider several approaches (such as [196, 58, 131]) to handle complications near the X-point. Experience gained in XGC can be of help. The second and third projects involve the use of nonstandard basis functions and sparse representations to improve efficiency. More details are in Sec. 3.1.

On the physics side, we will extend the code to include more complete physics, including recycling, neutrals, and radiation, using fast simpler models at first. Some packages and libraries can be shared with XGC. We have demonstrated an efficient way to include electromagnetic fluctuations using consistent basis functions for $A_{||}$ and $\nabla\phi$, and will implement this in the full code. We are working on improved models of sheath boundary conditions for gyrokinetics[169], and will implement those in Gkeyll and XGC for comparison with the full Vlasov approach in Sec. 2.3.1. As the code matures, there will be ongoing benchmarking to compare with XGC (and COGENT within its available capability) and build confidence in results of both codes and learn from each other. We can study some effects, like the impact of low-recycling lithium relative to high-recycling walls, in all years with different levels of fidelity as the code is improved.

2.5 Building a High-fidelity Boundary Physics Module, and interfacing with WDM and other SciDACs

(D'Azevedo, Hager, Worley, Ku, Chen, Myra, Ferraro, Churchill, Hoffman): This project will produce a unified high-fidelity boundary plasma simulation module "HBPS-module" that can be interfaced not only with a plasma-material interaction (PMI) SciDAC, but also can be used by a whole device modeling (WDM) framework through core-edge coupling, and interfaced with a Disruption modeling and other SciDAC projects. HBPS-module, especially XGC, will be "exascale-aware" to ensure readiness of our computational approach when exascale systems become available. We will establish connections and synergies with relevant DOE-supported efforts.

All three US gyrokinetic boundary physics codes (XGC, Gkeyll, and COGENT-via Hittinger) will be included in the HBPS module, with the user choices defined in the input file for validation of specific physics or cross-verification between codes. Liaisons with other SciDACs are funded members of this proposal (D. Curelli and R.M. Churchill for PMI, S. Parker, Y. Chen, D. Hatch and J. Myra for WDM, R, Hager for RF and energetic particles, N. Ferraro for disruption, and R. Hager for runaway electrons). Our HBPS module will be open to other fusion researchers, with the set of regression tests regularly expanded based on the usage.

Our research can also be interfaced with energetic particle, runaway electron and RF physics by extending the total-f gyrokinetic velocity range to high energies. For a runaway physics interface, XGC's nonlinear Fokker-Planck operator will need to be upgraded to be relativistic (in collaboration with the SciDAC SCREAM project). Our applied mathematics team has a clearly delineated plan to further improve the Fokker-Planck operator to make it more efficient at high energies. For an interface with a plasma Disruption SciDAC project, we can study the pedestal density limit physics and its relation to disruption. There is a possibility that turbulent electron heat flux may increase nonlinearly with the edge density and cool the plasma, leading to a plasma disruption. We can also study a possible reinforcing nonlocal interaction between the precursor modes (e.g., neoclassical tearing modes) in the core plasma and the dynamics of the boundary plasma. The low-n tearing mode capability in XGC has already been verified [78]. Sheath interaction with plasma particle and energy from disruption can be another topic.

2.6 Experimental Validation

(Greenwald, Maingi, Hughes, Labombard, Terry, Tynan, Churchill):

Introduction Even the gyrokinetic codes embody imperfect model equations and boundary conditions, thus a necessary step towards developing a predictive capability is demonstrating agreement, without bias, between simulations and experimental results. There is a compelling need to make these comparisons more systematic and more quantitative. Validation methodology for magnetic fusion has been reviewed by the leader (Greenwald) of this validation group and others [75, 152, 76]. Further, by identifying key discrepancies, validation can help guide and prioritize model improvement along the most productive avenues.

Experimental Validation Targets Our community-leading experimental validation team, led by M. Greenwald, has access to most of the world tokamak data base and has strong collaborative relations at both working and management levels. Specific validation targets will be chosen and planned according to the research plans listed in Sec. 2.1, and the time-evolving programmatic importance, the availability of experimental data and the availability of the computational resources. Potential targeted areas include: SOL/pedestal profiles, flows and fluctuations; parametric dependence of detachment thresholds; heat and particle loads; identification of conditions for achieving high-performance, ELM suppressed pedestal; and the tokamak density limit. With XGC being in all three pre-exascale programs, in addition to accessibility to the existing leadership class HPCs, an aggressive validation program is possible more than ever.

Description of Tokamak Facility Capabilities and Plans for Validation Since XGC is a total-f code, validation at all physics hierarchical levels is possible and desired: macroscopic level (profiles of plasma density n and temperature T, flow V and electric field $\mathbf{E}$); intermediate level (particle, heat and momentum fluxes); and microscopic level (fluctuations $\widetilde{n}, \widetilde{T}, \widetilde{\phi}, \widetilde{B}$). The more number of all level quantities are validated, the higher simulation accuracy can be expected. These validation quantities will be a function of heat and particle sources. We will employ advanced UQ methods (Sec. 3.1.7) with computer science workflows for in-situ in-memory validation analysis in the large-scale data environment, in collaboration with our UQ and computer science teams. Not only the simulation data, but also the experimental data will be subject to UQ analysis for higher fidelity validation, as we have already demonstrated [37]. The XGC team has built multiple synthetic diagnostics routines [40, 88] and will continue to do so as needed. Simulation data will be available to independent external validation collaborators.

The two existing major US facilities have mature and capable diagnostic sets suitable for testing the kind of predictions targeted above at all hierarchical levels. Additional relevant, high-quality data is also available from the C-Mod archive and through international collaborations. Energy and particle fluxes are typically obtained via transport analysis codes, though local edge particle sources can be obtained from atomic hydrogen line emission. Profile measurements include high resolution (better than 1% of normalized flux) time resolved observations of the pedestal $n_e, n_i, n_Z, T_e, T_i, V_\phi, E_r$. Comparable measurements are available in the SOL, though the presence of significant poloidal and toroidal variation means that these profiles are only sparsely sampled, typically at only a few locations. Measured quantities include $n_e, n_o, T_e, T_i, V_\phi, V_\theta, \phi$ (plasma potential), and radiation opacity. The machines are well equipped with fluctuation diagnostics as well, though fluctuations within the H-mode pedestal tend to be small and hard to observe. Measurements include local and line averaged $\widetilde{n_e}, \widetilde{T_e}, \widetilde{B}$ for both short and long wavelength modes. In the SOL, localized fluctuations for $\widetilde{n_e}, \widetilde{T_e}, \widetilde{\phi}$ are available. SOL data from probes can be limited in high performance discharges because of heat loading, but emerging techniques like gas-puff imaging are extending the range for measurements. For most of these quantities, the frequency and wavenumber spectra can be determined – though wavenumber resolution is often limited. Fluctuation data are often good enough (S/N, resolution, etc.) to perform nonlinear analysis, calculating bispectra, Reynold's stress, mode coupling (for example turbulence and zonal flows) and so forth.

3 Enabling-Technology Capabilities and Proposed Plans

While our enabling technology activities will be focused on HPC capabilities that exist today or are expected to be available in the next 3-5 years, we will adopt a long-term perspective and be "exascale-aware" to ensure readiness of our computational approach when exascale systems become available. We will establish connections and synergies with relevant DOE-supported efforts.

3.1 Applied Mathematics Applied mathematics efforts will be described in the most relevant areas to enhance the capability of (mostly for XGC, and for development of Gkeyll) physics fidelity, computational efficiency and portability utilizing full concurrency on the largest present and future computers: discrete formulations, time stepping, solvers, meshing, verification, and UQ.

3.1.1 Discrete formulations We consider both Lagrangian (PIC) and Eulerian (DG) representations of the gyrokinetic (GK) Vlasov equation, including Fokker-Planck Coulomb collisions, and propose strategies for alleviating current limitations in accuracy, efficiency, and exascale awareness. We use the word "Vlasov" to describe both discrete and continuum GK equations.

Discrete Vlasov formulations: Lagrangian (Chacon, Hauck, Carey, Chang, Ku, Hager):

The Lagrangian PIC representation employed by XGC is very powerful to sample high-dimensional spaces (such as multiscale phase space). It is naturally adaptive, very efficient computationally (particularly in massively parallel computers), and quite robust with only a weak sensitivity to the CFL condition. Nevertheless, its accuracy is typically limited by discrete particle noise, which limits the signal-to-noise ratio and may pollute subtle transport physics. Accuracy can be further compromised by the lack of strict conservation (mass, momentum, and energy), which may result in solution accuracy drift over long timescales.

In this project, we propose to explore conservative particle discretizations (local charge and global energy) as a way to enhance the fidelity of the PIC simulation over long time scale. Such conserving schemes require implicitness, which is also a focus topic in this proposal (Sec. 3.1.2). This work leverages significant experience by this proposal team in the development of such methods in the multidimensional electromagnetic, full PIC context [27, 29, 21].

Additionally, there is recent evidence that particle noise in collisionless PIC can be effectively ameliorated by suitable remapping strategies [192, 191, 138]. We will explore the use of such techniques in this project, and leveraging others currently being explored under independently funded projects at LANL (Chacon) and ORNL (Hauck).

Discrete Vlasov formulations: Eulerian (Hauck, Hittinger, Chacon, Hammett, Hakim):

We consider the Eulerian discontinuous Galerkin (DG) discretization method, implemented in the Gkeyll code [81, 169, 82]. DG methods benefit from a conservative formulation, high-order accuracy, and the ability to leverage general meshes and mesh refinement. They are easy to parallelize and can use limiters similar to those in finite volume [60, 151] to increase stability and enforce maximum principles. The variational framework of DG also enables rigorous mathematical analysis and preservation of structural properties at the continuum level.

DG methods have been applied to a variety of kinetic equations [51, 36], including recent formulations for gyrokinetics instantiated in the Gkeyll code [169, 82, 17]. With an appropriate choice of basis functions, DG can conserve energy and, with proper limiting, preserve positivity while maintaining high-order accuracy [197], even in general coordinates [65]. The main drawback with conventional DG is the large number of unknowns in each local cell, which in dimension d scales like $(k + 1)^d$ for basis functions of order k. However, these additional unknowns enable preservation of structural features and provide super-convergence in some quantities of interest.

To reduce the number of unknowns per cell, we will explore sparse basis representations [89] (related to [3]) within cells, with the minimal amount of enrichment needed to maintain formal order of accuracy and preserve important properties. This has the potential for very large speedup. We will design sparse quadrature routines that are adapted to these spaces. Finally, we will explore non-standard (i.e. non-polynomial) basis sets to capture nonlinear, low-dimensional, physically significant manifolds. We have found a way to implement this while preserving energy. Initial tests with exponential basis functions in 1D indicate an order of magnitude speedup for those cases [168].

Discrete treatment of collisions (Chacon, Adams, Chang, Hager, Ku, D'Azevedo):

XGC features an operator-split Landau-Fokker-Planck treatment of collisions on a v-space grid based on PDF reconstruction, implicit timestepping, and particle remapping to a velocity-space mesh [195, 79]. Collision effect is then remapped back to the particles by using the particle weights. The collisional step itself is conservative and naturally adaptive (velocity domains are normalized to the local thermal velocity), naturally dealing with disparate masses and temperatures. However, challenges remain. We focus here on the velocity-space discretization, reconstruction, and remapping steps, and discuss solver issues later (Sec. 3.1.4).

The PDF reconstruction and particle remapping steps are currently conservative enough for turbulence time scale, but not for the long transport time scale. During this project, we will explore more accurate conservative approaches for PDF reconstruction and particle remapping. The former are currently being explored by Chacon and collaborators under LDRD funding at LANL, using expectation-maximization [137] and Gaussian-mixture [11, 10] algorithms, and will be leveraged for this project if successful. For the latter, we will explore projection strategies [122] that ensure conservation in the sampling of the collisional correction.

The computational complexity of the Landau-Fokker-Planck implementation scales as N_v^2, with N_v the *total* number of velocity-space nodes [79]. As a result, only moderate meshes [$N_v \sim 2,000$] are used presently to keep the cost down, which limits the size of the velocity space domain to about $4v_{th}$ in each direction. This poses a significant challenge for the treatment of energetic particles (such as α particles). (Although this is not an urgent issue for the boundary plasma simulation goals proposed here, which does not include energetic-particles, this capability will enhance various WDM-interface capabilities of XGC; see Sec. 2.5.) To circumvent this, we will explore Eulerian approaches such as adapting recent work [150] that treats thermal α's and fusion α's as separate species, coupling them with pseudo-source terms. Alternatively, we will develop a PIC interface to the high-order accurate AMR discretization of Landau-Fokker-Planck in PETSc [90], which adaptively resolves the entire velocity space domain, using the finite element, PIC, and solver infrastructure in PETSc (Adams) [6]. We will also explore Lagrangian approaches, such as a meshless, noiseless (non-stochastic) Lagrangian collisional algorithm currently being developed at LANL under LDRD sponsorship (Chacon).

3.1.2 Timestepping (Chacon, Adams, Hauck, Hittinger, Ku, Hager, Hammett, Hakim):

Lagrangian Vlasov timestepping schemes One key proposed development in XGC is the implementation of a fully implicit algorithm. This development is motivated by recent success in multidimensional, electromagnetic full-PIC implementations [27, 29], where implicitness has been shown to achieve exact energy conservation and local charge conservation even for curvilinear mapped meshes [21]. In the gyrokinetic-PIC context, fully implicit algorithms are expected to solve the so-called Ampere cancellation problem [we already have preliminary evidence that this is the case in XGC; see Fig. 3(a)], which originates in the semi-implicit nature of the gyrokinetic (GK) advance, and forces the resolution of the electron skin depth everywhere in the domain. Our implementation follows the template of Refs. [29, 21], but specializes to the GK system in several important ways, such as the formulation of GK-specific preconditioners, and the formulation of energy and charge conserving GK particle-push strategies.

Vlasov timestepping in the presence of collisions More accurate time integration of the full gyrokinetic Vlasov-Fokker-Planck system will require advanced time-stepping techniques to address the multiple scales induced by collisions and various terms in the Vlasov equation. Because the natural time scale of each process may vary, any suite of methods must have the capability to (i) treat each individual operator explicitly or implicitly; (ii) leverage scale separation when it exists; and (iii) efficiently integrate multiple time scales without strong scale separation.

For problems with strong timescale separation, implicit-explicit (IMEX) methods [4, 143] provide efficient tools with formal accuracy up to third-order and the ability to capture stiff asymptotic limits without loss of accuracy. However, current methods are unable to preserve structural properties without reducing to first-order, or resolving the stiff time scales in the implicit components. For problems without strong scale separation, multirate methods [72, 45, 167, 160] increase efficiency by evaluating each operator according to its own intrinsic time scale. Methods based on Green's functions take advantage of exact solutions that may be available for some operators. Deferred corrections methods [92, 13, 134, 61, 39, 46] can be used to lift the order of many other methods by successive application to the error equation.

We propose to develop (i) high-order IMEX methods that preserve structural properties without resolving fast scales; (ii) multi-rate integrators for the explicit components; (iii) Green's function methods that explore the inversion of the advection operator treating the collision operator as a source term; and (iv) correction schemes for each of the above methods. Methods will be designed and analyzed to ensure uniform accuracy and proper behavior in relevant asymptotic limits.

3.1.3 Plasma-Material interfacing (Chacon, Shephard, Curreli, Hager, Churchill, Chang):

One of the key multiphysics couplings considered in this proposal is the scrape-off-layer plasma/plasma-material-interaction coupling through Debye sheath. Currently, XGC plans this coupling in a simple (albeit already sophisticated) way by containing the electrostatic hPIC code, that solves Debye sheath potential profile (see Sec. 2.3.1), as a subroutine in a similar way DEGAS2 has been coupled in. The hPIC code is currently electrostatic and explicit, requiring a uniform mesh representation that resolves Debye lengths everywhere several mm starting from the material surface, and an explicit (CFL-limited) time step. We propose to upgrade hPIC to an implicit algorithm that can employ much larger time steps [30, 31] and adaptive meshes that refine as they approach closer to the boundary [22], while exactly conserving local charge and global energy. Also, in the 1D Debye sheath potential problem (but with an arbitrary magnetic field incidence angle), the algorithm can be formulated in terms of the electric field, which obviates the need for a Poisson solve [30]. As a consequence, we expect to accelerate the hPIC Debye sheath simulation by one or two orders of magnitude, while enhancing the physical fidelity of the simulation by enforcing important conservation properties such as local charge and global energy [30].

3.1.4 Solver requirements (Adams, Chacon, Hittinger, D'Azevedo, Ku, Hager, Hammett):

At the present time, the PETSc PIC field solver in XGC takes less than 3% of total computing time, and is not much of an issue. The collision operator solver also does not take a significant fraction of the total time. However, we plan to upgrade both solvers to more accurate and robust ones in preparation for longer time electromagnetic simulations of larger problem size (ITER with electron gyro-scale grid) with multiple impurity species. The proposed developments towards fully implicit, electromagnetic simulations will demand commensurate solver advances. The fully implicit algorithms will demand effective preconditioners, for both collisional and collisionless components.

Lagrangian The collisional treatment in XGC is already implicit, but features a simple Picard iteration, which struggles to converge some times. To address this, we will accelerate the Picard iteration with Anderson Acceleration [188] (also known as Nonlinear GMRES) iterative solvers, already implemented in PETSc. We will also devise better preconditioning strategies that render the nonlinear iteration contractive for arbitrary timesteps. In particular, we will explore using penalization techniques [98] to accelerate the nonlinear iteration. These techniques formulate a very simple velocity-space diffusion operator which has the correct asymptotic limit, and can be used to accelerate the convergence of the expensive integro-differential Landau operator.

The implicit PIC collisionless (Vlasov) component, however, will demand novel solver solutions. Fluid preconditioners will be explored in this context, following Refs. [31, 29, 21]. Linear systems stemming from this treatment are of the Poisson type, but with non-trivially coupled sources that make the system anisotropic and stiff. We will begin by continuing the 3D solver development underway, using the operator split discretizations in XGC and PETSc's *FieldSplit* (block) preconditioner infrastructure [7, 6], with finite elements (FE) in the poloidal plane and finite differencing (FD) in the toroidal direction. The first step is to address the highly anisotropic grids used in XGC. We will exploit the toroidal FD structure of XGC meshes to develop scalable and efficient 3D "split" multigrid Laplacian solvers. If these solvers are not satisfactory we will develop the fully 3D discretizations and fast multigrid solvers in the Solver Integrated Tree-based Adaptive Refinement (SITAR) infrastructure in PETSc. We would add SITAR solvers into XGC by using the existing grids and maintaining the existing solver interface. Future work may include adding high order 3D FE discretizations and state-of-the-art AMR [176, 96, 157, 8] and hybrid GMG/AMG solvers [157, 129]. The next step, given an efficient 3D Laplacian solver, is to develop *FieldSplit* fluid preconditioners. We will continue to extend the existing solvers with new discretizations such as divergence, gradient, and curl operators in the implicit time integrators. We will investigate Schur-complement preconditioners for the coupled vector-potential/electrostatic-potential solve stemming from the implicit PIC preconditioning system. If these solvers, with XGC's split discretizations, are not sufficient we would, again as a risk mitigation strategy, investigate fast fluid solvers with 3D FE, finite volume [1], or discontinuous Galerkin discretizations in SITAR.

Eulerian Eulerian GK codes can benefit from the mesh-based collisional solver developments. The Eulerian Vlasov component can also benefit from IMEX timestepping strategies. This component is convective, and the need to respect convective timescales will allow only moderate timestep improvements vs. explicit CFLs, resulting in only mild nonlinearity. We will explore operator-split preconditioners [71], and we expect the use of Picard, Anderson, or JFNK solvers to be adequate.

3.1.5 Meshing Technologies (Shephard, Yoon, Hager, Ku, Porazik):

Future mesh-related developments will include enhancements to the mesh generation procedures as new XGC requirements arise. One area is to pursue enhancements to the two-scale mesh for higher fidelity in selected regions, boundary layer meshes, locally 3D meshes, etc. The desire to be able to couple XGC simulations with other simulations exists as described elsewhere in this proposal. This requires procedures to relate physical fields between multiple meshes and/or other discretizations. The FASTMath-developed PUMI [95] mesh and field structures tool can support transfer operations in parallel while tools such as the Data Transfer Kit [171] can be integrated with PUMI for general mesh-to-mesh transfer. In other cases, highly effective specific integration schemes will be implemented. For the M3D-C1/XGC coupled simulations (Sec. 2.1.6), we plan to take advantage of the fact that M3D-C1 already uses PUMI tools.

At present, XGC uses toroidal particle decomposition together with a special semi-2D particle decomposition on the poloidal planes. However, the mesh data uses only the toroidal decomposition for ions and no decomposition for the fast moving electrons due to the extreme expense in moving the mesh data when the particles cross the domain boundary. Due to the small number of mesh data, this method optimizes the computational efficiency. However, in the future, when the problem size increases significantly from the inclusion of electron gyro-radius scale mesh in ITER plasma, mesh data may increase to the point that a fully distributed scalable mesh may be needed. Thus, a major development over the next five years will be implementation of a scalable distributed mesh that supports the full set of PIC operations. Efforts during the past year have resulted in a new approach to distribute the mesh that is scalable and effectively tracks particles without excessive communication during a particle push operation. The mesh is distributed using the field-following information already accounted for in the domain definition, supplemented with sufficient layers of elements such that, for a given push, all particles will remain in the resident elements (Fig. 11). To take advantage of this mesh distribution and provide a mesh based PIC version of XGC, procedures for fast mesh-based search, field transfer between particles and mesh, and incremental load balance using neighbor transfer [172], must be developed and optimized. In addition, these procedures must be completely integrated into XGC to support its full range of simulation. Note that optimization of the mesh-based procedures should be able to take advantage of recent PUMI developments for efficient operation on many core [93] and GPU accelerated [94] systems.

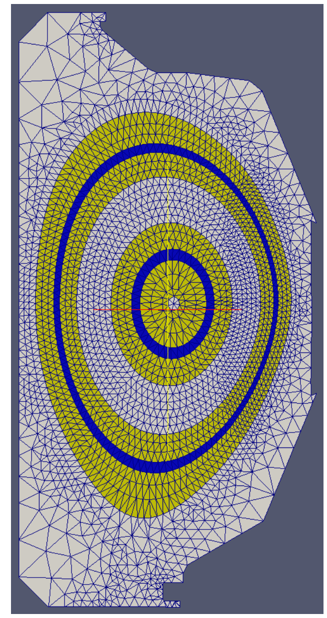


Figure 11: *Distributed mesh with layers of no-owned entities for particle operations.*

The introduction of a distributed mesh will also support the use of mesh adaptation, taking advantage of the SciDAC-developed parallel mesh-adaptation components [95, 94, 127, 123]. Unlike single-scale calculations where mesh adaptation is driven by the mesh discretization errors only, the multiscale nature of the PIC calculations requires consideration of the needs of both the particle and PDE field calculations.

3.1.6 ***Verification*** (Hittinger, Hauck, Ku, Hager, Hakim, Chang):

Verification is the process whereby correct implementation in software is demonstrated. It is the first step in systematic uncertainty quantification and a prerequisite to experimental validation. Verification presents several challenges: the exact output of a simulation code for all possible inputs is never known, error estimation techniques are difficult for multiscale and/or multiphysics codes, and it is difficult to design tests that exercise all paths for fully coupled, nonlinear models.

There are a variety of approaches to demonstrate code correctness. By far, the most common activity is code-to-code comparison, which is a weaker form of verification but allows for comparisons of complex problems. Comparison between very different approaches is particularly useful (in our case, continuum and particle approaches). Comparison between continuum and particle codes has been used successfully in core gyrokinetics to identify and correct issues [141], and the XGC family of codes has been benchmarked against δf [91, 77] (see Sec, 2.2 for an example) and full-f [54, 53, 159] continuum codes. XGC verification examples can be found in Ref. [117].

More quantitative approaches to code verification are based on order-of-convergence estimation. The most direct approach is to use an exact (or asymptotic) solution to estimate error in functionals of the solution and to consider a sequence of discrete problems with increasing resolution. Such an approach is common practice on subsets of code functionality; all three gyrokinetic edge codes have undergone various levels of order verification [44, 57, 115, 77]. Nevertheless, most exact solutions neglect key physical effects and/or couplings, and so the Method of Manufactured Solutions (MMS)

[106] was devised to provide more extensive testing. In this method, an exact solution is assumed, and the form of fictitious sources is determined in order to drive that solution. This approach has been used successfully for fluid codes [156, 59], but application to PIC codes to date has been quite limited [155]. Some early work on XGC verification in cylindrical geometry exists [115, 117].

We propose to pursue a program of benchmarking and order verification to ensure that the software we develop is correct. For several key problems of physical significance for the edge, such as global edge turbulence and plasma particle and heat flux from pedestal top to scrape-off layer, we will compare results from multiple codes and investigate and attempt to resolve discrepancies. For benchmarking of the global boundary plasma solution, we will include another US continuum edge code, COGENT, for a more extensive edge gyrokinetic code comparison; this will also benefit COGENT development, which is funded by the FES and ASCR base programs. All three gyrokinetic edge codes have already undergone various levels of order verification [44, 57, 115, 77]. GEM and GENE will be used for δf turbulence benchmarking in the steep pedestal (see Sec. 2.2). In addition, we will develop single-physics and multi-scale physics solutions on the edge using MMS and will conduct order convergence studies that ensure increased code coverage in the tests.

We further propose to build on recent work on MMS for PIC discretizations [155], enabling not only verification, but also a careful assessment of the impact of noise and noise-reduction strategies in the accuracy of the algorithm. We will first implement and test the method for a simple PIC algorithm in simple geometry, before extending it to the full gyrokinetic PIC algorithms in real geometries in the XGC codes. A close collaboration with our UQ team is expected.

3.1.7 Uncertainty Quantification (Moser, Carey, Michoski, Greenwald, Hager, Hittinger, Hauck, Klasky, Ku, D'Azevedo, Chang):

In this proposal, we will address two major types of uncertainty in the full-f particle (or continuum uncertainty, when Gkeyll is ready) simulation of the edge plasma. First is the uncertainty due to the sampling error associated with the PIC representation of particle distributions, which we propose to quantify and control as an integral part of simulations in XGC. The critical development here is the integration of resampling techniques that preserve the physically relevant characteristics of the particle distribution (which has already been examined by the UQ and XGC teams[66]) with estimates of the uncertainty introduced by the sampling on the predicted dynamics of the plasma. This will allow resampling to be performed adaptively to minimize this uncertainty. A close collaboration with the applied mathematics team is expected.

Second are uncertainties in a modest number of critical experimental inputs to a full-f boundary physics simulation and the real experiment, which are expected to have significant impact on the predictions made with the simulation: examples include parameters describing wall interactions and neutral recycling, heating sources and the imposed magnetic environment. The challenge here is that massively parallel high-fidelity simulations require extensive computational times. It is therefore impractical to perform a large number of simulations with the high fidelity (XGC) model to support uncertainty assessments. To address this issue, a "multi-fidelity" approach is proposed [148, 149] in which orders of magnitude cheaper lower-fidelity simulations are used to characterize uncertainties using available sample-based tools (e.g. Monte-Carlo or stochastic collocation), and potentially only a finite number of high-fidelity simulations are used to inform and/or validate the mapping of these low-fidelity uncertainty characterizations to the high-fidelity results. The low-fidelity simulation that might be used depends on the quantities of interest in the simulations. For example, it could be a low resolution version of the high-fidelity simulation, a reduced size simulation, a simulation in a partial space (such as toroidal wedge), or possibly others.

Several techniques to map and validate the uncertainty characterizations will be explored. The first is based on control variate techniques, in which the distribution representing the uncertainty in the low-fidelity output is augmented with a few samples of the difference between the low-fidelity and high-fidelity models [148]. The variance of this difference will be much smaller than the variance of the overall output if the low-fidelity model provides a reasonable approximation. A few samples of the difference will allow this to be confirmed and will allow the uncertainty derived from the low-fidelity model to be corrected. A second and complimentary approach applies when the lower fidelity model is a formal asymptotic approximation of the high-fidelity model. In this case, the asymptotic structure of the relationship between low- and high-fidelity models can be used to inform a representation of the difference, reducing the required number of samples of the difference, and allowing the cost of sampling the high- and low-fideltiy models to be balanced. This is a generalization of multi-level Monte Carlo algorithms [74]. Finally, a simple characterization of the change in the uncertainty going from low- to high-fidelity simulations can be postulated, parameterized and tested with a few high-fidelity simulations. This will build on past work to develop surrogates and extrapolate uncertainties in plasma simulations [132, 20]. All these mapping approaches will be pursued and others developed over the course of the project. A preliminary study has already been performed between the UQ and XGC team, to be submitted for publication [20].

3.2 Computer Science

The goal of the computer science efforts is to provide the support and infrastructure needed for the project codes to most effectively use the planned DOE systems in extreme scale science simulations and big physics data handling [5]. The subsections will be organized into I/O optimization including code coupling, campaign data management, fault tolerance and resilience, software engineering, and performance engineering and portability.

Next generation DOE systems are projected to provide a far greater increase in computational speed than in I/O bandwidth, as compared to current petascale systems [120, 142, 184]. This creates a time-critical need to optimize I/O to make sure that essential data can be effectively written to and read from the storage systems. Failure to meet this challenge will force our applications to risk losing important information vital to Scientific Discovery.

3.2.1 I/O optimizations for next generation HPCs. (Klasky, Choi): Main ADIOS development was initiated to support XGC. Now ADIOS is used by many DOE application teams for extreme scale I/O. ADIOS must continue to innovate to take full advantage of the new memory and storage technologies, and to provide the highest levels of performance. We will utilize the ADIOS hybrid-staging solutions to enable in-memory coupling between the gyrokinetic XGC code and the MHD M3D-C1 code for their coupled edge localized physics studies. Hybrid staging is another technology developed in a collaboration between the data management and XGC teams [99].

The storage systems on Summit, Aurora, and Cori will feature new technologies that our team must address to ensure I/O performance. New challenges include making effective use of the Burst Buffers, as implemented on each one of these machines, and effectively accounting for new memory and network technologies. This will pose a multitude of application specific R&D questions that need to be addressed to allow XGC to fully utilize the range of storage capabilities. Although the ADIOS team has done extensive research on data staging and using parallel file systems efficiently at scale, major application specific R&D tasks remain to be accomplished, such as managing the deep memory hierarchies and supporting the different burst buffer implementations. An overarching goal will be to utilize staging to offset the I/O bottleneck for analysis and visualization I/O.

A key requirement for XGC in the new Summit and Aurora is to dynamically manage data placement across the layers of the distributed memory/storage hierarchy, coordinating data movement and data sharing among the components of the application workflow so as to maximize their utility to the application and reduce access costs. Here we will explore new strategies and tune them to the needs of XGC. A large portion of this work will be to tune burst-buffer usage with XGC, inside of ADIOS, to ensure that I/O at scale will be kept efficient. This will allow for efficient Checkpoint Restart output as well as efficient output of analysis and visualization data.

XGC analysis and visualization I/O must also work well at scale, so we must ensure that ADIOS staging [183] can be fully utilized on the next LCF resources. Part of this work will be to create a new staging method with one-side MPI calls, which can contain visualization and analysis services. This will allow the coupling of various analysis and visualization codes to the XGC code, support the XGC/M3D-C1 coupled simulations, and support future coupling activities as they arise.

3.2.2 Management of campaign data (Klasky, Choi, Churchill): For the usability of the simulation results in scientific evaluations, V&V, and UQ operations, it is important to provide access to clearly identified results data, the input to the simulation, and even the source code. We aim to create a storage solution using ADIOS in a way that allows for adding the processed output, images, movies, source code and job input to the output data set, making them discoverable and accessible by ADIOS tools. These routines will be customized for the project code to ensure that we can support effective scientific discovery; thus, a metric of our success will be in how we can simplify the way the fusion scientist can work with the full range of data produced by their simulations.

We need two levels of metadata-abstraction above ADIOS' current metadata. The first level organizes a single campaign. ADIOS tools need to be extended (e.g. `bpls` to list the content of a campaign) and new ones created (e.g. to add an image to the campaign with related provenance information). A data movement/archival tool for the campaign also has to be provided so that end-users can move them around reliably. This level of metadata can be supported in the existing ADIOS metadata format through direct extension. The data products can be stored in the ADIOS BP formatted files as data elements (in a similar way as HDF5 can store images) or separately but having metadata to connect them to the rest of the dataset. The second level metadata is necessary to organize campaigns of the project and keep only basic information about each campaign (data variables with min/max information, campaign run information like input parameters) so that one can search this metadata to find simulation runs matching one's interest.

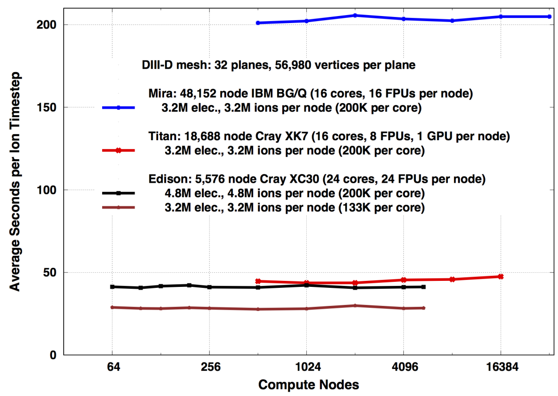
Finally, combining all these solutions for staging and data management, we will create an in-situ visualization workflow for running project codes with automatic plotting of diagnostic data. The visualization application will be executed along with the simulation and, using staging, will process the data on the fly and add the resulting images to the campaign dataset.

3.2.3 Fault tolerance and resilience (Klasky, Choi, Endeveve, Ku, Hager, D'Azevedo): Fault tolerance and resilience for production runs at scale has been a critical component of XGC's prior scientific campaigns. To begin, an efficient checkpoint/restart capability has been a driver for ADIOS development, and has enabled the largest ITER simulations in Titan. Beyond this, we have worked closely with the computing centers to identify XGC-specific hard-ware fault issues and to find solutions. Future work on fault tolerance within the project will primarily target improvements in checkpoint/restart, e.g. by taking advantage of new architectural features such as Burst Buffers and using staging effectively in both the checkpoint writes and the restart reads. We will also monitor the ASCR research portfolio for fault-tolerant capabilities that are relevant to these codes, collaborating as appropriate and including them as part of our new algorithms.

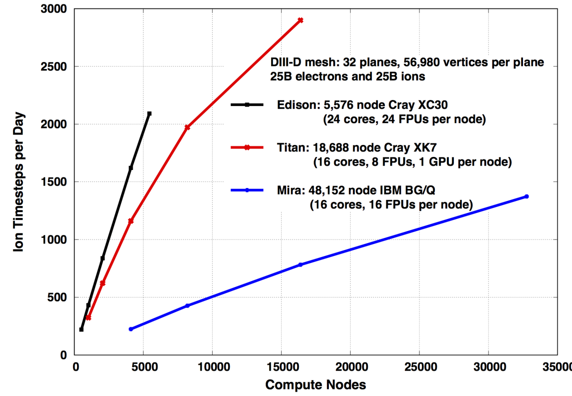
Some resilience issues have been detected in XGC's Fokker-Planck collision module, which manifest as larger-than-normal iteration counts on some mesh-nodes some times. Since we have a very large number of mesh-nodes (50M in ITER), We have dealt with it by aborting the local collision solve when these convergence issues appear, consider it in the error estimate, and let the simulation continue. We will work towards improving the resilience of the collision module via particle re-mapping and other enhancements to the collisional algorithms, and to account for errors using the UQ techniques as described in the enabling technologies section 3.

3.2.4 Software engineering (Kitware) (Hoffman, Galbreath, Churchill): The XGC, Gkeyll and ADIOS source repository is currently hosted on Bitbucket, but will be moved to GitHub to utilize its more advanced capabilities. We will develop a GitHub-based workflow that includes testing of development branches before they are merged into the master branch. In addition, nightly and continuous testing will be performed to ensure the stability and performance of the code base across all supported platforms. We will use the GitHub centralized **issue tracking system** for XGC/Gkeyll and application engagements, and apply an **agile scrum** [164, 163, 43] software development methodology. New features will be developed in 2–3 week sprints, selected from a backlog maintained by the scrum master. We have considerable experience with this approach in projects such as VTK [162].

A major portion of our effort will focus on the implementation of processes for ensuring software quality, improving performance, and building vital user and developer communities. To promote a more reliable and stable code base, we will leverage best-in-class software engineering practices relied upon for industry, developing an automated continuous integration and nightly testing infrastructure which simulates the diverse set of HPC environments representative of the project codes' (XGC and Gkeyll) deployment targets, starting with XGC. Included with the automated testing will be nightly documentation generation, including compelling examples. This will ensure both developers and users have access to up-to-date documentation with the ability to experiment with exercise consisting of working code. We will also update the project codes build system to enable better code modularization and reduce the difficulty of managing inter-code dependencies. Finally,



(a) *weak scaling in particle, strong scaling in mesh*



(b) *strong scaling in both particle and mesh*

Figure 12: *XGC performance scales well on all DOE Office of Science HPCs. Weak scaling in both particle count and mesh size shows similarly good performance. Some degradation in the strong scaling on Titan (b) is due to unrealistically small number of electrons in GPUs at high node count.*

we will improve the process of accepting and integrating community-developed contributions to the project codes by developing an infrastructure to facilitate code review and automated testing.

Similar to the project codes, to ensure the continued quality and robustness of ADIOS and PETSc's rigorous testing in the way it is used in the project codes is imperative. For this, we will integrate more expansive testing into the development workflow. Using a CMake and CTest for build management and CDash for web-based software quality reporting.

3.2.5 Performance Engineering (D'Azevedo, Worley, Adams, Ku, Hager, Abbot, Koskela)

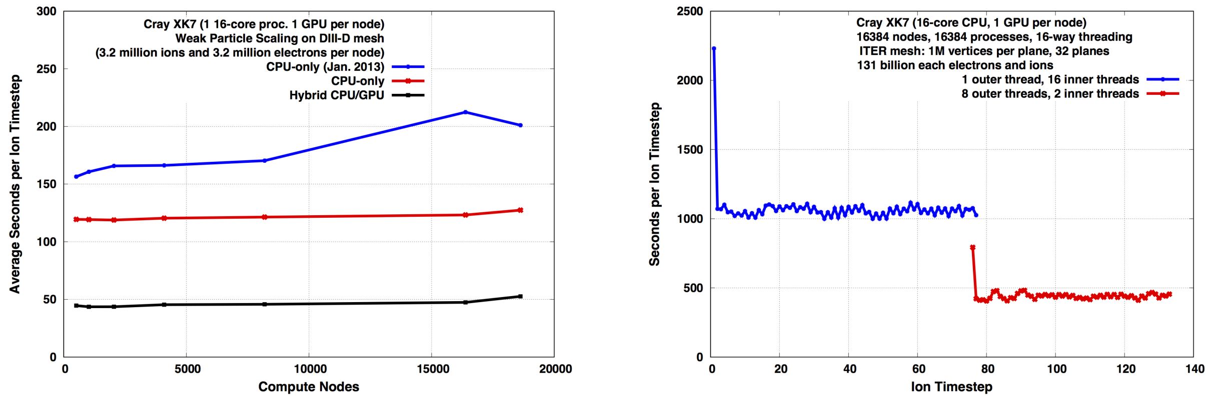
Our performance engineering practice will be "exacale-aware" to ensure readiness of our computational approach when exascale systems become available. We will establish connections and synergies with relevant DOE-supported efforts. Prior efforts have made XGC one of the premier science applications and fusion gyrokinetic codes, combining portable computational and algorithmic technologies to, for example, enable multiscale simulations of turbulence and transport dynamics of an ITER-scale fusion device on the largest US open-science systems at full scale: Titan, a Cray XK7 at the OLCF, and Mira, an IBM BG/Q at the ALCF. XGC achieves excellent scalability on all major leadership computing facilities (see Figure 12).

For systems containing GPU accelerators (e.g, Titan), the performance engineering team first ported the most computationally intensive kernel, the electron push, to the GPU. The initial implementation used CUDA Fortran and was integrated to enable concurrent use of multi-core CPUs and the NVIDIA GPU on XK7 (see Figure 13a). The treatment of nonlinear Fokker-Planck collision is another computationally intensive kernel that has achieved significant speedup, through both algorithm change and performance optimizations, including nested OpenMP [79] to target multi- and many-core processors (see Table 1). Heuristics for balancing the workload related to particle-based push and grid-based collision module while respecting other constraints with memory usage were also developed [194] (see Figure 13b). Topology-aware mapping of MPI tasks to take best advantage of the communication network has shown promise in reducing communication cost by 15% in some cases on Titan [175]. Similar topology-aware task mapping can be adapted for Summit and Aurora.

	Initial	V1	V2
Titan	178.3 s	72.3 s	54.8 s
Mira	214.2 s	121.2 s	103.2 s
Cori Phase I	41.0 s	17.7 s	14.4 s

Table 1: *Performance improvement of collision module. "V1" used an improved symmetry-exploiting algorithm, and "V2" used vectorization.*

XGC has been selected as pre-exascale code by all three DOE pre-exascale programs, at the ALCF, NERSC, and OLCF. XGC in the OLCF Center for Accelerated Application Readiness program (CAAR, with one postdoc support, S. Abbot) is being ported to and optimized on a prototype of the Summit system with multiple GPUs per node. XGC in the NERSC Exascale Science Applications Program (NESAP, with one postdoc support, T. Koskela) has been ported and is being optimized on the Intel Xeon Phi Knights Landing (KNL)-based Cori system, already



(a) *Weak scaling performance of XGC immediately after introduction of drift kinetic electron capability (blue), after optimizations to MPI communication algorithms (red), and after porting of electron push kernel to GPU (black). Recent performance improvements on GPU, not shown here, decrease the CPU-GPU time (black) by at least a factor of 2.*

(b) *Wallclock time per timestep for two checkpoint/restarts for a production XGC job. Number of outer and inner (nested) OpenMP threads changed between the restarts. The first timestep in each used particle-only load balancing. Subsequent steps also took into account load imbalance in the collision calculation (hybrid load balancing).*

Figure 13: *Performance impact of (a) porting electron push to GPU and of (b) introducing collision-cost-aware dynamic load balancing on Cray XK7 (Titan).*

enabling running production jobs at scale. The Aurora Early Science Program at ALCF (with one postdoc to be hired) targets Knights Hill (KNH) processors, the next generation Intel Xeon Phi, on the Aurora system. The focus in CAAR has been on exploring OpenACC compiler directives and GPU-specific optimizations (such as exploiting texture cache), whereas effective use of AVX-512 vectorization and use of high bandwidth MCDRAM has been the target in NESAP, also utilizing OpenMP 4. The insights from these two exercises suggest that the high level OpenACC and OpenMP 4.5 compilers are fragile or still not sufficiently mature to generate efficient code in all cases and a small number of performance sensitive routines that are optimized with architecture-specific features will be critical for high performance in the near term. The performance team will continue to explore the use of high-level compiler directives to maintain performance portability.

New performance challenges will arise, and be attacked, from the enhanced simulation capabilities proposed in this project. The computational cost in the collision module will increase as $O(K^2)$ with K plasma species. New science campaigns that will require an additional 2 impurities species may significantly increase the cost of the Fokker-Planck collision module. The performance team will also collaborate in the development of new physics components such as the fully implicit kinetic-electron electromagnetic solver, 6D sheath, and hybrid particle-fluid electromagnetic method to ensure high performance. New capabilities in coupling of XGC with the M3D-C1 implicit MHD code [69, 15], and in developing new numerical formulations in the discontinuous Galerkin discretization (Sec 2.4), will bring new opportunities for performance optimization. The future pre-exascale hardware will have very high floating point capability but will likely require high levels parallelism in dynamic task execution to mask high latencies in data movement. Ancillary supporting computation such as data analysis and compression may also be performed in the background. However, such dynamic task execution will complicate performance tuning and optimization.

The performance engineering team will continue to be active participants in the code development, algorithm improvement, performance tuning, and code optimization efforts to ensure that the scientific campaigns continue to make effective use of HPC resources at the highest-end. Particular attention will be paid to exploitation of the hardware characteristics of the many levels of deep memory hierarchies (in GPU device memory, MCDRAM, main DDR memory, and NVRAM) in the optimization of data movement, in collaboration with DM team. For example, approaches to be investigated include introducing techniques for overlapping data movement with concurrent computation to hide high latencies in MPI communication or data movement to GPU device memory, or maximizing data reuse while particle data are still residing on fast HBM or GPU device memory. Dynamic concurrent execution will introduce new challenges in balancing computational load and memory use across distributed nodes. We plan to extend and make robust the current heuristics for balancing work in particle push and collision module to more physics components. Performance engineering will be included in the software engineering workflow described in the previous subsection 3.2.4, with regular tests performed to ensure that new code development still maintains high performance and for early detection of anomalous performance caused by changes in compiler, software libraries or system upgrades. Integrated performance testing will require significant computing time to execute a required number of test steps using resources at near production scale. Such optimization/tuning exercises will be executed before major scientific campaigns.

An important element of the performance engineering activity is performance measurement, including the capability to track performance as the code base and scientific goals evolve. As pioneered in previous projects and XGC, we use performance measurement software that is embedded in the codes and always enabled, providing an application view of performance in the form of profile data checkpointed periodically during each computational experiment. Scripts were also developed that, when included in job scripts, archives both the performance and experiment provenance data, allowing performance tracking project-wide. These provide the basic tools of proposed performance engineering in the new project. Both technologies will be updated to improve support for accelerators and many-core processor architectures, including support for CUDA Fortran, OpenACC and nested OpenMP. However, these technologies target performance "triage", identifying performance issues or opportunity for performance optimization. For more detailed analysis and diagnosis, we will use more powerful community tools, such as HPCToolkit, VAMPIR, or TAU, and system or programming-model-specific tools.problems.

4 Project Timeline

The main project code XGC will be responsible for fulfilling the listed science milestones. Gkeyll will join in the listed science milestone activities as its capability develops in the later stage. Cross-verifications of XGC (with Gkeyll, GEM, GENE, COGENT) and the scouting simulations (by GEM and GENE) will be in support of and integral part of the science milestones, hence not listed separately. Major Enabling Technology milestones will be mixed in with the code development milestones. They are closely related. Usual support activities, which comprise much of the Enabling Technology duties and all of the Software Engineering duties, will not be listed here.

Major Reference Milestones for Science/Validation (Some studies may continue throughout the project period.)

Y1: Divertor Heat-Flux Width (on 27 PF Titan and 28PF Cori)
Q1: Complete XGC's electrostatic heat-flux width study by adding two high Bp JET discharges
Q2: Test ITER's electrostatic heat-flux physics by studying a numerically enlarged JET case
Q3: Electromagnetic (EM) turbulence correction to electrostatic heat-flux width in DIII-D/C-Mod/NSTX; transient heat-flux in the same geometries using M3DC1+XGC(neoclassical) coupling
Q4: EM turbulence correction to electrostatic heat-flux width in JET and ITER; transient heat-flux in JET/ITER using the M3DC1+XGC(neoclassical) coupling.

Y2: Pedestal structure and ELM stability (Titan and Cori, then on 200PF Summit in Q3-4)
Q1: T_e, T_i & n_e structures away from ELM instability on JET/ASDEX-U
Q2: Impact of stronger gas puffing and collisionality on relative shift between T_e and n_e.
Study the density limit physics at the same time in Q1 and Q2.
Q3: Study difference in gyrokinetic ELM stability between Q1 and Q2 plasma as pedestals grow; compare with M3D-C1 calculated ELM stability
Q4: Predict gyrokinetic pedestal structure for ITER and study gyrokinetic ELM stability; compare with M3D-C1 calculated ITER ELM stability

Y3: Impurity effect on pedestal structure and ELM stability (on 200PF Summit & Aurora)
Q1-Q4: Repeat Y2 Q1-Q4 studies with Tungsten and Tungsten+low-Z impurity species.
Also, study divertor detachment physics.

Y4: ELM control by RMPs (on 200PF Summit and Aurora)
Q1: Study RMP ELM control using M3DC1+XGC(turbulence) on DIII-D/ASDEX-U plasmas
Q2: Predict RMP ELM control in M3DC1+XGC(turbulence) framework for ITER

Q3: Gyrokinetic RMP ELM control in XGC(turbulence+MHD) on DIII-D/ASDEX-U plasmas
Q4: Predict gyrokinetic RMP ELM control in the XGC(turbulence+MHD) framework for ITER

Y5: Edge transport bifurcation and other timely ITER physics (on 200PF Summit and Aurora)
Q1: Simulate L-H transition on DIII-D/ASDEX-U/JET, study relative strength between turbulence-driven zonal-flow and orbit loss effects
Q2: Study tungsten effect on L-H transition on JET/ASDEX-U
Q3: Study L-H transition power threshold scaling and validate against experimental data
Q4: Predict L-H transition power threshold for ITER
Perform other timely ITER-urgent physics study throughout Y5.

Major reference milestones for code development and enabling technologies

Y1: Get XGC ready for implicit edge electromagnetic (E&M) simulation and improve performance on Cori; get ready for Summit computing in XGC; get ready for M3D-C1+XGC-neoclassical coupled simulation including meshing and data management; adaptive resampling UQ; improve collision solver; improve 3D solver; formulate Method of manufactured solution (MMS) for PIC; install the Debye sheath module hPIC in XGC with mesh adaptations and unified PETSc solver; install exponential basis functions and enhance 5D turbulence simulation capabilities in Gkeyll; Initial utilization of burst buffers at Cori and Summit for AdIOS in-situ data analysis and checkpoint restart I/O; Optimize XGC for deep memory hierarchies such as MCDRAM on Intel Xeon Phi and High Bandwidth Device memory on GPUs.

Y2: Get ready for detached divertor simulation in XGC; improve XGC performance on Summit including multiple impurity species; get XGC ready for Aurora; install particle-remapping technology in XGC; make hPIC routine implicit and optimize for Summit; improve fluid-gyrokinetic E&M pre-conditioner in XGC; study PIC distributed mesh; UQ for multi-fidelity hierarchies; Demonstrate MMS-PIC; improve general geometry capability and install a model X-point geometry in Gkeyll; Integrate in-situ analysis with staging methods in ADIOS framework; develop and optimize new methods in ADIOS for restart I/O; investigate the best use of NVLink direct communication between GPU and host CPU as well as benefits of MPI-one-sided communication, and if beneficial, implement new algorithms.

Y3: Complete the gyrokinetic RMP penetration and ELM control capability in XGC; improve XGC performance on Aurora; install adaptive mesh capability in the implicit hPIC routine; study IMEX/multi-rate methods; dynamics load-balancing of distributed mesh and particles; improve multi-fidelity UQ algorithms; Port MMS-PIC strategy to XGC; improve the realistic tokamak edge geometry capability in Gkeyll with sparse grid and higher resolution turbulence; initial implementation of task-based parallelism (such as using OpenMP task directives) to overlap data movement and communication as well as effective exploitation of CPU and GPU resources.

Y4: Complete higher-order, conservative interpolations in XGC; complete mesh adaptations including boundary layer and anisotropic meshes in XGC; complete realistic tokamak edge geometry capability in Gkeyll; apply multi-fidelity UQ algorithms to XGC and Gkeyll; Complete extension of ADIOS bpls utility to allow plug-ins to enable codes, physics analysis images and movies in ADIOS files. Implement dynamic load balancing heuristic and optimize coupling technology at scale.

Y5: Complete improvement of Fokker-Planck algorithm for efficient energetic particle collisions on Summit and Aurora; Complete dynamics load-balancing account for mesh adaption and particle migration; develop ADIOS tools for searching and exploring in the campaign storage, and visualize in web viewer; complete the edge physics module and make it available to WDM and other communities; determine and implement strategies to get XGC and the edge physics module ready for DOE's next generation exascale computers.

5 Management Plan

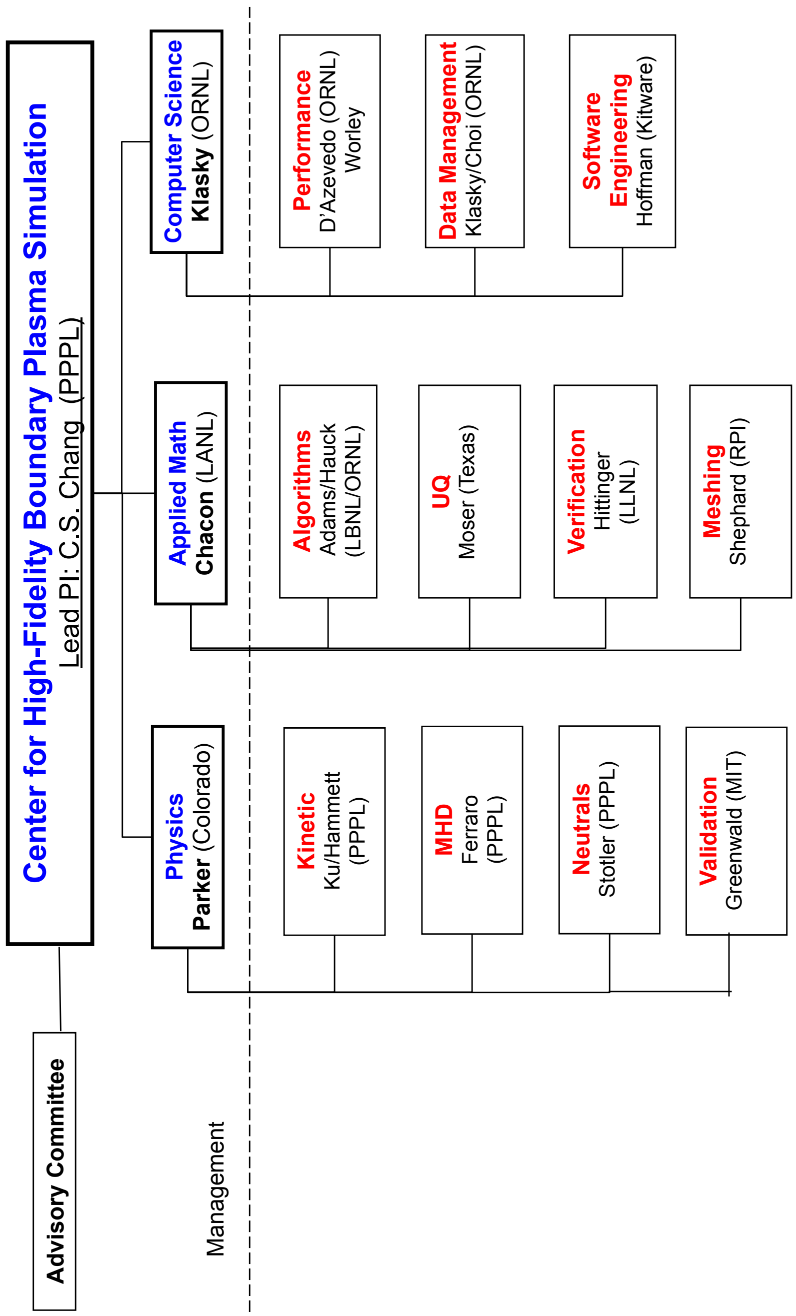
The Project PI, C.S. Chang has extensive experience in managing successful, large collaborative projects among computer scientists, applied mathematicians, and physicists. He will have overall responsibility for ensuring that proper cohesive and integrated activities are arranged and executed, and that the scientific and software development goals are well executed. Chang will make final decisions on project prioritization and personnel using a well-defined process based on input from the management team, which will include the members of the Executive Management Team (C.S. Chang, L. Chacon and S. Parker) and Group Leaders (see Organization Chart in Appendix 1). The executive management team members have significant management experience advancing the science that requires utilization of high performance computing. Key decisions made by the Executive Management Team on plans and priorities will be guided not only by the Group Leaders, but also by input from an external Program Advisory Committee, to evaluate success and failure to reconfigure the project as needed. There can be ad-hoc cross-cutting groups constructed upon needs in the time-varying technical challenges and scientific needs. Each Group Leader will provide a written quarterly report describing the progress and the plan. There will be biannual workshops for face-to-face discussions. Active collaboration with other SciDAC projects will be insured via funded liaison activities.

Responsibilities of Key Project Personnel: Many of the personnel have been members of the XGC team since the start of its HPC development in 2005. Most of the rest have been with the team for five years. Names in parentheses are the institutional PIs and Co-PIs.

PPPL: Project headquarters, led by **C.S. Chang**. PPPL Will execute large-scale production runs on all leadership class HPCs for centralized control of expensive computing resources. About ten proposal members at PPPL will share work with all FES and ASCR participants. PPPL will also develop synthetic diagnostics for validation.
LANL (L. Chacon) : Lead entire applied math related activities; also responsible for multirate, implicit kinetic algorithms, preconditioning, linear nonlinear solvers, Vlasov-Fokker-Planck Eq.
LBNL (M. Adams): In charge of the PETSc solvers and discretizations; will perform PETSc adaptive mesh refinement Landau collision operation; particle-mesh interface methods.
LLNL (J. Hittinger): Lead the mathematical verification activities, in particular, a posteriori error estimation for code and calculation verification of multiphysics codes; will also use the COGENT edge code for cross-verification of the project codes XGC/Gkeyll; investigate adaptive solvers.
ORNL (S. Klasky and E. D'Azevedo): S. Klasky will lead all computer science activities; his team is responsible for I/O, in-situ data analysis and in-memory XGC-M3DC1 data coupling. **E. D'Azevedo** is XGC's liaison with OLCF and CAAR; will lead code optimization on existing HPCs and porting/optimizing codes on Summit and Aurora. **C. Hauck** will contribute to Discontinuous Galerkin development in Gkeyll, multi-fidelity UQ algorithms, and exploration of time stepping approaches for Vlasov-Fokker-Planck equation.
Kitware (B. Hoffman): in charge of software engineering. original author of CMake.
Lodestar (J. Myra): analysis and interpretation of scrape-off layer turbulence from project codes.
UCSD (G. Tynan): experimental validation of edge physics; will help identify proper discharges and assist in data analysis.
U. Colorado Boulder (S. Parker): will lead all physics activities; will also be responsible for GEM-XGC cross-verification tests and exploratory simulations using his GEM code in steep edge pedestal; participate in XGC turbulence data analysis and physics study.
U. Colorado Denver (V. Carey): advanced UQ for large-scale XGC particle simulations.
U. Illinois at UC (D. Curreli): will be the XGC liaison with plasma-material interaction codes; will install his Debye sheath code in XGC as a subroutine and be in charge of this physics.
U. Texas at Austin (R. Moser and D. Hatch): R. Moser will lead the UQ activities and **D. Hatch** will be responsible for exploratory studies and cross-verification of electromagnetic turbulence solutions with XGC (and Gkeyll) in pedestal using the GENE code.
MIT (M. Greenwald): will lead experimental validation group; will also work with the UQ team.
PH Worley Consulting (P. Worley): responsible for (a) parallel algorithm design, implementation, and optimization, (b) performance evaluation of parallel applications and computer systems, and (c) software and performance engineering.
RPI (M. Shephard): in charge of meshing; will also be responsible for XGC's unstructured mesh interaction with particle structures.

There are also XGC personnel supported by Pre-Exascale Programs, whose sole responsibilities are porting & optimizing XGC on Summit (S. Abbot), CORI (T. Koskela), and Aurora (to be hired).

Appendix 0 Organizational Chart



Appendix 1 Biographical Sketches

In alphabetical order by name after lead PI:

1. C. S. Chang
2. M. F. Adams
3. V. Carey
4. L. Chacon
5. Y. Chen
6. J. Y. Choi
7. D. Curreli
8. E. D'Azevedo
9. S. Ethier
10. N. M. Ferraro
11. M. Greenwald
12. G. W. Hammett
13. D. R. Hatch
14. C. D. Hauck
15. J. A. F. Hittinger
16. B. Hoffman
17. S. A. Klasky
18. S. Ku
19. R. Maingi
20. R. D. Moser
21. J. R. Myra
22. S. E. Parker
23. D. A. Russell
24. M. S. Shephard
25. D. P. Stotler
26. G. R. Tynan
27. P. H. Worley

Choong-Seock (C-S) Chang

cschang@pppl.gov

February 2017

Education and Training:

Ph.D.	Physics	May 1979	The University of Texas at Austin, USA
B.S.	Physics	Feb. 1974	Seoul National University, Korea

Postdoctoral training position: none

Research and Professional Experience:

Managing Principal Research Physicist, Princeton Plasma Physics Laboratory; 2011-present,
and Deputy-Head, NSTX Boundary Physics Research; present
Research Professor (with Rolling Tenure), Courant Institute of Math. Sciences, NYU, 1988-2011
Professor of Physics, Korea Advanced Institute of Science and Technology, 1986-2011
Staff Scientist, Applied Microwave Plasma Concept, Carlsbad, CA, 1983-1986
Senior Scientist, General Atomics, La Jolla, CA, 1979 – 1983

Five Selected Synergistic Activities

Chair, DOE FES/ASCR Exascale Requirement Review and Report, Jan.-Dec. 2016.
Head, SciDAC-3 Partnership Center for "Edge Plasma Simulation (EPSI);" ending.
Associate Head for Scientific Computing, ECP High-fidelity Whole Device Modeling; present.
Head, Proto-FSP and SciDAC-2 Centers for Plasma Edge Simulation (CPES), 2005-2011.
Theory Coordinating Committee, US DOE Office of Fusion Energy Science, present.

C.S. Chang has extensive experience in successfully leading multiple large-scale, multi-institutional and multidisciplinary teams composed of fusion energy scientists, applied mathematicians, and computer scientists; which include the Proto-Type Fusion Simulation Center for Plasma Edge Simulation, SciDAC-2 Center for Plasma Edge Simulation (CPES), SciDAC-3 Center for Edge Plasma Simulation (EPSI), the recent DOE FES/ASCR Exascale Requirement Review workshop and report activities, and others. His advanced computational science research teams have delivered multiple distinguished results; e.g., the adaptive ADIOS I/O tool by his data management team that won a 2013 R&D 100 award and the XGC edge gyrokinetic code. XGC is one of the premier science application codes, with multiple large-scale INCITE and ALCC awards, making production runs at full-scale on both of the largest US open-science systems: the Cray XK7 Titan at OLCF, the IBM BG/Q Mira at ALCF with excellent scalability.

C.S. Chang is a Fellow of the American Physical Society. He is serving and has served as an International Honorable Advisory Committee member for Association of Asia Pacific Physical Society Division of Plasma Physics, the Organizer of US-Japan Fusion Exascale Computing Workshops, a Council member of US Burning Plasma Organization, an Executive Committee member of the US Transport Task Force, a User Group Executive Council of Oak Ridge Leadership Computing Facility (OLCF), the Advisory Committee Chair of the fusion SciDAC GPS Center, and other leading roles. He also led two DOE FES National Theory/Simulation Milestone Research projects, recently, and participate as a core member in multiple FES and ASCR Milestone activities. He has given more than 20 invited and plenary talks, keynote speeches, and tutorial lectures at major international conferences over the last 5 years. He has supervised more than 20 Ph.D.'s and similar number of postdoctoral scientists, and has published over 200 scientific papers in major refereed journals.

Ten Relevant Publications

- C.S. Chang, S. Ku, G.R. Tynan, R. Hager, R.M. Churchill, I. Cziegler, M. Greenwald, A. E. Hubbard, J. W. Hughes, "A fast L-H bifurcation dynamics in a tokamak edge plasma gyrokinetic simulation, Invited Talk, 2016 IAEA-FEC, Submmited to Phys. Rev. Lett, arXiv:1701.05480
- C.S. Chang, S. Ku, A. Loarte, V. Parail, F. Köchl, M. Romanelli, R. Maingi, J.-W. Ahn, T. Gray, J. Hughes, B. LaBombard, T. Leonard, M. Makowski, J. Terry, "Gyrokinetic projection of the divertor heat-flux width from present tokamaks to ITER," submitted to Nucl. Fusion, arXiv:1701.05507
- Lingfei Wu, Kesheng Wu, Alex Sim, Michael Churchill, Jong Y. Choi, Andreas Stathopoulos, C.S. Chang, and Scott Klasky, Towards Real-Time Detection and Tracking of Blob-Filaments in Fusion Plasma Big Data," IEEE Transactions on Big Data (2016) 1–1. http://doi.org/10.1109/TBDATA.2016.2599929
- S. Ku, R. Hager, C.S. Chang et al., "A new hybrid Lagrangian numerical scheme for gyrokinetic simulation of tokamak edge plasma," J. Comp. Physics 315, 467-475 (2016)
- E.S. Yoon and C.S. Chang, "A Fokker-Planck-Landau collision equation solver on two-dimensional velocity grid and its application to particle-in-cell simulation," Phys. Plasmas 21, 032503 (2014)
- R. Hager and C.S. Chang, "Gyrokinetic neoclassical study of the bootstrap current in the tokamak edge pedestal with fully nonlinear Coulomb collisions," Physics of Plasmas 23, 042503 (2016)
- B.J. Battaglia, Keith Burrell, Choong-Seock Chang, John deGrassie, B. Grierson, Richard Groebner, Robert Hager, "Improved kinetic neoclassical transport calculation for a low-collisionality QH-mode pedestal," Plasma Physics and Controlled Fusion 58, 085009 (2016)
- C. S. Chang, S. Ku, P. H. Diamond, Z. Lin, S. Parker, T. S. Hahm and N. Samatova, "Compressed ion temperature gradient turbulence in diverted tokamak edge," Phys. Plasmas 16, 056108 (2009)
- C. S. Chang, Seunghoe Ku, and H. Weitzner, "Numerical study of neoclassical plasma pedestal in a tokamak geometry," Phys. Plasmas (APS Invited Talk Issue) 11, 2649 (2004).
- C.S. Chang and F.L. Hinton, "Effect of Impurity Particles on the Finite-Aspect-Ratio Ion Thermal Conductivity in a Tokamak," Letter, Phys. Fluids 29, 3314 (1986); "Effect of Finite Aspect Ratio on the Neoclassical Ion Thermal Conductivity in the Banana Regime," Letter, Phys. Fluids 25, 1493 (1982)

List of Collaborators for the last four years outside of PPPL

J.W. Ahn (ORNL), H. Bui (Rutgers), J. Canik (ORNL), P. Catto (MIT), W. Choe (KAIST, Korea), D. Ernst (MIT), M. Greenwald (MIT), A. Hubbard (MIT), J. Hughes (MIT), F. Jenko (ECP collaborator, UCLA), T. Jin (Rutgers), D. Hatch (U. Texas at Austin), G.T.A. Huijsmans (ITER), S. Janhunen (University of Saskatchewan, Canada), F. Koechl (U. Wien, Austria), A.H. Kritz (Lehigh); B. Labombard (MIT), M. Landreman (U. Maryland); A. Loarte (ITER), M. Makowski (LLNL), A. Pankin (LLNL), V. Parail (JET), M. Parashar (Rutgers), T. Rafiq (Lehigh), M. Romanelli (JET), A. Sim (LBNL), L. Sugiyama (MIT), J. Terry (MIT), T. Watanabe (JIFT meeting co-orgnizer, Nagoya Univ.), K. Wu (LBNL), X. Xu (LLNL), F. Zhang (RPI), I. Ziegler (U. York)

PhD Advisor: R. Hazeltine (U. Texas at Austin)
Postdoctoral Advisees staying in scientific research out side of PPPL: J. Kwon (NFRI, Korea); J. Lang (Intel); S. Janhunen (U. Saskatchewan, Canada);
PhD Advisees staying in fusion research: G. Park, H. Jhang, S. Han, S. Koh (NFRI)

MARK F. ADAMS

609 Gott Street • Ann Arbor, MI 48103 • (609) 206-2040 • mfadams@lbl.gov

EDUCATION

Ph.D. in Civil Engineering — 1998
  University of California, Berkeley
  Co-chairs: Prof. R.L. Taylor and Prof. James Demmel
B.A. in Architecture — 1983
  University of California, Berkeley

PROFESSIONAL EXPERIENCE

Software Engineer — 2013-present
  Scalable Solvers Group
  Computational Research Division
  Lawrence Berkeley National Laboratory
Adjunct Research Scientist — 2013-present
  Department of Applied Physics and Applied Mathematics
  Columbia University
Research Scientist — 2004-2013
  Department of Applied Physics and Applied Mathematics
  Columbia University
Technical Staff — 2002-2004
  Computer Sciences and Mathematics Center
  Sandia National Laboratories
John von Neumann Research Fellow — 2000-2002
  Computer Sciences and Mathematics Center
  Sandia National Laboratories
Postdoctoral Appointment — 1999-2000
  Department of Computer Science
  University of California, Berkeley
  with Prof. James Demmel, Department of Computer Science
Graduate Student Researcher — 1996-1998
  Department of Computer Science
  University of California, Berkeley
Summer Intern — 1998
  Center for Applied Scientific Computing
  Lawrence Livermore National Laboratory

PUBLICATIONS

1. *Electrostatic Gyrokinetic Simulation of Global Tokamak Boundary Plasma and the Generation of Nonlinear Intermittent Turbulence*, submitted to Nuclear

Fusion, S. Ku, R. Churchill, C.S. Chang, R. Hager, E. Yoon, M.F. Adams, E. D'Azevedo and P. Worley.
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4. *Algebraic Multigrid Techniques for Strongly Indefinite Linear Systems from Direct Frequency Response Analysis in Solid Mechanics*, Computational Mechanics, Vol. 39, No. 4, p. 497-507, 2007, M. F. Adams.
5. *Performance of Particle in Cell Methods on Highly Concurrent Computational Architectures*, J. of Phys.: Conference Series, No. 78, 2007, M. F. Adams, S. Ethier and N. Wickmann.
6. *Conservative Discretization of the Landau Collision Integral*, arXiv:1611.07881, 2016, E. Hirvijoki and M. F. Adams.
7. *PETSc Users Manual*, Technical Report ANL-95/11−Revision 3.7, Argonne National Laboratory, 2016, S. Balay, S. Abhyankar, M. F. Adams, J. Brown, P. Brune, K. Buschelman, L. Dalcin, V. Eijkhout, W. D. Gropp, D. Kaushik, M. G. Knepley, L. C. McInnes, K. Rupp, B. F. Smith, S. Zampini, H. Zhang and H. Zhang.
8. *Exascale Computing Without Threads*. Whitepaper for the DOE High Performance Computing Operational Review (HPCOR) on Scientific Software Architecture for Portability and Performance, 2015, M. G. Knepley, J. Brown, L. C. McInnes, B. Smith, K. Rupp and M. F. Adams.
9. *Overview of the PETSc Library*. Whitepaper for the DOE High Performance Computing Operational Review (HPCOR) on Scientific Software Architecture for Portability and Performance, 2015, M. G. Knepley, J. Brown, L. C. McInnes, B. Smith, K. Rupp and M. F. Adams.

Synergistic Activities:
1. "Extending PETSc's Composable Hierarchically Nested Linear Solvers", ASCR Math base program.
2. "Simulation Center for Runaway Electron Avoidance and Mitigation", SciDAC funded FES partnership.
3. "FASTMath", ASCR SciDAC institute.

Collaborators and Co-editors:
1. Dylan Brennan, Princeton University
2. Jed Brown, Colorado University at Boulder
3. Boyce Griffith, University of North Carolina at Chapel Hill
4. Stefan Henneking, Georgia Institute of Technology
5. Robert Hagar, Princeton Plasma Physics Laboratory
6. Eero Hirvijoki, Princeton Plasma Physics Laboratory
7. Tobin Isaac, Rice University

8. Matt Knepley, Rice University
9. Xiaowei Sherry Liu, University of Pennsylvania
10. Dan Martin, Lawrence Berkeley National Laboratory
11. Peter McCorquodale, Lawrence Berkeley National Laboratory
12. Lois Curfman McInnes, Argonne National Laboratory
13. Karl Rupp, Vienna University of Technology
14. Ravi Samtaney, KAUST University
15. Barry Smith, Argonne National Laboratory
16. David Trebotich, Lawrence Berkeley National Laboratory
17. Rich Vuduc, Georgia Institute of Technology
18. Garth Wells, Cambridge University, United Kingdom
19. Hong Zhang, Argonne National Laboratory

Graduate and Postdoctoral Advisors and Advisees:

1. Stefan Henneking, Georgia Institute of Technology

Curriculum Vitae
Varis Carey

Education

1993	B.S., Mathematics, University of Texas at Austin
1997	M.S., Mathematics, University of Texas at Austin
2005	PhD., Applied Mathematics, Cornell University

Research and Professional Experience

2015-current	Assistant Professor, Department of Mathematical and Statistical Sciences, University of Colorado Denver
2012-2015	Research Associate, Institute for Computational Engineering and Sciences, University of Texas at Austin
2009-2012	Research Scientist I, Colorado State University, Department of Mathematics(joint with Atmospheric Sciences)
2009	Oden Fellow, Institute for Computational Engineering and Sciences, University of Texas at Austin
2005-2009	Postdoctoral Fellow, Colorado State University

Synergistic Activities

Contributor and presenter at Uncertainty quantificaiton and verification and validation conferences.

Co-organizer, Rocky Mountain Workshop on Uncertainty Quantification (2015).

Relevant Recent Publications

A Posteriori Analysis and Adaptive Error Control For Multiscale Operator Decomposition Solution of Elliptic Systems I: Triangular Systems, V.Carey, D. Estep, and S. Tavener SINUM, 47 (2009) 740-761.

Blockwise Adaptivity for Time Dependent Problems based on Coarse Scale Adjoints ,V.Carey, D. Estep, A. Johansson, M. Larsson, and S. Tavener), SIAM Scientific Computing(SISC), 32(2010), 2121-2145

A Posteriori Analysis and Adaptive Error Control For Multiscale Operator Decomposition Solution of Coupled Semilinear Systems, V. Carey, D. Estep, and S. Tavener, Int. J. Numer. Meth. Engng., (2013) 94, 826-849

A posteriori error analysis of two stage computation methods with application to efficient resource allocation and the Parareal Algorithm, V. Carey, J. Chowhurdy, D. Estep, J. Sandelin, and S. Tavener), SINUM 54, 5: 2016.

Sensitivity Analysis for Time Dependent Problems: Optimal Checkpoint-Recompute HPC Workflows V.Carey, H. Abbasi, I. Rodero and H. Kola), (Proceedings of Works 2014, Supercomputing 14, November 16,2014).

Collaborators and Co-Editors

Hasan Abbasi, Amazon, Seattle
Paul Bauman, SUNY-Buffalo
Peer-Timo Bremer, Lawrence Livermore National Laboratory
Troy Butler, University of Colorado Denver
C.S. Chang, Princeton Plasma Physics Laboratory(PPPL)
Jehanzeb Chowdhurdy, Dept. of Mathematics, University of New Mexico
Donald Estep, Dept. of Statistics, Colorado State University
Danial Faghigi, ICES, UT-Austin
Robert Hager, PPPL
August Johansson, Simla, Norway
Salomon Janhunen, PPPL
Hemant Kola, Sandia Livermore
Mats Larson, Dept. of Mathematics, Umea University, Sweden
Craig Michoski, ICES, UT-Austin.
Robert Moser, ICES, UT-Austin
Ivan Rodrigo, Dept. of Computer Science, Rutgers Univeristy
Simon Tavener, Dept. of Mathematics, Colorado State University

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Graduate and Professionals Advisors

Donald Estep, Colorado State University
Lars Wahlbin, Cornell University
Mary F. Wheeler, ICES, UT-Austin

Curriculum Vitae of Luis Chacón

Applied Mathematics and Plasma Theory Group, Theoretical Division
Los Alamos National Laboratory, MS K717
Los Alamos, NM 87545
Phone: (505) 667-8453 (Office), (505) 665-5757 (Fax)
e-mail: chacon@lanl.gov

Research background and current research interests

Broad-based interest in computational physics algorithm development and implementation, with an evolving interest in computational co-design. Detailed contributions in the areas of: modern scalable algorithms for fluid and kinetic modeling of plasmas; moving-grid methods, adaptive mesh refinement; and implicit algorithms, Newton-Krylov methods, multilevel techniques. Broad-based interest in computational and theoretical plasma physics at the macroscopic scale, the kinetic scale, and across these scales (multi-scale). Detailed contributions to MFE, magnetic reconnection, and inertial electrostatic confinement.

Education and Training

1997 - 2000	Ph.D. in Nuclear Eng., U. of Illinois at Urbana-Champaign, adviser G. H. Miley
1995 - 1997	M.S. in Nuclear Eng., U. of Illinois at Urbana-Champaign, adviser G. H. Miley
1988 - 1994	M.S.,B.S. in Industrial Eng., Polytechnic U. of Madrid, Spain, adviser A. Crespo

Research and Professional Experience

2012 -	Scientist 5, Los Alamos National Laboratory
2008 - 2012	Research Scientist 4, Oak Ridge National Laboratory
2004 - 2008	Technical Staff Member, Los Alamos National Laboratory
2002 - 2004	Limited-term Staff Member, Los Alamos National Laboratory
2000 - 2002	Director Postdoctoral Fellow, Los Alamos National Laboratory
1994 - 1995	Research Assistant, Institute of Nuclear Fusion, Polytechnic U. of Madrid

Honors and awards

2000	ANS Fusion Energy Division "Best Student Paper Award"
1999 - 2002	Director Postdoctoral Fellow at Los Alamos National Laboratory
1997 - 1999	Fellow of the Spanish Ministry of Education
1995 - 1996	Fellow of the La Caixa Fellowship Program

Synergistic Activities

- Associate editor, Journal of Computational Physics (2013 - current)
- Executive editor, Journal of Computational Physics (2015 - current)
- Ongoing collaboration with the Theory Team of the Reversed Field Pinch experiment (RFX) in Padova, Italy. Ongoing collaboration with Prof. Raul Sanchez at U. Carlos III in Madrid, Spain, on particle-based gyrokinetic methods. Ongoing collaboration with CS Chang at PPPL on particle gyrokinetic methods. Ongoing collaboration with Prof. T. Manteuffel at UC-Boulder on methods for MHD.
- Member of the Exascale Mathematics Working Group (Jan. 2013-Feb. 2014)
- Member of the Executive Committee of the International Conference of Numerical Simulation of Plasmas (ICNSP) since March 2015
- Member of the Executive Committee of the International Sherwood Fusion Theory Conference since 2008 (vice-chair, 2010-11; chair, 2011-12).
- Member of the American Physical Society (APS), the Society for Industrial and Applied Mathematics (SIAM).
- Referee of J. Comput. Phys., SIAM J. Sci. Comput., Comput. Phys. Comm., Computers and Fluids, Phys. Plasmas, Phys. Rev. Lett., Phys. Rev. E, J. Geophys. Res., J. Plasma Physics.

Publications and invited presentations summary

Metrics:	2120 citations, h-index: 26 (source: Google Scholar)
85	Published Refereed Journal Papers
14	Conference Proceedings
2/23	Plenums/Invited Talks
20	Invited talks at minisymposia
26	Colloquia and seminars
100+	Conference presentations

Selected publications:

[1] L. Chacón, G. Chen, D. A. Knoll, C. Newman, H. Park, W. Taitano, J. A. Willert, G. Womeldorff, "Multiscale high-order/low-order (HOLO) algorithms and applications," *J. Comput. Phys.*, **330**, 21-25 (2017). **Invited manuscript for the 50th anniversary of JCP.**

[2] L. Chacón, A. Stanier, "A scalable, fully implicit algorithm for the low-β extended MHD model," *J. Comput. Phys*, **326**, 763âĂŞ772 (2016)

[3] L. Chacón, G. Chen, "A curvilinear, fully implicit, conservative electromagnetic PIC algorithm in multiple dimensions," *J. Comput. Phys.*, **316**, 578âĂŞ597 (2016)

[4] J. N. Shadid, R. P. Pawlowski, E. C. Cyr, R. S. Tuminaro, L. Chacón, P. D. Weber, "Scalable Implicit Incompressible Resistive MHD with Stabilized FE and Fully-coupled Newton-Krylov-AMG," *Comp. Meth. App. Mech. and Eng.*, **304**, 1-25 (2016)

[5] A. Stanier, W. Daughton, L. Chacón, H. Karimabadi, J. Ng, Y.-M. Huang, A. Hakim, A. Bhattacharjee, "Role of ion kinetic physics in the interaction of magnetic flux-ropes," *Phys. Rev. Lett.*, **115**, 175004 (2015)

[6] G. Chen, L. Chacón, "A multi-dimensional, energy- and charge-conserving, nonlinearly implicit, electromagnetic Vlasov-Darwin particle-in-cell algorithm," *Comput. Phys. Comm.*, **197**, 73-87 (2015)

[7] A. Stanier, Andrei N. Simakov, L. Chacón, and W. Daughton, "Fluid vs. kinetic magnetic reconnection with strong guide fields," *Phys. Plasmas*, **22**, 101203 (2015)

[8] A. Stanier, Andrei N. Simakov, L. Chacón, and W. Daughton, "Fast magnetic reconnection with large guide fields," *Phys. Plasmas*, **22**, 010701 (2015)

[9] D. Bonfiglio, M. Veranda, S. Cappello, D. F. Escande, L. Chacón, "Helical self-organization in 3D MHD modelling of fusion plasmas," *Plasma Phys. Controlled Fusion*, **57**, 044001 (2015)

[10] L. Chacón, D. del Castillo-Negrete, and C. D. Hauck, "An asymptotic-preserving semi-Lagrangian algorithm for the time-dependent anisotropic heat transport equation," *J. Comput. Phys.*, **272**, 719 (2014)

Collaborators and Co-authors: M. Adams (LBL) , B. Afeyan (Polymath) , B. Albright (LANL) , D. Bonfiglio (Consorzio RFX) , S. Cappello (Consorzio RFX) , C. S. Chang (PPPL) , A. Christlieb (Michigan State University) , W. Daughton (LANL) , D. del-Castillo-Negrete (ORNL) , G. L. Delzanno (LANL) , E. Endeve (ORNL) , J. Fernandez (LANL) , Z. Guo (LANL) , C. D. Hauck (ORNL) , J. Hittinger (LLNL) , S. Hirshmann (ORNL) , S. Klasky (ORNL) , G. Lapenta (Katholieke Universiteit Leuven) , T. Manteuffel (UC-Boulder) , C. McDevitt (LANL) , K. Molvig (LANL) , H. Park (LANL) , R. Pawlowski (SNL) , R. Petrasso (MIT) , B. Philip (ORNL) , R. Sánchez (U. Carlos III, Madrid) , J. N. Shadid (SNL) , A. N. Simakov (LANL) , X. Tang (LANL) , L. Yin (LANL)

Graduate and Postdoctoral Advisors and Advisees: G. H. Miley (U. of Illinois at Urbana-Champaign) , D. C. Barnes (Coronado Consulting) , J. M. Finn (LANL) , D. A. Knoll (LANL) , C. Leibs (UC-Boulder) , M. Berrill (ORNL) , G. Chen (LANL) , B. Keenan (LANL) , A. Stanier (LANL) , W. Taitano (LANL) , N. Vinyard (LANL) , A. Zocco (Oxford U./Culham)

YANG CHEN

RESEARCH/PROFFESIONAL EXPERIENCE:

- Fellow of the American Physical Society, 2013
- Sr. Research Scientist, Fellow of Center for Integrated Plasma Studies, Dept. of Physics, Univ. of Colorado at Boulder, 2005
- Research Scientist, Dept. of Physics, Univ. of Colorado at Boulder, 1998-2005
- Ph. D., Plasma Physics, Princeton University, November 1998. Nonlinear simulation of elergetic particle driven Toroidicity-induced Alfvén Eigenmodes.

SELECTED PUBLICATIONS:

- **Y. Chen**, J. Chowdhury, N. Maksimovic, S. E. Parker and W. Wan, "Gyrokinetic-ion drift-kinetic-electron simulation of the (m = 2, n = 1) cylindrical tearing mode," Phys. Plasmas 23, 056101 (2016)
- **Y. Chen**, J. Chowdhury, S. E. Parker and W. Wan, "Finite Larmor radius effects on the (m=2, n=1) cylindrical tearing mode," Phys. Plasmas 22, 042111 (2015)
- **Y. Chen**,T. Munsat, S. E. Parker, W. W. Heidbrink, M. A. Van Zeeland, B. J. Tobias, and C. W. Domier, "Gyrokinetic simulations of reverse shear Alfvén eigenmodes in DIII-D plasmas," Phys. Plasmas 20, 012109 (2013)
- W. Wan, S. E. Parker, **Y. Chen**, Z. Yan, R. J. Groebner, and P. B. Snyder, "Global Gyrokinetic Simulation of Tokamak Edge Pedestal Instabilities," Phys. Rev. Lett. 109, 185004 (2012)
- **Y. Chen**, S. E. Parker, J. Lang and G-Y. Fu, "Linear gyrokinetic simulation of high-n toroidal Alfvén eigenmodes in a burning plasma," Phys. Plasmas 17, 102504 (2010)
- W. Wan, S. E. Parker, **Y. Chen**, F. W. Perkins, "Natural fueling of tokamak fusion reactor," Phys. Plasmas **17**, 040701 (2010)
- **Y. Chen** and S. E. Parker, "Electromagnetic gyrokinetic delta-f particle-in-cell simulation with realistic equilibrium profiles and geometry," Journal of Computational Physics 220 (2007) 839-855
- **Y. Chen**, S. E. Parker et. al., "Simulations of turbulence transport with kinetic electrons and electromagnetic effects from the Summit Framework," Nucl. Fusion 43 1-7 (2003)
- **Y. Chen** and S. E. Parker, "A δf particle method for gyrokinetic simulations with kinetic electrons and electromagnetic perturbations," Journal of Computational Physics 189(2), 463-475 (2003)
- **Y. Chen**, R. White, "collisional δf method", Phys. Plasmas 4(10), 1997.

SYNERGISTIC ACTIVITIES:

- Participated in several SciDAC projects. Applied GEM to simulate NSTX, DIII-D and C-Mod plasmas and compared simulation results with imaging data.

Significant collaborators and co-authors in the past 48 months: Guo-Yong Fu (PPPL), C-S Chang (PPPL), Scott Parker(Univ. Colorado), Tobin Munsat (Univ. Colorado), Michael Van Zeeland (GA), William Heidbrink (Univ. California, Irvine), Jugal Chowdhury (PPPL) Benjamin Sturdevant (Univ. Colorado)

PH.D. Advisor: Roscoe White

Jong Youl Choi

Oak Ridge National Laboratory
One Bethel Valley Road
P.O. Box 2008, MS 6057
Oak Ridge, TN 37831-6057

Phone: (865) 241-1436
Fax: (865) 241-4811
E-mail: choij@ornl.gov

Biographical Sketch

Jong Youl Choi is a researcher working in Scientific Data Group, Computer Science and Mathematics Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, Tennessee, USA. He earned his Ph.D. degree in Computer Science at Indiana University Bloomington in 2012 and his MS degree in Computer Science from New York University in 2004.
His areas of research interest span data mining and machine learning algorithms, high-performance data-intensive computing, parallel and distributed systems. More specifically, he is focusing on researching and developing data-centric machine learning algorithms for large scale data management, in-situ/in-transit data processing, and data management for code coupling.

Education

Ph.D. in Computer Science (2012), Indiana University, Bloomington, Indiana, USA. (Advisor: Geoffrey Fox)
M.S. in Computer Science (2004), New York University, New York, New York, USA.

Select Professional Experience

2012 – Present, HPC Data Research Scientist, Scientific Data Group, Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee
2012, Post-doc, Univ. of Tennessee, Knoxville, Tennessee, Working in Scientific Data Group, Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee
2007, Research Internship, Technical Computing, Microsoft Research, Redmond, Washington
2006, Research Internship, Computer Communications and Applications Laboratory, Ećole Polytechniques Fédérales de Lausanne (EPFL), Lausanne, Switzerland

10 Related Publications

1. Lingfei Wu, Kesheng John Wu, Alex Sim, Michael Churchill, Jong Y Choi, Andreas Stathopoulos, Choong-Seock Chang, and Scott Klasky. Towards real-time detection and tracking of spatio-temporal features: Blob-filaments in fusion plasma. IEEE Transactions on Big Data, 2(3):262–275, 2016.
2. Qing Liu, Jeremy Logan, Yuan Tian, Hasan Abbasi, Norbert Podhorszki, Jong Youl Choi, Scott Klasky, Roselyne Tchoua, Jay Lofstead, Ron Oldfield, et al. Hello ADIOS: the challenges and lessons of developing leadership class I/O frameworks. Concurrency and Computation: Practice and Experience, 26(7):1453–1473, 2014.
3. Melissa Romanus, Fan Zhang, Tong Jin, Qian Sun, Hoang Bui, Manish Parashar, Jong Choi, Saloman Janhunen, Robert Hager, Scott Klasky, et al. Persistent data staging services for data intensive in-situ scientific workflows. In Proceedings of the ACM International Workshop on Data-Intensive Distributed Computing, pages 37–44. ACM, 2016.
4. David Pugmire, James Kress, Jong Choi, Scott Klasky, Tahsin Kurc, Randy Michael Churchill, Matthew Wolf, Greg Eisenhower, Hank Childs, Kesheng Wu, et al. Visualization and analysis for near-real-time decision making in distributed workflows. In 2016 IEEE International Parallel and

Distributed Processing Symposium Workshops (IPDPSW), pages 1007–1013. IEEE, 2016.
5. Jong Youl Choi, Tahsin Kurc, Jeremy Logan, Matthew Wolf, Eric Suchyta, James Kress, David Pugmire, Norbert Podhorszki, Eun-Kyu Byun, Mark Ainsworth, et al. Stream processing for near real-time scientific data analysis. In Scientific Data Summit (NYSDS), 2016 New York, pages 1–8. IEEE, 2016.
6. James Kress, Scott Klasky, Norbert Podhorszki, Jong Choi, Hank Childs, and David Pugmire. Loosely coupled in situ visualization: A perspective on why it's here to stay. In Proceedings of the First Workshop on In Situ Infrastructures for Enabling Extreme-Scale Analysis and Visualization, pages 1–6. ACM, 2015.
7. Ye Jin, Mingliang Liu, Xiaosong Ma, Qing Liu, Jeremy Logan, Norbert Podhorszki, Jong Youl Choi, and Scott Klasky. Combining phase identification and statistic modeling for automated parallel benchmark generation. In Proceedings of the 20th ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming, pages 269–270. ACM, 2015.
8. Yanwei Zhang, Qing Liu, Scott Klasky, Matthew Wolf, Karsten Schwan, Greg Eisenhauer, Jong Choi, and Norbert Podhorszki. Active workflow system for near real-time extreme-scale science. In Proceedings of the first workshop on Parallel programming for analytics applications, pages 53–62. ACM, 2014.
9. Roselyne Tchoua, Jong Choi, Scott Klasky, Qing Liu, Jeremy Logan, Kenneth Moreland, Jingqing Mu, Manish Parashar, Norbert Podhorszki, David Pugmire, et al. Adios visualization schema: A first step towards improving interdisciplinary collaboration in high performance computing. In eScience (eScience), 2013 IEEE 9th International Conference on, pages 27–34. IEEE, 2013.
10. Jong Youl Choi, Hasan Abbasi, David Pugmire, Norbert Podhorszki, Scott Klasky, Cristian Capdevila, Manish Parashar, Michael Wolf, Jian Qiu, and Geoffrey Fox. Mining hidden mixture context with ADIOS-P to improve predictive pre-fetcher accuracy. In E-Science (e-Science), 2012 IEEE 8th International Conference on, pages 1–8. IEEE, 2012.

Select Synergistic Activities

1. Researcher in the CODAR ECP project for data reduction
2. Development of staging and python coupling module for XGC and XGC analysis in the ADIOS Project (https://www.olcf.ornl.gov/center-projects/adios)
3. Researcher in the ICEE project for remote workflow development for fusion data

Recent Collaborators

John Wu, Alex Sim (LBNL); CS Chang (PPPL); Tahsin Kurc (Stoony Brook); Manish Parashar (Rutgers); Matthew Wolf, Greg Eisenhauer (Georgia Tech); Krishnendu Chakrabarty (Duke); Soonwook Hwang (KISTI);

Graduate Advisors

Professor Geoffrey Fox, Indiana University

Davide Curreli
Assistant Professor
Department of Nuclear, Plasma and Radiological Engineering
University of Illinois at Urbana-Champaign
104 S. Wright St. Urbana IL 61801
http://npre.illinois.edu/directory/profile/dcurreli

Education

2011, PhD Space Science and Technology, University of Padova, Italy
2007, MS Aerospace Engineering, University of Padova, Italy
2004, BS Aerospace Engineering, University of Padova, Italy

Professional Experience

2015–Present	NCSA Fellow, National Center for Supercomputing Applications, NCSA
2014–Present	Faculty Affiliate, Computer Science and Engineering, UIUC
2013–Present	Assistant Professor, Department of Nuclear, Plasma and Radiological Engineering, UIUC
2012–2013	Postdoctoral Research Associate, Center for Plasma Material Interaction, UIUC
2011–2012	Postdoctoral Research Fellow, University of Padova, Italy
2009–2010	Research Scholar, Francis F. Chen's Low Temperature Plasma Technology Lab, UCLA

Publications

1. S. Keniley, D. Curreli, *Dynamic Coupling of Boltzmann Plasma Model to Surface Erosion Model for Kinetic Treatment of Plasma-Material Interactions*, Fusion Science and Technology 71, 93-102, January 2017. http://dx.doi.org/10.13182/FST16-117
2. R. Khaziev, D. Curreli, *Ion energy-angle distribution functions at the plasma-material interface in oblique magnetic fields*, Phys. Plasmas, 22(4):043503, 04/2015. http://dx.doi.org/10.1063/1.4916910
3. P. Fiflis, D. Curreli, D.N. Ruzic, *Direct time-resolved observation of tungsten nanostructured growth due to helium plasma exposure*, Nuclear Fusion 55(3): 033020, 04/2015. http://dx.doi.org/10.1088/0029-5515/55/3/033020
4. W. Xu, D. Curreli, and D. Ruzic, *Computational Studies of Thermoelectric MHD Driven Liquid Lithium Flow in Metal Trenches*, Fusion Engineering and Design, 89(12):2868, 2014. http://dx.doi.org/10.1016/j.fusengdes.2014.06.008
5. S. Jung, M. Christenson, D. Curreli, C. Bryniarski, D. Andruczyk, D.N. Ruzic, *Development of a high energy pulsed plasma simulator for the study of liquid lithium trenches*, Fusion Engineering and Design, 89(12):2822, 2014. http://dx.doi.org/10.1016/j.fusengdes.2014.02.061
6. M Mozetič, K Ostrikov, D N Ruzic, D Curreli, U Cvelbar, A Vesel, G Primc, M Leisch, K Jousten, O B Malyshev, J H Hendricks, L Kövér, A Tagliaferro, O Conde, A J Silvestre, J Giapintzakis, M Buljan, N Radić, G Dražić, S Bernstorff, H Biederman, O Kylián, J Hanuš, S Miloševič, A Galtayries, P Dietrich, W Unger, M Lehocky, V Sedlarik, K Stana-Kleinschek, A Drmota-Petrič, J J Pireaux, J W Rogers, and M Anderle, *Recent advancement in Plasma Science and Applications* – Review Paper, J. Phys. D: Appl. Phys. 47 153001, 2014. http://dx.doi.org/10.1088/0022-3727/47/15/153001
7. W. Xu, P. Fiflis, M. Szott, K. Kalathiparambil, S. Jung, M. Christenson, I. Haehnlein, A. Kapat, D. Andruczyk, D. Curreli, D.N. Ruzic, *Vertical flow in the Thermoelectric Liquid Metal Plasma Facing Structures (TELS) facility at Illinois*, Journal of Nuclear Materials 463:1181, 12/2014. http://dx.doi.org/10.1016/j.jnucmat.2014.12.045
8. Francis F. Chen and Davide Curreli, *Central peaking of magnetized gas discharges*, Phys. of Plasmas 20, 057102, 2013. http://dx.doi.org/10.1063/1.4801740
9. W. Xu, D. Curreli, D. Andruczyk, T. Mui, R. Switts, D.N. Ruzic, *Heat transfer of TEMHD driven lithium flow in stainless steel trenches*, Journal of Nuclear Materials, 07/2013,438:S422–S425, 2013. http://dx.doi.org/10.1016/j.jnucmat.2013.01.085

10. D. Curreli and Francis F. Chen, *Equilibrium theory of cylindrical discharges with special application to helicons*, Phys. Plasmas 18, 113501, 2011. http://dx.doi.org/10.1063/1.3656941

Synergistic Activities

- Co-PI SciDAC Project on Plasma-Surface Interactions: Bridging from the Surface to the Micron Frontier through Leadership Class Computing
- Faculty Fellow, National Center for Supercomputing Applications, 2015-2016, Development of an HPC platform for plasma-material interactions and nano-structuring; *Blue Waters Exploratory Allocation 2015*, National Center for Supercomputing Applications
- *Organizer*, Mini-Conference on Modeling and Measuring Plasma Material Interactions at the APS-DPP American Physical Society, Division of Plasma Physics, Savannah, Georgia, 2015
- *Organizer,* Mini-Course on Fundamentals of Plasma-Material Interactions and Plasma Edge Physics in Magnetic Fusion, IEEE 20th Pulsed Power Conference (PPC) and the IEEE 26th Symposium on Fusion Engineering (SOFE), Austin, Texas USA, 2015; *Organizer,* Mini-Course on "Plasma-Material Interactions: Fundamentals and Applications", 27th IEEE Symposium On Fusion Engineering, Shanghai, China, 2017
- IAEA Coordinated Research Project (CRP) on Plasma-Wall Interaction with Irradiated Tungsten and Tungsten Alloys in Fusion Devices, 2013-2018

Collaborators and Co-editors (alphabetical order)
E. Ahedo (Universidad Politecnica de Madrid); A. Cardinali (ENEA Frascati); J.P. Allain (University of Illinois - Urbana); D. Andruczyk (University of Illinois - Urbana); J. Carlsson (PPPL); J. Canik (ORNL); E. Cazzola (University of Surrey); V. Chan (General Atomics); C.S. Chang (PPPL); G. Delzanno (LANL); R. Deangelis (ENEA, Frascati); R. Ding (General Atomics); D.A. Gates (PPPL); D. Green (ORNL); K. Hammond (University of Missouri); S. Jung (Applied Materials); S. Kapoor (University of Illinois - Urbana); V. Lancellotti (TU Eindhoven); M. Landreman (University of Maryland); G. Lapenta (KU Leuven, Belgium); A. Lasa (ORNL); S. Markidis (KTH Royal Institute of Technology: Stockholm); M. Mozetic (Institute of Surface Engineering and Optoelectronics); S. Mujumdar (University of Illinois - Urbana); H. Radousky (LLNL); T. Rose (LLNL); S. Srivastava (Applied Research Institute, Illinois); P. Snyder (General Atomics); J.R. Sporre (IBM); X. Tang (LANL); B. Wirth (University of Tennessee).

Graduate and Postdoctoral Advisors (alphabetical order)
Chen, Francis F. (University of California Los Angeles), Enrico Lorenzini (University of Padua, Italy), Daniele Pavarin (University of Padua, Italy), David N. Ruzic (University of Illinois Urbana Champaign)

Graduate and Postdoctoral Advisees (alphabetical order)
S. Keniley (University of Illinois - Urbana), M. Finko (University of Illinois - Urbana), K. Gimbel (University of Illinois - Urbana), R. Khaziev (University of Illinois - Urbana), S. Marcinko (University of Illinois - Urbana).

Eduardo D'Azevedo

Computational and Applied Mathematics Group
Oak Ridge National Laboratory
Oak Ridge, TN 37831-6211

Phone: 865-576-7925
E-mail: dazevedoef@ornl.gov

Eduardo D'Azevedo has developed and optimized algorithms and application software for advanced high performance computing systems for over 25 years. He is currently the task lead for optimizing the XGC fusion application code for GPU as part of the Center for Accelerated Application Readiness (CAAR) program for ORNL Summit system and for Intel Xeon Phi as part of NERSC Exascale Science Applications Program (NESAP). He developed the parallel external memory algorithms for dense matrix computations that take advantage of GPU acceleration. Previously, he has developed mathematical libraries and solvers such as the out-of-core and compact storage in ScaLAPACK library in support of the DOE fusion and materials program. His activities include parallel algorithm design and implementation, application performance optimization, algorithms development, and application performance modeling and prediction.

Education

Ph.D. Computer Science, Faculty of Mathematics, University of Waterloo, 1989.
M. Math, Computer Science, Faculty of Mathematics, University of Waterloo, 1985.
B. Math, Computer Science, Combinatorics & Optimization, University of Waterloo, 1984.

Employment

Research Mathematician, ORNL, Oak Ridge, TN, 6/1991–present
Postdoctoral Fellow, ORNL, Oak Ridge, TN, 4/1990–6/1991
Postdoctoral Fellow, University of Waterloo, 1989–3/1990

Awards and Synergistic Activities

ORNL Significant Event Award, Simulation of Superconductivity , 2009
Gordon Bell Award, SC08
ORNL Significant Event Award, Numerical Formulation of the Hirsch-Fey Quantum Monte Algorithm, 2006
ORNL Awards Night, Recognition of Scientific Research by a Team, 2003

Selected Publications

B. Messer, E. D'Azevedo, J. Hill, W. Joubert, M. Berrill, C. Zimmer, "MiniApps Derived from Production HPC Applications Using Multiple Programming Models", *The International Journal of High Performance Computing Applications*, accepted.

R. Hager, E. S. Yoon, E. D'Azevedo, et al, "A fuly non-linear multi-species Fokker-Planck-Landau collision operator for simulation of fusion plasma", Journal of Computational Physics, 315, p644-660, 2016.

E. D'Azevedo, K. Chan, S. Su, K. Wong, "Scalable Out-of-Core Solvers on a Cluster" in *High Performance Parallelism Pearls*, J. Reinders, J. Jeffers editors pp. 443-455, 2015, Morgan Kaufmann publishers

K. Wong, E. D'Azevedo, H. Hu, S. Su, "Solving a large scale radiosity problem on GPU-based parallel computers", Journal of Computational and Applied Mathematics, 270:109120, 2014

E. D'Azevedo, J. Hill, "Parallel LU Factorization on GPU Cluster", Procedia Computer Science, Volume 9, 2012, Pages 67-75, 2012

E. D'Azevedo, S. Fata, "On the effective implementation of a boundary element code on graphics processing units using an out-of-core LU algorithm", Engineering Analysis with Boundary Elements 36(8):12461255, 2012

R. F. Barrett, T. Chan, E. D'Azevedo, R. Wong, "Complex version of high performance computing LINPACK benchmark (HPL)", Concurrency and Computation Practice and Experience 22(5):573-587, 2010

G. Alvarez, M. S. Summers, D. E. Maxwell, M. Eisenbach, J. S. Meredith, J. M. Larkin, J. Levesque, T. A. Maier, P. R. C. Kent, E. F. D'Azevedo, T. C. Schulthess, "New algorithm to enable 400+ TFlop/s sustained performance in simulations of disorder effects in high-T_c superconductors", Proceedings of the 2008 ACM/IEEE conference on Supercomputing, **Gordon Bell Award**

E. D'Azevedo, M. R. Fahey, R. T. Mills, "Vectorized Sparse Matrix Multiply for Compressed Row Storage Format", Lecture Notes in Computer Science Volume 3514, 2005, pp 99-106

E. F. Jaeger, L. A. Berry, et al., "All-orders spectral calculation of radio-frequency heating in two-dimensional toroidal plasmas", Phys. Plasma 8, 1573(2001)

Recent Collaborators and Other Affiliations

S. Abbott (ORNL), M. Berrill (ORNL), J. Candy (GA), C. Chang (PPPL),M. Gorentla Venkata (ORNL), R. Hager (PPPL), J. Hill (ORNL), C. Hsu (ORNL),Y. Idomura (JAEA), N. Imam (ORNL), W. Joubert (ORNL), P. Kent (ORNL), S. Ku (PPPL),Y. Li (ORNL), T. McDaniel (UT), M. B. Messer (ORNL),T. Mintz (ORNL), B. Philip (ORNL), S. Pophale (ORNL), S. Powers (ORNL), S. Sreepathi (ORNL), P. Wang (Nvidia), K. Wong (UT), P. Worley (ORNL), E. Yoon (RPI), C. Zimmer (ORNL)

Graduate and Postdoctoral Advisors and Advisees

Postdoctoral Advisor: M. Heath (University of Illinois at Urbana-Champaign)

Thesis Advisor: R. B. Simpson (University of Waterloo, Ontario, Canada)

Postdoctoral Advisee: none

Graduate Student Advisees: none

Stéphane Ethier

Deputy head, Computational Plasma Physics Group
Princeton Plasma Physics Laboratory
P.O. Box 451, Princeton, NJ 08543
ethier@pppl.gov

Education:

1989, B.Sc. honors in Physics at University of Montreal, Montreal, Canada.
1991, M.Sc. in Solid State Physics at University of Montreal, Montreal, Canada.
1996, Ph.D. in Plasma Physics at "Institut National de Recherche Scientifique INRS-Energie et Materiaux", Montreal, Canada. Supervisor : Prof J.-P. Matte

Professional experience:

Deputy head of the Computational Plasma Physics Group, HPC Team Lead (10/12 – present)
Senior Computational Scientist (10/07 – 10/12)
Lead Computational Scientist (10/04 – 10/07)
Computational Scientist rank IV and V (10/98 – 10/04)
Princeton Plasma Physics Laboratory, Princeton, NJ 08543
Work focus: *High Performance Computing*

Postdoctoral Fellow (1996 – 1998), Princeton University
Applied Physics Group, Mechanical Aerospace Engineering Department
Princeton, NJ 08544
Supervisor: Prof. Szymon Suckewer
Project: *Develop collisional-radiative code for Molybdenum-based X-ray laser.*

Book Contributions:

- "Performance Tuning of Scientific Applications", Chapman &Hall/CRC Computational Sciences Series, David Bailey, Robert Lucas, Samuel Williams Editors, Chap. 6: Large-Scale Numerical Simulations on High-End Computational Platforms, ISBN 9781439815694, 2010.
- "Petascale Computing: Algorithms and Applications", Chapman &Hall/CRC Computational Sciences Series, David A. Bader Editor, Chapter 1: Performance Characteristics of Potential Petascale Scientific Applications, 2007.

Selected Refereed Publications:

- W. Tang, B. Wang, **S. Ethier**, G. Kwasniewski, T. Hoefler, K. Ibrahim, K. Madduri, S. Williams, L. Oliker, C. Rosales-Fernandez, T. Williams, "*Extreme Scale Plasma Turbulence Simulations on Top Supercomputers Worldwide*", SC16, Proceedings of 2016 International Conference for High Performance Computing, Networking, Storage and Analysis (2016).
- **Stephane Ethier**, Choong-Seock Chang, Seung-Hoe Ku, Wei-li Lee, Weixing Wang, Zhihong Lin, and William Tang, *"NERSC's Impact on Advances of Global Gyrokinetic PIC Codes for Fusion Energy Research"*, Computing in Science & Engineering, vol. 17, no. 3, p. 10-21 (2015).
- B. Wang, **S. Ethier**, W. Tang, T. Williams, K. Ibrahim, K. Madduri, S. Williams, L. Oliker, "*Kinetic Turbulence Simulations at Extreme Scale on Leadership-Class Systems*", SC13, Proceedings of 2013 International Conference for High Performance Computing, Networking, Storage and Analysis (2013).
- Kamesh Madduri, Jimmy Su, Samuel Williams, Leonid Oliker, **Stephane Ethier**, and Katherine Yelick, "Optimization of Parallel Particle-to-Grid Interpolation on Leading Multicore Platforms", IEEE TRANSACTIONS ON PARALLEL AND DISTRIBUTED SYSTEMS, **23**, 1915 (2012).
- K. Madduri, E. Im, K. Ibrahim, S. Williams, **S. Ethier**, L. Oliker, "*Gyrokinetic Particle-in-Cell Optimization on Emerging Multi- and Manycore Platforms* ", SC11, Proceedings of 2011

International Conference for High Performance Computing, Networking, Storage and Analysis (2011).

- Robert Preissl, Nathan Wichmann, Bill Long, John Shalf, **Stephane Ethier**, Alice Koniges, "*Multithreaded Global Address Space Communication Techniques for Gyrokinetic Fusion Applications on Ultra-Scale Platforms*", SC11, Proceedings of 2011 International Conference for High Performance Computing, Networking, Storage and Analysis, 2011.
- Kamesh Madduri, Eun-Jin Im, Khaled Z. Ibrahim, Samuel Williams, **Stephane Ethier**, Leonid Oliker, "*Gyrokinetic particle-in-cell optimization on emerging multi- and manycore platforms*", Parallel Computing, volume 37, pp. 501-520 (2011).
- **S. Ethier**, M. Adams, J. Carter, L. Oliker,*"Petascale Parallelization of the Gyrokinetic Toroidal Code",* VECPAR: High Performance Computing for Computational Science, June 2010.
- K. Madduri, S. Williams, **S. Ethier**, L. Oliker, J. Shalf, E. Strohmaier, K. Yelick, *"Memory-Efficient Optimization of Gyrokinetic Particle-to-Grid Interpolation for Multicore Processors"*, In Proceedings SC09, Seattle, WA (2009).
- **S. Ethier**, W.M. Tang, R. Walkup, L. Oliker, "*Large-scale gyrokinetic particle simulation of microturbulence in magnetically confined plasmas*", IBM Journal of Research and Development **52**, 105 (2008).
- L. Oliker, A. Canning, J. Carter, C. Iancu, M. Lijewski, S. Kamil, J. Shalf, H. Shan, E. Strohmaier, **S. Ethier**, T. Goodale, " *Scientific Application Performance on Candidate Petascale Platforms*", In Proceedings IPDPS 2007, Long Beach, CA (2007) (**Best Paper Award**).

Synergistic Activities: Chair of the NERSC Users Group Executive Committee (2009-2015); member of the NERSC Policy Board (2010); member of the editorial board of Computational Science & Discovery; member of the OLCF User Council; member of Sigma-Xi, ACM, and APS.

Collaborators and co-authors: {L. Oliker, S. Williams, K. Ibrahim, K. Yelick, J. Shalf, A. Koniges, M. Adams, H. Shan, Z. Zhao (LBNL)}, K. Madduri (Penn State), B. Wang (Princeton U.), {S-H Ku, C.S. Chang, R. Hager, W.X. Wang, W.M. Tang, D. Stotler, E. Startsev, W.W. Lee, J. Chen, E. Feibush (PPPL)}, {S. Klasky, P. Worley, Ed D'Azevado, M. Wolf, J. Turner, J. Choi (ORNL)}, {T. Williams, R. Latham, R. Ross, J. Jenkins, S. Habib, A. Heitmann, H. Finkel (ANL)}, {T. Germann, L. Chacon, G. Chen, W. Daughton, G. Shipman (LANL)}, {J. Hittinger, J. Belak, M. Dorr, S. Futral (LLNL)}, {F. Jenko, G. Merlo (UCLA)}, Z. Lin (UC-Irvine), {T. Neuroth, K-L Ma, F. Sauer, Y. Zhang (UC-Davis)}, R. Ganesh (IPR India), G. Heisenhauer (GA Tech), {A. Malony, K. Huck, C. Wood (U. Oregon)}, M. Parashar (Rutgers U), {T. Hoefler, G. Kwasniewski (ETH Zurich)}, {C. Trott, S. Plimpton (SNL)}, C. Rosales-Fernandez (TACC).

Brief Biosketch: Dr. Stephane Ethier is a principal computational physicist with expertise and interest in high performance computing on large-scale systems, particle-in-cell methods for magnetic fusion research, GPU programming, data management, and other related fields. He is the deputy head of the Computational Plasma Physics Group at the Princeton Plasma Physics Laboratory where he leads the high performance computing team. He has worked on many HPC- related projects in collaboration with computer scientists, data management experts, applied mathematicians, and HPC specialists in DOE and at universities.

Nathaniel M. Ferraro

Education and Training

PhD, Princeton University, Astrophysical Sciences, Program in Plasma Physics (2008)
MS, Dartmouth College, Physics (2003)
BA, Dartmouth College, Physics and Mathematics (2002)

Research and Professional Experience

Research Scientist, Princeton Plasma Physics Laboratory (2015—present)
Scientist, General Atomics (2011—2015)
Postdoctoral Fellow, Oak Ridge Institute for Science and Education (2008-2011)

Selected Publications

N.M. Ferraro, S.C. Jardin, L.L. Lao, M.S. Shephard, F. Zhang, "Multi-Region Approach to Free-Boundary 3D Tokamak Equilibria and Resistive Wall Instabilities." *Phys. Plasmas* **23**, 056114 (2016)

N.M. Ferraro, T.E. Evans, L.L. Lao, R.A. Moyer, R. Nazikian, D.M. Orlov, M.W. Shafer, E.A. Unterberg, M.R. Wade, A. Wingen, "Role of plasma response in displacement of the tokamak edge due to applied non-axisymmetric fields." *Nucl. Fusion* **53**, 073042 (2013)

N.M. Ferraro, "Calculations of two-fluid linear response to non-axisymmetric fields in tokamaks." *Phys. Plasmas* **19**, 056105 (2012)

N.M. Ferraro, "Symmetries of resistive and two-fluid magnetohydrodynamics under reversals of toroidal field, current, and rotation." *Phys. Plasmas* **19**, 014505 (2012)

N.M. Ferraro, S.C. Jardin, P.B. Snyder. "Ideal and resistive edge stability calculations with M3D-C1." *Phys. Plasmas* **17**, 102508 (2010)

N.M. Ferraro, S.C. Jardin. "Calculations of two-fluid magnetohydrodynamic axisymmetric steady-states," *J. Comp. Sci.* **228**(20), 7742 (2009)

N.M. Ferraro. "Finite Larmor radius effects on the magnetorotational instability," *Astrophys. J.* **662**, 512 (2007)

N.M. Ferraro, S.C. Jardin. "Finite element implementation of Braginskii's gyroviscous stress with application to the gravitational instability," *Phys. Plasmas* **13**(9), 092101 (2006)

N.M. Ferraro, B.N. Rogers, "Turbulence in low-β reconnection," *Phys. Plasmas* **11**(9), 4382 (2004)

Synergistic Activities

Center for Tokamak Transients Simulations SciDAC (proposed)
NSTX-U Macroscopic Stability Topical Science Group

Collaborators and Co-Authors

J Callen (Wisconsin), G Canal (GA), X Chen (GA), SJ Diem (ORNL), TE Evans (GA), IT Chapman (CCFE), GTA Huijsmans (ITER), J King (DOE), LL Lao (GA), B Lyons (ORAU), J Lore (ORNL), O Meneghini (GA), S Mordijck (William & Mary), DM Orlov (UCSD), P Piovesan (RFX), C Paz-Soldan (GA), MW Shafer (ORNL), M Shephard (RPI), A Turnbull (GA), MA Van Zeeland (GA), RE Waltz (GA), MR Wade (GA), R Wilcox (ORNL), A Wingen (ORNL)

Graduate and Postdoctoral Advisors

Rogers BN (Dartmouth), Jardin SC (PPPL), Snyder PB (GA)

Appendix I Biographical Sketch: Martin Greenwald

Education and Training

Undergraduate	Massachusetts Institute of Technology; Cambridge, MA	Physics BS 1973
Undergraduate	Massachusetts Institute of Technology; Cambridge, MA	Chemistry BS 1973
Graduate	University of California Berkeley, Berkeley CA	Ph.D. Physics 1978

Research and Professional Experience:

Oct. 1978 – Present Deputy Director (since 2015) and Senior Research Scientist (since 2000) - MIT Plasma Science & Fusion Center

Selected Publications Relevant to Work Under this Proposal:

- N.T. Howard, C. Holland, A.E. White, M. Greenwald, J. Candy, A.J. Creely, " *Multi-scale gyrokinetic simulations: Comparison with experiment and implications for predicting turbulence and transport*", Phys. Plasmas 23, 056109, 2016.
- M. Greenwald, "*Alcator C-Mod and the High-Field Approach to Fusion*" in Magnetic Fusion Energy – Chapter 10 From Experiments to Power Plants, George Neilson Editor, published by Woodhead Publishing, 2016.
- Sung, C., White, A. E., Mikkelsen, D. R., Greenwald, M., Holland, C., Howard, N. T., Churchill, R., Theiler, C., Alcator C-Mod Team, *"Quantitative comparison of electron temperature fluctuations to nonlinear gyrokinetic simulations in C-Mod Ohmic L-mode discharges"*, Phys. Plasmas 23, 042303, 2016.
- M. Chilenski, M. Greenwald, Y. Marzouk, N. Howard, A. White, J. Rice, J Walk, *"Improved profile fitting and quantification of uncertainty in experimental measurements of impurity transport coefficients using Gaussian process regression"*, Nuclear Fusion 55, 023012, 2015.
- M. Greenwald et al., *"20 Years of Research on the Alcator C-Mod Tokamak",* APS-DPP Review published in Phys. Plasmas 21, 110501, 2014.
- N.T. Howard, C. Holland, A.E. White, M. Greenwald, J. Candy, *"Synergistic cross-scale coupling of turbulence in a tokamak plasma"*, Phys. Plasmas 21, 112510, 2014.
- M. Greenwald, T. Fredian, D. Schissel, J. Stillerman, *"A metadata catalog for organization and systemization of fusion simulation data"*, Fusion Engineering and Design **87**, 2205-2208, 2012
- M. Greenwald, "*Verification and validation for magnetic fusion",* APS-DPP Tutorial, published in Phys. Plasmas 17, 058101, 2010

- P.W. Terry, M. Greenwald, J-N. Leboeuf, G. McKee, D. Mikkelsen, W. Nevins, D. Newman, D. Stotler, *"Validation in fusion research"*, Phys. Plasmas 15, 062503, 2008
- M. Greenwald, *"Beyond Benchmarking – How Experiments and Simulations Can Work Together in Plasma Physics"* Computer Physics Communications, 164, 1-8, 2004.

Synergistic Activities

- Co-chair for DOE workshop "Fusion Energy Sciences Exascale Requirements Review" January, 2016
- Co-chair for DOE workshop "Data Management, Visualization and Analysis of Experimental and Observational Data" Sept, 2015
- Member BPO working group on validation
- Coordination of experimental transport program on Alcator C-Mod tokamak
- Associate Editor – Physics of Plasmas (2006 -)

Identification of potential conflicts of interest or bias in selections of reviewers:

Outside Collaborators & Coauthors: Abla G (GA), Bader A (U. Wisc.), Barnard H (LBNL), Barnes M, (Oxford), Bergerson W (UCLA), Bespamyatnov I (U.T. Austin), Bitter M (PPPL), Brower D (UCLA), Candy J (GA), Canik J (ORNL), Churchill RM (PPPL), Coviello EN (GA), Cziegler I (U. York), Delgado-Aparicio L (PPPL), Diallo A (PPPL), Diamond PH (UCSD), Dominguez A (PPPL), Duval BP (EPFL), Switzerland, Ellis R), (PPPL, Fisch NJ (PPPL), Flanagan SM (GA), Garcia OE (U. Tromso, Norway), Gates D (PPPL), Goetz J (U. Wisc.), Groebner RJ (GA), Grulke O (IPP Greifswald, Germany), Hill KW (PPPL), Holland C (UCSD), Izzo V (UCSD), Kessel C (PPPL), Kotschenreuther M (U.T. Austin), Krasheninnikov SI (UCSD), Kritz AH (Lehigh), Kube R (U. Tromso, Norway), Liao K (U.T. Austin), Lipschultz B (U. York, UK), Loarte A (ITER), Ma Y(ITER), Mahajan S (U.T. Austin), Manduchi G (ENEA, Assoc. Consorzio RFX), Mauel ME (Columbia U.), McDermott RM (IPP Garching, Germany), Meneghini O (GA), Mikkelson D (PPPL), Myra JR (Lodestar), Nelson-Melby E (Raytheon), Ochoukov R (IPP Garching, Germany), Osborne T (GA), Pace D (GA), Pankin AY (Tech X Co.), Parra F(Oxford), Petty CC (GA), Phillips PE (U.T. Austin), Pitcher S (ITER), Podpaly YA (LLNL), Poli F (PPPL), Rafiq T (Lehigh U.), Reinke ML (ORNL), Rognlien T (LLNL), Romosan A (LBNL), Rowan WL (U. T. Austin), Ryutov D (LLNL), Schissel DP (GA), Schmidt A (LLNL), Scott SD (PPPL), Shoshani A (LBNL), Smick N (GT Advanced Technology), Snipes JA (ITER), Snyder PB (GA), Soukhanovskii V (LLNL), Staebler GM (GA), Stepanov D (ITER), Stotler DP (PPPL), Takase Y (U. Tokyo), Tang V (LLNL), Theiler C (EPFL, Switzerland), Tronchin-James A (LLNL), Tsujii N (U. Tokyo), Umansky M (LLNL), Walker ML (GA), Waltz RE (GA), Wilson JR (PPPL), Wurden G (LANL), Xu XQ (LLNL), Zarnstorff M (PPPL), Zweben S(PPPL)

Recent Graduate and Postdoctoral Advisees

Howard Yuh (Nova Photonics)
Nathan Howard (MIT)
Mark Chilenski (MIT)

Fabio Riva (EPFL, Switzerland)

Graduate Advisor
Wulf Kunkel (deceased)

Gregory W. Hammett
Princeton Plasma Physics Laboratory +1-609-243-2495
100 Stellarator Road, Princeton, NJ 08540 hammett@pppl.gov
http://w3.pppl.gov/~hammett

Education and Training

Ph.D.	Princeton University, Astrophysical Sciences, Program in Plasma Physics Physics, 1986
M.S.	Princeton University, Astrophysical Sciences, Program in Plasma Physics Physics, 1982
B.A.	Harvard University, Physics, 1980

Research and Professional Experience

1997-	Principal Research Physicist, Theory Division, PPPL
1995-	Lecturer, Program in Plasma Physics, Princeton University (Lecturer with Rank of Professor since 2001)
2008-	Associated Faculty, Applied and Computational Mathematics, Princeton University
2013	Trinity Term, Visiting Research Fellow, Merton College, Oxford
2013, Spring,	Director of Graduate Studies, Princeton Program in Plasma Physics
2010, Summer	Visiting Fellow, Isaac Newton Inst. for Mathematical Sciences, Cambridge
2005, Spring	Long Term Participant, Kavli Inst. for Theoretical Physics, Santa Barbara
2004, Fall	Miller Visiting Research Professor, Astronomy Dept., U. California Berkeley
2001-2002	Visiting Scientist, Department of Physics, Imperial College, London Visiting Scientist, Joint European Torus, UK
1993- 1997	Research Physicist, Theory Division, Princeton Plasma Physics Laboratory
1986-1993	Research Physicist, Tokamak Fusion Test Reactor, Princeton Plasma Physics Laboratory
1987-1991	Visiting Scientist, Joint European Torus, Oxfordshire, England
1976-1979	Summer Jobs with Grumman Aerospace, in factories and research
1976-1980	Programmer, Harvard Business School Multinational Enterprise Project

Selected Publications

"Gyrokinetic continuum simulation of turbulence in a straight open-field-line plasma" E. L. Shi, G. W. Hammett, T. Stoltzfus-Dueck, A. Hakim, subm. to J. Plasma Physics, 2017. Arxiv.

"Scrape-Off Layer Turbulence in Tokamaks Simulated with a Continuum Gyrokinetic Code" A. Hakim, E.L. Shi, I.G. Abel, G.W. Hammett, T. Stoltzfus-Dueck, Proceedings of the 26th IAEA Fusion Energy Conference (2016, Kyoto, Japan). Arxiv.

"A Gyrokinetic 1D Scrape-Off Layer Model of an ELM Heat Pulse", E.L. Shi, A. H. Hakim, G. W. Hammett, Phys. Plasmas 22, 022504 (2015). Arxiv

"Direct multiscale coupling of a transport code to gyrokinetic turbulence codes, with comparisons to tokamak experiments", M. Barnes, I. G. Abel, W. Dorland, T. Goerler, G.W. Hammett, and F. Jenko, Phys. Plasmas 17, 056109 (2010).

"On 1D diffusion problems with a gradient-dependent diffusion coefficient", S.C. Jardin, G. Bateman, G.W. Hammett, L.P. Ku, J. Comp. Phys. 227 (2008) 8769.

"Report of the Study Group GK2 on Momentum Transport in Gyrokinetics", J. A. Krommes and G. W. Hammett, Technical Report PPPL-4945, October, 2013.

"Effects of plasma shaping on nonlinear gyrokinetic turbulence", E.A. Belli, G.W.Hammett and W. Dorland, Phys. Plasmas 15 (2008) 092303.

"An Iterative Semi-Implicit Scheme with Robust Damping", N.F. Loureiro, G.W. Hammett, J. Comp. Phys. 227 (2008) 4518.

"Applications of large eddy simulation methods to gyrokinetic turbulence", A. Bañón Navarro, B. Teaca, F. Jenko, G. W. Hammett, T. Happel and ASDEX Upgrade Team, Phys. Plasmas 21, 032304 (2014).

"Suppressing Electron Turbulence and Triggering Internal Transport Barriers with Reversed Magnetic Shear in the National Spherical Torus Experiment", J. L. Peterson, R. Bell, J. Candy, W. Guttenfelder, G. W. Hammett, S. M. Kaye, B. LeBlanc, D. R. Mikkelsen, D. R. Smith, and H. Y. Yuh, Phys. Plasmas 19, 056120 (2012). 2011 APS-DPP Invited Talk.

For a complete list, see w3.pppl.gov/~hammett/papers

Synergistic Activities

Have taught graduate courses at Princeton in Computational Plasma Physics, Turbulence and Nonlinear Processes in Plasmas, Irreversible Processes in Plasmas (covers collision operator and transport theory), and General Plasma Physics I.

Give lectures in various 1-week schools, including the NUF and SULI 1 week summer school in plasma physics for college students at PPPL, and at the 2014 ITER Summer School for graduate students and postdocs in Aix-en-Provence.

Past P.I. for the Center for the Study of Plasma Microturbulence SciDAC project (ended 2016) and participant in several other SciDAC projects.

Reviewer of grant proposals for government agencies and for many scientific journals.

Member of PPPL Research Council.

Collaborators and Co-editors

Co-authors and collaborators in past 48 months:
I. G. Abel (Chalmers), Justin Ball (Oxford, EPFL Lausanne), J. A. Baumgaertel (LANL), A. Bañón Navarro (UCLA and Max-Planck Institute for Plasma Physics, Michael Barnes (Oxford), R.E. Bell (PPPL), J. Candy (General Atomics), Stephen C. Cowley (Oxford), P. J. Dellar (Oxford), W. Dorland (U. Maryland), W. Guttenfelder (PPPL), A. Hakim, (PPPL), E. G. Highcock (Oxford, and Chalmers University of Technology), G.G. Howes (Iowa), F. Jenko (UCLA and Max-Planck-Institut Fur Plasmaphysik), S.M. Kaye (PPPL), J. A. Krommes (Princeton), B.P. LeBlanc (PPPL), Nuno F Loureiro (MIT), D.R. Mikkelsen (PPPL), W.M. Nevins (LLNL), J. T. Parker (Oxford), Felix I Parra (Oxford), J.L. Peterson (LLNL), Y. Ren (PPPL), Paulo Rodrigues (Instituto de Plasmas e Fusa0̃o Nuclear, University of Lisbon, Portugal) (no direct interaction), A. A. Schekochihin (Oxford), E. L. Shi (Princeton), T. Stoltzfus-Dueck (PPPL), T. Happel (Max-Planck Institute for Plasma Physics) (no direct interaction), B. Teaca (U. Coventry, UK), J.M. TenBarge (U. Maryland), D. Told (UCLA and Max-Planck-Institut Fur Plasmaphysik), H. Yuh (Nova Photonics, Princeton). (No co-editors in past 24 months).

Graduate Advisors:

Robert Kaita and Randy Wilson (PPPL)
(did not do a postdoc)

Graduate Advisees:

W.D. Dorland (Maryland)
M.A. Beer (Johns Hopkins)
S.A. Smith (LANL, last known, then business consulting)
P.B. Snyder (General Atomics)
E.A. Belli (General Atomics)
P. Sharma (Indian Institute of Science, Bangalore)
J.L. Peterson (LLNL)
Nadine Kremer (Business consulting in Germany)
J.A. Baumgaertel (LANL)
E. M. Granstedt (Tri Alpha)
E. L. Shi (current at Princeton)
N. Mandell (current at Princeton)

David R. Hatch
Research Scientist, Institute for Fusion Studies, University of Texas at Austin 512 720 1281
1 University Station C1500, Austin, TX 78712-0262 drhatch@austin.utexas.edu

Education and Training

Ph.D. Physics, University of Wisconsin-Madison, 2010

B.S. Mathematics (4.0), Utah State University, 2006

Physics (4.0), Utah State University, 2005

Research and Professional Experience

Institute for Fusion Studies, University of Texas at Austin

2015 - present	Research Scientist
2013 - 2015	Research Associate

Max Planck Institute for Plasma Physics; Garching, Germany

2011 - 2012	Postdoctoral Research Associate

University of Wisconsin-Madison

2006 - 2010	Graduate Research Assistant

Selected Publications

[1] D. R. Hatch, M. Kotschenreuther, S. Mahajan, P. Valanju, X. Liu, "A gyrokinetic perspective on the JET-ILW pedestal," Nuclear Fusion, 57, 36020 (2017).

[2] D. R. Hatch, M. Kotschenreuther, S. Mahajan, P. Valanju, F. Jenko, D. Told, T. Gorler, S. Saarelma, "Microtearing turbulence limiting the JET-ILW pedestal," Nuclear Fusion 56, 104003 (2016).

[3] D. R. Hatch, D. Told, F. Jenko, H. Doerk, M. G. Dunne, E. Wolfrum, E. Viezzer, M. J. Pueschel, and the ASDEX-Upgrade team, "Gyrokinetic study of ASDEX-Upgrade inter-ELM pedestal profile evolution," Nuclear Fusion 55, 063028 (2015).

[4] D. R. Hatch, F. Jenko, A. Bañón Navarro, V. Bratanov, "Transition between Saturation Regimes of Gyrokinetic Turbulence," Physical Review Letters 111, 175001 (2013).

[5] D. R. Hatch, M. J. Pueschel, F. Jenko, W. M. Nevins, P. W. Terry, H. Doerk, "Origin of Magnetic Stochasticity and Transport in Plasma Microturbulence," Physical Review Letters 108, 235002 (2012).

[6] D. R. Hatch, D. del-Castillo-Negrete, P. W. Terry, "Analysis and compression of six-dimensional gyrokinetic datasets using higher order singular value decomposition," Journal of Computational Physics 231, 4234 (2012).

[7] D. R. Hatch, P. W. Terry, F. Jenko, F. Merz, W. M. Nevins, "Saturation of Gyrokinetic Turbulence Through Damped Eigenmodes," Physical Review Letters 106, 115003 (2011).

[8] J. Citrin, J. Garcia, T. Goerler, F. Jenko, P. Mantica, D. Told, C. Bourdelle, D. R. Hatch, J. Hogeweij, T. Johnson, M. J. Pueschel, M. Schneider, "Electromagnetic stabilization of tokamak microturbulence in a high-beta regime," Plasma Phys. Control. Fusion 57, 014032 (2014).

[9] M. J. Pueschel, P. W. Terry, F. Jenko, D. R. Hatch, W. M. Nevins, T. GÃűrler, D. Told, "Extreme Heat Fluxes in Gyrokinetic Simulations: A New Critical β," Physical Review Letters 110, 155005 (2013).

[10] H. Doerk, F. Jenko, M. J. Pueschel, D. R. Hatch, "Gyrokinetic Microtearing Turbulence," Physical Review Letters 106, 155003 (2011).

Synergistic Activities

Panelist, FES/ASCR Exascale Review Meeting, 2016

Executive Committee Member, Sherwood Fusion Theory Conference, 2016-present

Panelist, National Science Foundation, 2014

Journal Referee: Communications in Computational Physics; Computer Physics Communications; Nature Communications; Nuclear Fusion; Physics of Plasmas

Speaker on fusion energy at physics workshop for Austin-area high school students, 2015

Collaborators and Co-editors in past 24 months
A. Bañón Navarro (UCLA), S. Brunner (EPFL), J. Citrin (Difer—Netherlands), D. del Castillo-Negrete (ORNL), H. Doerk (IPP-Garching), W. Dorland (Maryland), M. Dunne (IPP-Garching), D. Ernst (MIT), T. Goerler (IPP-Garching), G. Hammett (PPPL), R. Hazeltine (UT-Austin), J. Hillesheim (Culham), A. Hubbard (MIT), J. Hughes (MIT), M. Kotschenreuther (UT-Austin), F. Laggner (IPP-Garching), S. Mahajan (UT-Austin) , G. Merlo (UCLA), C. Michoski (UT-Austin), P. Morrison (UT-Austin), B. Moser (UT-Austin), W. Nevins (LLNL-retired), M.J. Pueschel (UW-Madison), S. Saarelma (Culham), D. Told (IPP-Garching), P. Valanju (UT-Austin), F. Waelbroeck (UT-Austin), E. Wolfrum (IPP-Garching)

Graduate and Postdoctoral Advisors and Advisees
T. Bernard (UT-Austin—PhD advisee), V. Bratanov (UT-Austin—postdoc advisee), E. Hassan (Ain Shams University, Egypt—PhD advisee), F. Jenko (IPP/UCLA—postdoc advisor), X. Liu (UT-Austin–PhD advisee), P. W. Terry (UW-Madison—PhD advisor)

Biographical sketch for Cory D. Hauck

Address

Department of Mathematics
University of Tennessee
219 Ayres Hall, 1403 Circle Dr
Knoxville, TN
Phone: (865) 574-0730, Fax: (865) 241-9915,
Email: **cdhauck@math.utk.edu**

Education and Training

2006	Ph.D.	Applied Mathematics	University of Maryland	College Park, MD
2004	M.S.	Electrical Engineering	University of Maryland	College Park, MD
1997	B.S.	Mathematics and Physics	University of South Carolina	Columbia, SC

Research and Professional Experience

2016 –	Associate Professor (Joint Faculty), Department of Mathematics, University of Tennessee
2012 – 2016	Assistant Professor (Joint Faculty), Department of Mathematics, University of Tennessee
2011 –	Research Staff, Oak Ridge National Laboratory
2009 –	Householder Fellow, Oak Ridge National Laboratory
2006 – 2009	Postdoctoral Research Associate, Los Alamos National Laboratory

Publications

1. M.P. Laiu, C. D. Hauck, R.G. McClarren, D.P. O'Leary, A.L. Tits, *Positive filtered P_N moment closures for linear kinetic equations*, SIAM J. Numer. Anal 54 (2016), pp. 3214-3238.
2. M. Frank, C. D. Hauck, and K. Küpper, *Convergence of filtered spherical harmonic equations for radiation transport*, Commun. Math. Sci., 14 (2016), pp. 1443-1465.
3. E. Endeve, C. D. Hauck, and Y. Xing, and A. Mezzacappa, *Bound-preserving discontinuous Galerkin methods for conservative phase space advection in curvilinear coordinates*, J. Comput. Phys., 287 (2015), pp. 151-183.
4. L. Chacon, D. del Castillo-Negrete, and C. D. Hauck, *An asymptotic-preserving semi-Lagrangian algorithm for the time-dependent anisotropic heat transport equation*, Journal of Computational Physics, 272 (2014), pp. 719-746
5. C. D. Hauck and R. G. McClarren, *A scattering-based hybrid method for time dependent, linear, kinetic transport equations*, SIAM J. Multiscale Modeling and Analysis, 11 (2013), pp. 1197-1227.
6. H. Schaeffer, R. Caflisch, C. D. Hauck, S. Osher, *Sparse dynamics for partial differential equations*, Proceedings of the National Academy of Sciences, 110 (2013), pp. 6634-6639.
7. E. Olbrant, C. D. Hauck, and M. Frank, *A realizability-preserving, discontinuous Galerkin method for the M_1 model of radiative transfer*, J. Comput. Phys., 231 (2012), pp. 56125639.
8. C. D. Hauck and R. B. Lowrie, *Temporal regularization of the P_N equations*, SIAM J. Multiscale Modeling and Analysis, 7 (2009), pp. 1497-1524.
9. C. D. Hauck, C. D. Levermore, and Andre Tits, *Convex duality and entropy-based moment closures*, SIAM J. Control Optim, 47 (2008), pp. 1977-2015.
10. J. Haack and C. D. Hauck, *Oscillatory Behavior of Asymptotic-Preserving Splitting Methods for a Linear Model of Diffusive Relaxation*, Kinetic and Related Models, 1 (2008), pp. 573-590.

Synergistic Activities

1. **Journal Work**: Associate Editor, *Multiscale Modeling and Simulation*, 2016 – present; Reviewer for *ACM Transactions on Mathematical Software*, *Analysis and Mathematical Physics*, *Communications on Computational Physics*, *Communications in Mathematical Sciences*, *Journal of Computational Physics*, *Journal of Scientific Computing*, *Journal of Theoretical and Computational Transport*, *Journal of Uncertainty Quantification*, *SIAM Journal on Applied Mathematics*, *SIAM Journal on Numerical Analysis*, *SIAM/ASA Journal of Uncertainty Quantification*, *SIAM Journal on Scientific Computing*, *SIAM Review*, *Zeitschrift für Angewandte Mathematik und Physik*

2. **Project Management**: PI, Department of Energy (Advanced Scientific Computing Research), Applied Mathematics, Projects on *Hybrid Methods for Complex Particle Systems* and *Moment Methods for Kinetic Equations*; PI, National Science Foundation, Computational Mathematics, Project on *Optimization-Based Moment Models for Multiscale Kinetic Equations* Node Leader, NSF Research Network on *Kinetic Description of Emerging Challenges in Multiscale Problems of Natural Sciences.*

3. **Invited and Plenary Lectures**: Conference on *Numerical approximations of hyperbolic systems with source terms and applications*, RWTH Aachen, September 2013; Short Course on *Numerical topics in collisional kinetic equations: moment models, asymptotic preserving methods, and hybrid approaches*, Aachen Institute for Advanced Study in Computational Engineering Science EU Regional School, July 2015; Workshop on *Uncertainty quantification in kinetic and hyperbolic problems*, University of Wisconsin, May 2015; Workshop on *Boundary-value problems and multi-scale coupling methods for kinetic equations*, University of Wisconsin, April 2016.

4. **Service and Organization**: Chair, Householder Seminar Series, UTK/ORNL; Member, Householder Fellowship committee, Oak Ridge National Laboratory; Chair, Conference on *Scalable methods for kinetic equations*, Oct 19 - 23, 2015, Oak Ridge, Tennessee; Chair, Annual Meeting of the SIAM Southeastern Atlantic Section, March 22-24, 2013, Knoxville / Oak Ridge, TN; Chair, Workshop on *Moment Methods in Kinetic Theory III*, Oct 2017, Oak Ridge, Tennessee; Technical Committee, Workshop on *Algorithm and Model Verification And Validation For Kinetic Plasma Simulation Codes*, November 12-15, 2012, East Lansing, Michigan; Panel Member, DOE *Workshop on Integrated Simulations for Magnetic Fusion Energy Sciences*, June2-4, 2015, Rockville, MD; Mini-symposia organizer at SIAM AN09, SIAM AN10, SIAM CSE11, SIAM CSE13.

5. **Honors and awards**: Career Award, ASCR, Office of Science, Department of Energy, 2015; Alton S. Householder Fellowship, Oak Ridge National Laboratory, 2009–2011; NSF VIGRE research grant 2005; Carolina Scholar, 1993 – 1997; National Merit Scholarship, 1993 – 1997.

Collaborators and Other Affiliations for Cory D. Hauck

Collaborators (last 48 months) and Co-editors (last 24 months)

Graham Alldredge (RWTH-Aachen); Rick Archibald (Oak Ridge National Laboratory); Richard Barnard (Oak Ridge National Laboratory); Russel Caflisch (UCLA); Luis Chacon (Los Alamos National Laboratory); Zheng Chen (Oak Ridge National Laboratory); Andrew Christlieb (Michigan State University); Diego del-Castillo-Negrete (Oak Ridge National Laboratory); Giacomo Dimarco (University of Ferrara); Eirik Endeve (Oak Ridge National Laboratory); Rodney Fox (Iowa State University); Martin Frank (RWTH-Aachen); Irene Gamba (University of Texas-Austin); Kris Garrett (Los Alamos National Laboratory); Jeff Haack (Los Alamos National Laboratory); Judith Hill (Oak Ridge National Laboratory); Jingwei Hu (Purdue University); Ming-Tse Paul Laiu (University of Tennessee); Raphaël Loubère (Université de Toulouse);

Ryan McClarren (Texas A & M University); Tony Mezzacappa (University of Tennessee); Michael Murillo (Michigan State University); Dianne O'Leary (University of Maryland); Stan Osher (UCLA); Hayden Schaeffer (Carnegie Mellon); Weiran Sun (Simon Fraser University); Qiwei Sheng (California State-Bakersfield); Yi Sun (University of South Carolina); Ilya Timofeyev (University of Houston); André Tits (University of Maryland); Zhi-Jian Wang (University of Kansas); Clayton Webster (Oak Ridge National Laboratory); Yulong Xing (UC-Riverside); Dongbin Xiu (Ohio State University)

Graduate and Postdoctoral Advisors and Advisees

C. David Levmore (University of Maryland); Robert B. Lowrie (Los Alamos National Laboratory); André L. Tits (University of Maryland) Graham W. Alldredge (Freie Universität Berlin); Richard Barnard (Oak Ridge National Laboratory); Zheng Chen (Oak Ridge National Laboratory); C. Kris Garrett (Los Alamos Laboratory); Vincent Heningburg (University of Tennessee); Ming-Tse Paul Laiu (University of Tennessee); Qiwei Sheng (California State-Bakersfield)

Jeffrey Hittinger

Contact Information

Center for Applied Scientific Computing
Lawrence Livermore National Laboratory
7000 East Avenue, L-561
Livermore, CA 94550

Phone: (925)–422–0993
Fax: (925)–423–2993
E-mail: hittinger1@llnl.gov

Education and Training

Ph.D., Aerospace Eng. & Sci. Computing, 2000, University of Michigan

M.S., Applied Mathematics, 1997, University of Michigan

M.S.E., Aerospace Engineering, 1994, University of Michigan

M.S., Mechanical Engineering, 1993, Lehigh University

Research and Professional Experience

Deputy Devision Leader (acting), Center for Applied Scientific Computing, Lawrence Livermore National Laboratory, 2016–Present.

Group Leader, Scientific Computing Group, Lawrence Livermore National Laboratory, 2013–Present.

Computational Scientist, Lawrence Livermore National Laboratory, 2002–Present.

Postdoctoral Research Staff Member, Lawrence Livermore National Laboratory, 2000–2002.

Selected Publications

M. Dorf, M. Dorr, J. Hittinger, R. Cohen, T. Rognlien, “Continuum kinetic modeling of the tokamak plasma edge,” Phys. Plasmas, 23 (2016), pp. 056102.

P. McCorquodale, M. Dorr, J. Hittinger, P. Colella, “High-order finite-volume methods for hyperbolic conservation laws on mapped multiblock grids,” J. Comput. Phys., 288 (2015), pp.181–195.

J. M. Connors, J. W. Banks, J. A. F. Hittinger, C. S. Woodward, “Quantification of errors for operator-split advection-diffusion calculations,” Comput. Methods Appl. Mech. Engrg. 272 (2014), 181–197.

M. Dorf, R. Cohen, M. Dorr, T. Rognlien, J. Hittinger, J. Compton, P. Colella, D. Martin and P. McCorquodale, “Simulation of Neoclassical Transport with the Continuum Gyrokinetic Code COGENT,” Phys. Plasmas, 10 (2013), pp. 012513.

M. A. Dorf, R. H. Cohen, M. Dorr, T. Rognlien, J. Hittinger, J. Compton, P. Colella, D. Martin and P. McCorquodale, “Numerical Modelling of Geodesic Acoustic Mode Relaxation in a Tokamak Edge,” Nucl. Fusion, 53 (2013), pp. 063015.

J. A. F. Hittinger and J. W. Banks, “Block-Structured Adaptive Mesh Refinement Algorithms for Vlasov Simulation,” J. Comput. Phys., 241 (2013), pp. 118–140.

J. W. Banks, J. A. F. Hittinger, J. M. Connors, and C. S. Woodward, “Numerical Error Estimation for Nonlinear Hyperbolic PDEs Via Nonlinear Error Transport,” Comput. Meth. App. Mech. Engin., 213-216 (2012), pp. 1–15.

P. Colella, M. R. Dorr, J. F. Hittinger and D. F. Martin, “High-order, Finite-volume Methods in Mapped Coordinates,” J. Comput. Phys., 230 (2011), pp. 2952–2976.

J. W. Banks and J. A. F. Hittinger, “A New Class of Non-Linear, Finite-Volume Methods for Vlasov Simulation,” IEEE Trans. Plasma Sci., 38 (2010), pp. 2198–2207.

M. R. Dorr, F. X. Garaizar, and J.A.F. Hittinger, “Simulation of Laser Plasma Filamentation Using Adaptive Mesh Refinement,” Journal of Computational Physics, 177 (2002), pp. 233–263.

Synergistic Activities

Co-PI, High-Resolution Methods for Phase Space Problems in Complex Geometries, DOE ASCR Applied Math Base Program.

Investigator, High-Fidelity Whole Device Modeling of Magnetically Confined Fusion Plasmas, DOE Exascale Computing Project

Collaborators and Co-editors in past 24 months

Collaborators

William Arrighi, David Beckingsale, Richard Berger, Timo Bremer, Thomas Chapman, Mikhail Dorf, Milo Dorr, Debo Ghosh, Richard Klein, Chunhua Liao, Wonjae Lee, Peter Lindstrom, Scott Lloyd, John Loffeld, Don Lucas, Daniel Osei-Kuffuor, Daniel Quinlan, Tom Rognlien, Geoff Sanders, Markus Schordan, Carol Woodward (LLNL); Mark Adams, Phil Colella, Dan Martin, Peter McCorquodale, Andrew Myers, Peter Schwartz, Brian van Straalen (LBNL); Jeff Banks (RPI); Stefan Brunner (EPFL); Amitava Bhattercharjee, Choong-Seock Chang, Stephane Ethier (PPPL); Ed DâĂŹAzevedo, Scott Klasky (ORNL); Ron Cohen (CompX); Anshu Dubey, Andrew Siegel (ANL); Steve Guzik, Michelle Mills Strout (Colorado State); Catherine Olschanowsky (Boise State); Scott Parker (U. Colorado); Frank Jenko, Ben Winjum (UCLA)

Co-editors

Paul Hovland, Sven Leyffer, Lois Curfman McInnes, Elia Merzari, Rob Ross, Rick Stevens, Stefan Wild (ANL); Babara Chapman (BNL); Luis Chacon, Gary Grider (LANL); Jon Bashor, John Bell, Silvia Crivelli, Esmond Ng, John Shalf (LBNL); Lori Diachin, Rob Falgout, Dean Williams (LLNL); Jack Dongarra, Al Geist, Jeffrey S Vetter, Clayton Webster (ORNL); Choong-Seock Chang (PPPL); Adolfy Hoisie (PNNL); James Ang, Ron Brightwell, Erik Debenedictus, James Laros, Mike Heroux (SNL); Eric Stahlberg (NIH); Scott A Lathrop (NCSA); Laura Carrington (SDSC); Michael Sprague, Ray Grout (NREL); Robert Colwell (DARPA); William Carlson (Institute for Defense Analysis); Don Estep (Colorado State); Keren Bergman (Columbia); Paul Bonoli (MIT); Harper Langston (NYU); Vivek Sarkar (Rice); Frank Jenko (UCLA); Paul Fischer (UIUC); Robert Lucas (USC); Robert Moser (UT Austin); Thomas Sterling (U. Indiana); Stanislav Boldyrev (U. Wisconsin); Peter Kogge (Notre Dame); Robert Schreiber (HP); George Chiu, Paul Coteus, Rud Haring, KH Kim (IBM); Shekhar Borkar (Intel); Dean Klein, Richard Murphy (Micron); William Dally (NVIDIA); Richard Lethin (Reservoir Labs); Henri Calandra (Total SA); Jon Hiller (Science and Technology Associates)

Graduate and Postdoctoral Advisors and Advisees

P. Roe (U. Michigan), A. Messiter (U. Michigan), B. Van Leer (U. Michigan), M. Dorr (LLNL)

Debo Ghosh, John Loffeld, Genia Vogman (LLNL); James Adler (Tufts); Jeff Banks (RPI); Jeff Connors (UConn); Johann Dahm (U. Michigan); Mikhail Khodak (Princeton); Martina Prugger (U. Innsbruck); David Seal (US Naval Academy); Yoshifumi Suzuki (Altair Engineering)

Bill Hoffman
Bill.hoffman@kitware.com
518 881-4905
28 Corporate Drive
Clifton Park, NY, 12065

Education

1992 MS Computer Science, Rensselaer Polytechnic Institute

1990 Bachelor of Computer Science, University of Central Florida

Employment

CTO Kitware Inc. (1998-present)

Bill is the CTO and a founder of Kitware, and oversees the IT infrastructure of the company. In addition, he contributes at a high level to many of the ongoing software efforts at Kitware. As part of the leadership of Kitware Inc. he has had a huge impact on open source software contributing to many important open source tools used extensively by the scientific community. He was part of the architecture team for the Insight Toolkit (ITK), a contributor to the Visualization Toolkit (VTK), and created the CMake build system. While at GE, he created an open source computer vision package called TargetJR which became VXL and contributed the numerical library VNL which ITK is built on. CMake in particular has had a huge impact on the ability to share and collaborate with scientific software. For example, Bill helped create a CMake build system for LAPACK which enabled greater cross-platform access to this key numerical library (http://www.netlib.org/lapack/lawnspdf/lawn270.pdf). These tools are the bedrock on top of which numerous scientific efforts over the past two decades have been built.

Individual Contributor GE CRD (1990-1998)

Recent Collaborators

Terry Yoo (NIH/NLM) Roscoe Bartlett (Sandia National Labs)
Dan Quinlan (LLNL)
Justin Too (LLNL) Jim Ahrens LANL

Synergistic Activities

- Project lead for Toyota Research Institute (TRI) / MIT's Project Drake software process project. https://blog.kitware.com/enhancing-software-quality-with-ci-in-the-cloud/. Using CMake/CTest/CDash and Jenkins and AWS to create fast turnaround continuous integration testing system.
- Project lead for Kitware's software support for Google Tango project. software process project. Using CMake/CTest/CDash and Jenkins to build and test software for the Google Tango project.

- Project lead for Sandia CMake/CTest/CDash support contract.
- Project lead for CASL CMake/CTest/CDash support contract.

Publications

- **Hoffman B.**, Martin K., Schroeder W., Geveci B., Brown A., Wilson G., Bryant R., Crook J., Ramey C., Seltzer M., Bostic K., Moir K., Davis C., Chansler R., Kuang H., Radia S., Scvachko K., Srinivas S., Brown C.T., Canino-Koning R., Ivov E., Lattner C., Ochtman D., Marcus A., Ziade T., Cesarini F., Gross A., Sheehy J., Steward S., Allman E., Bryant R., Lagar-Cavilla A., Tang A., Madeley D., Laudicina A., Mavrinac A., Horstmann C., Freire J., Koop D., Santos E., Shimooka R., White D., The Architecture of Open Source, 2011
- Hanwell M., **Hoffman B.**, King B., Distributed Version Control: The Future of History, Kitware Source, Oct-2010
- **Hoffman B.**, Kitware Quality Software Process, Kitware Source, Oct-2008
- Martin K., **Hoffman B.**, An Open Source Approach to Developing Software in a Small Organization, IEEE Software, 2007
- Martin K., **Hoffman B.**, Mastering CMake: A Cross-Platform Build System, second edition, Kitware Inc., 2004
- Hoffman W., Martin K., The CMake Build Manager, Dr. Dobb's Journal, M and T PUBLISHING INC, 2003
- Martin K., **Hoffman B.**, Mastering CMake: A Cross-Platform Build System, Kitware Inc, 2003
- Martin K., Hoffman W., Geveci B., Creating Libraries For Multiple Programming Languages, Dr. Dobb's Journal. February 2002. , Feb-2002
- Schroeder W.J., Avila L.S., Martin K.M., Hoffman W., Law C., The Visualization Toolkit User's Guide, Kitware, Inc., 2001
- Schroeder W., Avila L., Hoffman W., Visualizing with VTK: A Tutorial, IEEE Computer Graphics And Applications, Sep-2000
- Hoffman W., Curwen R., Pseudo-Incremental Linking for C/C++, Dr. Dobb's Journal, M and T PUBLISHING INC, Oct-1999
- Rothwell C., Mundy J., **Hoffman B.**, Representing Objects using Topology, 1996
- Rothwell C., Rothwell C., Mundy J., Nguyen V-D., Mundy J., **Hoffman B.**, Hoffman B., Robotvis P., Driving Vision by Topology, Proc. International Symposium on Computer Vision, 1995
- Mundy J., Huang C., Liu J., Hoffman W., Forsyth D., Rothwell C., Zisserman A., Utcke S., Bournez O., MORSE: A 3D object recognition system based on geometric invariants, Proc. DARPA Image Understanding Workshop, 1994

Curriculum Vitae
Scott A. Klasky
Contact Information

Professional Preparation

Ph.D. in Physics (1994), University of Texas, Austin, TX.
B.S. in Physics (1989), Drexel University.

Appointments

2014 – Present, Distinguished Scientist, ORNL
2014 – Present, Adjunct Faculty, Georgia Technical University, Atlanta GA.
2012 – Present, Group Leader: Scientific Data, Computer Science and Mathematics, ORNL,
2009 – Present, Adjunct Professor, Dept. of Electric and Computer Science, University of Tennessee Knoxville, Knoxville TN.
2007 – Present, Adjunct Professor, Dept. of Information Technology, North Carolina State University, Raleigh, NC.
2005 – Present, Visiting Professor, Dept. of Electrical and Computer Engineering, Rutgers University, Piscataway NJ.
2005 – 2011, Senior Research Scientist, and End-to-End Task Lead, Oak Ridge National Laboratory, Oak Ridge, TN.
1999 – 2005, Senior Research Scientist, Princeton Plasma Physics Laboratory, Princeton NJ.
1995 – 1999, Senior Research Scientist, Syracuse University (Northeast Parallel Architecture Center, Syracuse NJ.

Five Publications Most Relevant to This Proposal

1. J. F. Lofstead, S. Klasky, K. Schwan, N. Podhorszki, C. Jin, Flexible io and integration for scientific codes through the adaptable io system (adios) in Proceedings of the 6th international workshop on Challenges of large applications in distributed environments, ACM, pp. 15–24. (229 citations, 1/24/2017)
2. H. Abbasi, M. Wolf, G. Eisenhauer, S. Klasky, K. Schwan, F. Zheng. Datastager: scalable data staging services for petascale applications. *Cluster Computing* 2010, *13*, 277–290. (193 citations, 1/24/2017)
3. J. Lofstead, F. Zheng, S. Klasky, K. Schwan, Adaptable, metadata rich IO methods for portable high performance IO in Parallel & Distributed Processing, 2009. IPDPS 2009. IEEE International Symposium on, IEEE, pp. 1–10. (125 citations, 1/24/2017)
4. F. Zheng, H. Abbasi, C. Docan, J. Lofstead, Q. Liu, S. Klasky, M. Parashar, N. Podhorszki, K. Schwan, M. Wolf, PreDatA–preparatory data analytics on peta-scale machines in Parallel & Distributed Processing (IPDPS), 2010 IEEE International Symposium on, IEEE, pp. 1–12. (104 citations, 1/24/2017)
5. J. Lofstead, F. Zheng, Q. Liu, S. Klasky, R. Oldfield, T. Kordenbrock, K. Schwan, M. Wolf, Managing variability in the IO performance of petascale storage systems in Proceedings of the 2010 ACM/IEEE International Conference for High Performance Computing, Networking, Storage and Analysis, IEEE Computer Society, pp. 1–12. (111 citations, 1/24/17)

Research Interests and Expertise

Dr. Klasky has over 25 years of experience in designing and creating middleware, visualization, mathematical algorithms, and numerical simulations for high performance- data intensive computing. Dr. Klasky leads many large efforts, and has funding of over $6M/year, and serves as the technical lead and coordinator on all of these projects. Scott is one of the world's leaders in Research into Data Intensive

Science, and is the lead of the ADIOS project, used by many of the largest data producers in the world. Dr. Klasky is starting to lead a new effort which combines the use of Service Oriented Arthictures for High End Computing with advanced data streaming techniques which can process voluminous data from remote resources and efficiently use all of the devices.

The core mission around my work is to perform research and development in core solutions for data intensive computing. I lead a large team of over 75 scientists to research and build data handling infrastructure for moving, reducing, analyzing, visualizing, and understanding massive amounts of data produced by current and next generation facilities, both computational and experimental. My approach is rooted in deep engagements with real science end-users. As such, my team is a strong partner with leading application teams to co-design new algorithms, middleware, and end-to-end systems. My overarching goal is to create infrastructure that enables new capabilities for scientists to make Timely (Near-Real-Time) and Quality-based decisions.

Synergistic Activities

1. Head of the ADIOS Project, (https://www.olcf.ornl.gov/center-projects/adios/
2. Co-PI on the SDAV SciDAC data institute.
3. Co-PI on the CODAR ECP project.
4. PI of the ECP ADIOS project.
5. Co-PI on the ECP WDM project.

Collaborators (*past 5 years including name and current institution*)-ORNL are conflicts

Abbasi, Hasan, Amazon
Adams, Mark, LBNL
Agrawal, Ankit, NWU
Ahrens, James, LANL
Aiken, Alexander, Stanford
Altintas, Ilkay, UCSD
Bell, John, LBNL
Bennett, Janine, SNL
Bethel, Wes, LBNL
Brugger, Eric, LLNL
Chen, Jackie, Sandia
Childs, Hank, U. Oregon
Choudhary, Alok, NWU
Ethier, Stephane, PPPL
Feibush, Elliott, PPPL
Fox, Geoffrey, U Indiana
Gavrilovska, Ada, GT
Geveci, Berk, Kitware
Grout, Ray, NREL
Hanrahan, Patrick, Stanford
Hansen, Charles, U. Utah
Johnson, Chris, U. Utah
Kolla, Hemanth, SNL
Kothe, Doug, ORNL
Kurc, Tahsin, SBU SUNY
Latham, Rob, ANL
Lee, Wei-Li, PPPL
Liao, Wei-keng, NWU
Liu, Qing, Oak Ridge National Laboratory
Lofstead, Jay, Sandia National Laboratories
Logan, Jeremy, UTK
Ludaescher, Bertram, UCD
Ma, Xiaosong, Qatar Research Foundation
Ma, Kwan-Liu, U.C. Davis
Maccabe, Arthur, Oak Ridge National Laboratory
Matzner, Richard, U Texas Austin
McCormick, Patrick, LANL
Moreland, Kenneth, SNL
Moser, Robert, U. T. Austin
Oldfield, Ron, SNL
Papka, Michael, ANL
Parker, Scott, U. of Colorado
Pascucci, Valerio, U. of Utah
Peterka, Tom, ANL
Quinlan, Dan, LLNL
Ross, Rob, ANL
Saltz, Joel, SBU
Samatova, Nagiza, NCSU
Sanderson, Allen, Utah
Shalf, John, LBNL
Shen, Han-Wei, OSU
Shephard, Mark, RPI
Shoshani, Arie, LBNL
Siegel, Andrew, ANL
Taufer, Michela, U. Delaware
Tchoua, Roselyne, Chicago
Vishwanath, Venkat, ANL
Widener, Patrick, SNL
Wolf, Matthew, GT Tech
Wu, Kesheng, LBNL
Yu, Weikuan, U. Flo

Seung-Hoe Ku

Princeton Plasma Physics Laboratory, Princeton, NJ 08543-0451
sku@pppl.gov • 609-243-2684

Professional Preparation

Ph. D in Physics, Korea Advanced Institute of Science and Technology, June 2004
M. S. in Physics, Korea Advanced Institute of Science and Technology, Feb. 1998
B. S. in Physics, Korea Advanced Institute of Science and Technology, Feb. 1996
Postdoctoral training, Courant Institute of Math. Science, New York Univ. (2005 – 2006)
Postdoctoral training, Korea Advanced Institute of Science and Technology, (2004 – 2005)

Appointments

Research Physicist, Princeton Plasma Physics Laboratory (2011-present)
Research Scientist, Courant Institute of Math. Science, New York University (2006 – 2011)

Biosketch

Seung-Hoe Ku is a computational physicist, studying plasma turbulence and transport on full scale Titan, Mira and Edison. He is a leading expert in extreme scale computing on both GPU-dominant and CPU-dominant architectures. He is the lead author and manager of the modern gyrokinetic particle-in-cell code XGC that is a flagship code at PPPL, and its simplified version XGC0 that is used by experimentalists for kinetic transport analysis. Since the inception of the XGC-code, he has been working with multi-disciplinary scientists including applied mathematicians (algorithms, solvers, meshing) and computer scientists (performance engineering, multi-hardwae porting, data management, MPI/OpenMP/Cuda/OpenACC programming languages, etc.). He has given many invited and plenary talks at major scientific conferences. He has been serving in the Executive Committee, International Conference on Numerical Simulation of Plasmas (ICNSP) since 2015.

Ten Relevant Publications

1. S. Ku, R. Hager, C.S. Chang, “A new hybrid-Lagrangian numerical scheme for gyrokinetic simulation of tokamak edge plasma”, J. Computational Physics, 325, 467 (2016)
2. R. Hager, E.S. Yoon, S. Ku, E.F, D’Azevedo, P.H. Worley and C.S. Chang, “A fully non-linear multi-species Fokker-Planck-Landau collision operator for simulation of fusion plasma”, J. Computational Physics, 315, 644 (2016)
3. F. Zhang, R. Hager, S. Ku, Choong-Seock Chang , Stephen C. Jardin, Nathaniel M. Ferraro, E. Seegyoung Seol, Eisung Yoon, Mark S. Shephard, “Mesh generation for confined fusion plasma simulation”, Engineering with computers, 32, 285 (2016)
4. S. Lakshminarasimhan, N. Shah, S. Ethier, S. Ku, C-S Chang, S. Klasky, R. Latham, R. Ross, N. Samatova, "Isabela for effective in situ compression of scientific data", Concurrency and Computation: Practice and Experience, 25, 524 (2013)
5. S. Ku, J. Abiteboul, P.H. Diamond, G. Dif-Pradalier, J.M. Kwon, Y. Sarazin, T.S. Hahm, et. al. “Physics of intrinsic rotation in flux-driven ITG turbulence”, Nuclear Fusion, 52, 063013 (2012)
6. S. Ku, C.S. Chang, P.H. Diamond, “Full-f gyrokinetic particle simulation of ITG turbulence with a strong central heating in realistic tokamak geometry”, Nuclear Fusion, 49, 115021 (2009)

7. M. F. Adams, S. Ku, P. Worley, E. D'Azevedo, J. C. Cummings, C.S. Chang, "Scaling to 150K cores: recent algorithm and performance engineering developments enabling XGC1 to run at scale", Journal of Physics: Conference Series, 180, 012036 (2009)
8. Y. Chen, S. E. Parker, G. Rewoldt, S. Ku, G.Y. Park, C.S. Chang, Coarse-graining the electron distribution in gyrokinetic simulations, Phys. Plasmas, 15, 055905 (2008)
9. S. Ku, C.S. Chang, M. Adams, et al. "Gyrokinetic particle simulation of neoclassical transport in the pedestal/scrape-off region of a tokamak plasma," SCIDAC 2006:Scientific discovery through advanced computing 46, 87 (2006)
10. Seung-Hoe Ku, Hoyul Baek, and C. S. Chang, Property of an X-point generated velocity-space hole in a diverted tokamak plasma edge, Phys. Plasmas, 11, 5626 (2004)

Collaborators (past 5 years including name and current institution)

C.S. Chang, Princeton Plasma Physics Lab., Graduate and Postdoctoral advisor
P. H. Diamond, University of California, San Diego
E.S. Yoon, Rensselaer Polytechnic Institute
M. Adams, Lawrence Berkeley National Laboratory
S. Koh, National Fusion Research Institute, Korea
J.M. Kwon, National Fusion Research Institute, Korea
S. Klasky, Oak Ridge National Laboratory
P. Norbert, Oak Ridge National LaboratoryP. Worley, Oak Ridge National Laboratory
E. D'Azevedo, Oak Ridge National Laboratory

PhD Advisor: C.S. Chang (PPPL)
Postdoctoral Advisor: C.S. Chang (PPPL)

Dr. Rajesh Maingi Biographical Sketch (Principal Investigator)

Education and training:

Ph.D, Dept. of Nuclear Engineering, N.C. State University, 1992

Thesis title: "Coupled 2-D Edge Plasma and Neutral Gas Simulations of Tokamak Scrape-off Layers"

B.S. Dept. of Nuclear Engineering, N.C. State University, 1987

Research and Professional Experience:

2012-present: staff member, Princeton Plasma Physics Laboratory; title: Division Head
2013-present: Adjunct Professor, Dept. of Nuclear Engineering, UT-Knoxville
1997-2012: staff member, Oak Ridge National Lab; title: Distinguished R & D Staff
1992-1997: postdoctoral research associate, ORNL on-site at General Atomics at DIII-D

Relevant recent publication list:

1. R. Maingi, "Edge Transport Barrier Without Large Edge Localized Modes: Control, Performance, and Extrapolability Issues for ITER", *Nucl. Fusion* **54** (2014) 114016.
2. J.S. Hu, G.Z. Zuo, J. Ren, Q.X. Yang, Z.X. Chen, H. Xu, L.E. Zakharov, **R. Maingi**, C. Gentile, X.C. Meng, Z. Sun, W. Xu,Y. Chen, D. Fan, N. Yan, Y.M. Duan, Z.D. Yang, H.L. Zhao, Y.T. Song, X.D. Zhang, B.N. Wan, J.G. Li and EAST Team, "First Results of the Use of a Continuously Flowing Lithium Limiter in High Performance Discharges in the EAST Device", *Nucl. Fusion* **56** (2016) 046011.
3. J. S. Hu, Z. Sun, H. Y. Guo, J. G. Li, B. N. Wan, H. Q. Wang, S. Y. Ding, G. S. Xu, Y. F. Liang, D. K. Mansfield, **R. Maingi**, X. L. Zou, L. Wang, J. Ren, G. Z. Zuo, L. Zhang, Y. M. Duan, T. H. Shi, L. Q. Hu and East team, "New Steady-State Quiescent High-Confinement Plasma in an Experimental Advanced Superconducting Tokamak", *Phys. Rev. Lett.* **114** (2015) 055001.
4. R. Maingi, T.H. Osborne, M.G. Bell, R.E. Bell, D.P. Boyle, J.M. Canik, A. Diallo, R. Kaita, S.M. Kaye, H.W. Kugel, B.P. LeBlanc, S.A. Sabbagh, C.H. Skinner, V.A. Soukhanovskii, The NSTX Team, "Dependence of recycling and edge profiles on lithium evaporation in high triangularity, high performance NSTX H-mode discharges", *J. Nucl. Mater.* **463** (2015) 1134.
5. J. Li, H. Y. Guo, B. N.Wan, X. Z. Gong, Y. F. Liang, G. S. Xu, K. F. Gan, J. S. Hu, H. Q.Wang, L.Wang, L. Zeng, Y. P. Zhao, P. Denner, G. L. Jackson, A. Loarte, **R. Maingi**, J. E. Menard, M. Rack, and X. L. Zou, "A long-pulse high-confinement plasma regime in the Experimental Advanced Superconducting Tokamak", *Nature Phys.* **9** (2013) 817.
6. R. Maingi, D.P. Boyle, J.M. Canik, S.M. Kaye, C.H. Skinner, J.P. Allain, M.G. Bell, R.E. Bell, S.P. Gerhardt, T.K. Gray, M.A. Jaworski, R. Kaita, H.W. Kugel, B.P. LeBlanc, J. Manickam, D.K. Mansfield, J.E. Menard, T.H. Osborne, R. Raman, A.L. Roquemore, S.A. Sabbagh, P.B. Snyder, and V.A. Soukhanovskii, "The effect of progressively increasing lithium coatings on plasma discharge characteristics, transport, edge profiles and ELM stability in the National Spherical Torus Experiment", *Nucl. Fusion* **52** (2012) 083001.
7. R. Maingi, T.H. Osborne, B.P. LeBlanc, R.E. Bell, J. Manickam, P.B. Snyder, J.E. Menard, D.K. Mansfield, H.W. Kugel, R. Kaita, S.P. Gerhardt, S.A. Sabbagh, F.A. Kelly, and the NSTX research team, "ELM suppression through density profile modification with lithium wall coatings in the NSTX", *Phys. Rev. Lett.* **103** (2009) 075001.
8. R. Maingi, S.M. Kaye, C.H. Skinner, D.P. Boyle, J.M. Canik, M.G. Bell, R.E. Bell, T.K. Gray, M.A. Jaworski, R. Kaita, H.W. Kugel, B.P. LeBlanc, D.K. Mansfield, T.H. Osborne, S.A. Sabbagh, and V.A. Soukhanovskii, "The continuous improvement of H-mode discharge performance with progressively increasing lithium coatings in NSTX", *Phys. Rev. Lett.* **107** (2011) 145004.

9. R. Maingi, R.E. Bell, J.M. Canik, S.P. Gerhardt, S.M. Kaye, B.P. LeBlanc, T.H. Osborne, M.G. Bell, E.D. Fredrickson, K.C. Lee, J.E. Menard, J.-K. Park, S.A. Sabbagh, and the NSTX team, "Triggered confinement enhancement and pedestal expansion in high confinement mode discharges in the NSTX", *Phys. Rev. Lett.* **105** (2010) 135004.
10. R. Maingi, C.E. Bush, R. Kaita, H.W. Kugel, A.L. Roquemore, S.F. Paul, V.A. Soukhanovskii, and the NSTX team, "Divertor Heat Flux Scaling with Heating Power and Plasma Current in H-mode Discharges in the National Spherical Torus Experiment", *J. Nucl. Mater.* **363-365** (2007) 196.

Synergistic Activities

1. Served as Chairman of the 2015 FES Workshop on Plasma-Materials Interactions
2. Serves as Chairman of the International Tokamak Physics Activity (ITPA) Pedestal and Edge Physics Topical Group, and on the ITPA Coordinating Committee, 2013-
3. Serves on the International Advisory Committee for the H-mode Workshop, 2015-
4. Participated in APS Distinguished Lecturer in Plasma Physics Program, 2013-2015
5. Served as technical Program Co-chair, TOFE meeting, Anaheim CA, 2014

Collab. Institution	Collaborator Names (PPPL and ORNL collaborators not included)
ASIPP, China	J.S. Hu, J.G. Li, B.N. Wan, L. Wang, G.S. Xu, G.Z. Zuo, Z.X. Liu, Z. Sun, J. Ren
CCFE	A. Kirk, H. Meyer, S. Saarelma
General Atomics	R. Buttery, C. Chrobak, T. Evans, H.Y. Guo, D. Hill, T. Leonard, R. Groebner, G. Jackson, T. Osborne, P. Parks, T.Petrie, P. Snyder, M. Wade
IPP-Garching	P. Lang, E. Wolfrum, T. Eich
LLNL	M. Fenstermacher, C. Lasnier, M. Makowski, A. McLean, V. Soukhanovskii, X. Xu
MIT	A. Hubbard, M. Greenwald, J. Hughes, B. LaBombard, J. Terry, D. Whyte, G. Wright
UCSD	J. Boedo, D. Orlov, M. Tillack
UI-UC	D. Ruzic, J.P. Allain. D. Andruczyk
UT-Austin	M. Kotschenreuther, S. Mahajan, P. Valanju
UT-Knoxville	B. Wirth, S. Zinkle, K.F. Gan
UW-Madison	O. Schmitz, K. Flesch, G. McKee, Z. Yan

A. Loarte & R. Pitts (ITER Org.), H. Urano & N. Oyama (JAEA) G. Huijsmans (CEA), S. Sabbagh (Columbia U.), K. Tritz (Johns Hopkins U.), L. Zakharov (LiWF), J. Myra (Lodestar), A. Pankin (Tech-X), S. Kubota (UCLA), R. Raman (U. Washington), D. Boyle & A. Fil (Princeton U.), D. Bannerjee & P. Zhu (USTC-China)

Graduate and Postdoctoral advisors and Advisees, and students:

NC State U.	J. Gilligan, O. Hankins (Ph.D. thesis advisors)
Retired	P. Mioduszewski (Postdoctoral fellowship advisor)
Postdoc Advisees	D. Battaglia (PPPL), J-W. Ahn (ORNL), T.K. Gray (ORNL), A. Diallo (PPPL), M. Coury (PPPL), V. Soukhanovskii (LLNL)
Students	J. Surany, V. Ayyala, D. Sukhin, T.K. Gray, D. Boyle, J. Rhoads, B. Meckley
Co-Editors:	T. Rognlien, LLNL

Graduate and Postdoctoral advisors and Advisees:

NC State U. J. Gilligan, O. Hankins (Ph.D. thesis advisors)

Retired P. Mioduszewski (Postdoctoral fellowship advisor)

Robert D. Moser
Department of Mechanical Engineering
Institute for Computational Engineering and Sciences (ICES)
The University of Texas at Austin, 1 University Station, C0200 Austin, Texas 78712
email: rmoser@ices.utexas.edu

Education:

MIT	Mechanical Engineering	B.S.	June 1978
Stanford	Mechanical Engineering	M.S.	June 1981
Stanford	Mechanical Engineering	Ph.D.	June 1984

Professional Experience:

9/09-pres.	Deputy Director, Institute for Computational Engineering and Sciences, University of Texas, Austin, TX
1/05-pres.	Professor of Mechanical Engineering, and Institute for Computational Engineering and Sciences, University of Texas, Austin, TX
6/95-1/05	Professor of Theoretical and Applied Mechanics, University of Illinois, Urbana, IL.
8/99-8/00	Interim Head, Department of Theoretical and Applied Mechanics, University of Illinois, Urbana, IL.
4/87-6/95	Research Scientist, NASA Ames Research Center, Moffett Field CA.
4/85-4/87	Reservoir Engineer, Sohio Petroleum Co., Dallas, TX.
6/84-4/85	Research Scientist, NASA Ames Research Center, Moffett Field CA.

Selected Publications:

Faghihi, D. & Carey, V. & Michoski, C. & Hager, R. & Janhunen, S. & Chang, C-S & Moser, R. D. 2017 A Particle Down-Sampling Method with Application to Multifidelity Plasma Particle-in-Cell Simulations, Under consideration for publication in *Computer Physics Communications*.

Sprague, M., Boldyrev, S., Chang, C., Fischer, P., Grout, R., Gustafson, W., Hittlinger, J., Merzari, E., & Moser, R. D., 2016 Outcomes from the DOE Workshop on Turbulent Flow Simulation at the Exascale, 46th AIAA Fluid Dynamics Conference, *AIAA 2016-3321*.

Wu, S., Angelikopoulos, P., Papadimitriou, C., & Moser, R. D., Koumoutsakos, P. 2016 A hierarchical Bayesian framework for force field selection in molecular dynamics simulations, *Philosophical Transactions of the Royal Society of London A: Mathematical, Physical, and Engineering Sciences*, **374**, 20150032.

McDougall, D., Malaya, N. & Moser, R. D. 2015 The Parallel C++ Statistical Library for Bayesian Inference: QUESO, *Handbook of Uncertainty Quantification*, Springer International Publishing, Switzerland.

Moser, R. D. & Oliver, T. (2015) Validation of Physical Models in the Presence of Uncertainty, *Handbook of Uncertainty Quantification*, Springer International Publishing, Switzerland.

Lee, M. & Moser, R. D. 2015 Direct numerical simulation of turbulent channel flow up to $Re_\tau \approx 5200$, *J. Fluid Mech.*, **774**, 395-415.

Oliver, T., Terejanu, G., Simmons, C., & Moser, R. D. 2014 Validating Predictions of Unobserved Quantities, Computer Methods in Applied Mechanics and Engineering, *CMAME*, **283**, 1310-1335.

Oliver, T., Malaya, N., Ulerich, R. & Moser, R. D. 2014 Estimating Uncertainties in Statistics Computed from Direct Numerical Simulation, *Phys. of. Fluids*, **26**, 035101.

Oliver, T. A. & Moser, R. D. 2012 Accounting for uncertainty in the analysis of overlap layer mean velocity models, *Phys. of Fluids*, **24**, 075108.

Cheung, S. H., Oliver, T. A., Prudencio, E. E., Prudhomme, S. & Moser, R. D. 2011 Bayesian Uncertainty Analysis with Applications to Turbulence Modeling, *Reliability. Eng. System Safety*, **96**, 1137-1149.

Synergistic Activities:

Developed a new advanced course on Uncertainty Quantification (2014)

Reviewer for *Journal of Fluid Mechanics, Journal of Computational Physics, Physics of Fluids, AIAA Journal, Journal of Fluids Engineering, Theoretical and Computational Fluid Dynamics*

Member of AIAA, SIAM, Fellow of APS (DFD)

Chair of the Division of Fluid Dynamics, American Physical Society (2017)

Deputy Director of the Institute for Computational Engineering and Sciences and Director of the Center for Predictive Engineering and Computational Sciences (PECOS) at the Univeristy of Texas at Austin.

Collaborators & Other Affiliatio:

Collaborators & Co-editors: Abbasi, Hasan , Oak Ridge National Lab; Adams, Mark, Columbia; Allen, Mark G., Georgia Tech; Angelikopoulos, Panagiotis, Computational Science & Engineering Laboratory; Babuska, Ivo, University of Texas at Austin; Barone, Matthew, Sandia National Lab; Battaglia, Devon , Princeton; Beaman, Jr., Joseph, University of Texas at Austin; Bell, John, Lawrence Berkeley National Lab; Biros, George, University of Texas at Austin; Boldyrev, Stanislav, University of Wisconsin-Madison; Brown, Garry, Princeton; Burns, Randal, The Johns Hopkins University; Calise, Anthony, Georgia Tech; Carey, Varis, University of Colorado Denver; Chang, C.S., Princeton; Chang, Henry, University of Delaware; Chen, Jacqueline, Sandia National Lab; Clemens, Noel, University of Texas at Austin; Cummings, Julian, MSC Software; DAzevedo, Ed, Oak Ridge National Lab; Dawson, Clint, University of Texas at Austin; Debusschere, Bert, Sandia National Lab; Demkowicz, Leszek, University of Texas at Austin; Eldred, Michael, Sandia National Lab; Estep, Donald, Colorado State University; Eyink, Gregory, The Johns Hopkins University; Ezekoye, Ofodike, University of Texas at Austin; Feng, Yusheng, University of Texas at San Antonio; Fischer, Paul, University of Illinois at Urbana-Champaign; Gattiker, James, Los Alamos National Laboratory; Ghanem, Roger, University of Southern California; Ghattas, Omar, University of Texas at Austin; Girolami, Mark, Warwick University; Glezer, Ari, Georgia Tech; Goldstein, David, University of Texas at Austin, Graham, Jason, The Johns Hopkins University; Greenwald, Martin, MIT; Grout, Ray, National Renewable Energy Laboratory; Gunzburger, Max, Florida State; Gustafson, William, PNNL; Hanrahan, Pat, Stanford University; Hesthaven, Jan, Brown University; Higdon, Dave, Los Alamos National Lab; Hittlinger, Jeffery, Lawrence Livermore National Laboratory, Heinkenschloss, Matthias, Rice University; Howell, John, University of Texas at Austin; Hughes, Thomas J.R., University of Texas at Austin; Jee, Solkeun, Gwanju Institute of Science and Technology; Jimenez, Javier, Universidad Politecnica de Madrid; Juanes, Ruben, MIT; Kanov, Kalin, Bloomberg LP; Kenny, Joseph, Sandia National Lab; Kirk, Benjamin, NASA; Klasky, Scott, Oak Ridge National Lab; Knio, Omar, Duke University; Koumoutsakos, Petros, ETH Zurich; Kritz, Arnold, Lehigh University; Lalescu, Cristian, The Johns Hopkins University; Leonard, Tony, CalTech; Ling, Julia, Sandia National Lab; Majumdar, Amitava, San Diego Supercomputer Center; Mallick, Bani, Texas A&M University; Martin, Michael, Department of Energy; Marzouk, Youssef, MIT; Massa, Luca, University of Texas at Arlington; McCormick, Patrick, Los Alamos National Lab; McDougall, Damon, University of Texas at Austin; Meneveau, Charles, The Johns Hopkins University; Merzari, Elia, Argonne National Labs; Najm, Habib, Sandia National Lab; Oden, J.

Tinsley, University of Texas at Austin; Oliver, Todd, University of Texas at Austin; Papadimitriou, Christos, University of California at Berkeley; Parashar, Manish , Rutgers; Parker, Scott, University of Colorado Boulder; Pascucci, Valerio, University of Utah; Pearlstein, Arne, University of Illinois at Urbana-Champaign; Philpott, Andrew, University of Auckland; Prudencio, Ernesto, Schlumberger; Quinlan, Dan, Lawrence Livermore National Lab; Raman, Venkat, University of Michigan; Riley, James, University of Washington; Roberts, Nate, Argonne National Labs; Rodin, Greg, University of Texas at Austin; Samatova, Nagiza, North Carolina State University; Schulz, Karl, Intel; Schwan, Karsten, Georgia Tech; Shalf, John, Lawrence Berkeley National Lab; Shephard, Mark, Rensselaer; Shoshani, Arie, Lawrence Berkeley National Lab; Sillero, Juan, McKinsey & Company; Simmons, Christopher, University of Texas at Austin; Sprague, Michael, National Renewable Energy Laboratory; Stogner, Roy, University of Texas at Austin; Stuart, Andrew, Cal Tech; Szalay, Alex, The Johns Hopkins University; Taleff, Eric, University of Texas at Austin; Tempone, Raul, King Abdullah University of Science and Technology; Tynan, George, University of California San Diego; Varghese, Philip, University of Texas at Austin; Wang, Qiqi, MIT; Wilcox, Karen, MIT; Williamson, Rodney, University of Texas at Austin; Worley, Patrick, Oak Ridge National Lab; Yang, Xiang, The Johns Hopkins University; Yeung, P.K., Georgia Tech; Ying, Lexing, Stanford University

Advisors: Parviz Moin, Stanford; William R. C. Reynolds, Stanford

Thesis & Postdoc Advisees:

Alawieh, Leen, Lawrence Berkeley National Lab; Bauman, Paul, University of Buffalo; Bhattacharya, Amitabh, Indian Institute of Technology, Bombay; Borodai, Stanislov, GlobalSim, Inc.; Chan, Jesse, Rice University; Chang, Henry, University of Delaware; Cheung, Sai Hung, Nanyang Technological University; Das, Arup, Unknown; Deram, Nora, Enthought Scientific Computing Solutions; Doyeux, Vincent, IMFT Toulouse; Ellis, Truman, Sandia National Labs; Estacio-Hiroms, Kemelli, University of North Texas; Fitzsimmons, Nicholas, Texas Advanced Computing Center; Garg, Vikram, University of Texas at Austin; Guarini, Stephen, Riverbed Technology; Haering, Sigfried, University of Texas at Austin; Hira, Jeremy, CFD-Adapco; Hossain, Shaolie, The Methodist Hospital Research Institute; Jagodzinski, Jeremy, University of Texas at Austin; Jee, Sol Keun, Gwanju Institute of Science and Technology; Kwok, Wai-Yip, Synopsys, Inc.; Langford, Jacob, Unknown; Lee, Myoungkyu, University of Texas at Austin; Lee, Sei Young, Yonsei University; Lopez, Vanessa, IBM; Lopez-Mejia, Omar Dario, Los Andes University Bogota; Loulou, Patrick, Domtar; Malaya, Nick, AMD; Maurente, Andre, Universidade Federal do Rio Grande do Norte; Miki, Kenji, GE Global Research; Morrison, Rebecca, MIT; Neves, John, Unknown; Panesi, Marco, University of Illinois at Urbana-Champaign; Plessis, Sylvain, University of Texas at Austin; Reinisch, Guillaume, University of Texas at Austin; Sharma, Manu, Infinity Aerospace; Terejanu, Gabriel, University of South Carolina; Topalian, Victor, University of Texas at Austin; Ulerich, Rhys, Two Sigma Investments; Venugopal, Prem, GE Global Research; Volker, Stefan, Unknown; West, Anthony, Sun Microsystems; Yang, Shan, Microsoft; Zandonade, Paulo, Unknown; Zhou, Jun, CBM International, Inc.

Biographical Sketch

James R. Myra

Education

University of Maryland: Ph.D., Physics (1979)

- Doctoral Thesis: “Nonlinear electrostatic ion cyclotron waves,” Thesis Advisor: C.S. Liu

University of British Columbia: M.S., Physics (1977)

- Recipient of National Research Council of Canada’s 1967 Science Scholarship (five-year portable graduate scholarship)
- Master’s Thesis: “Stimulated Scattering in a Plasma Filling an Optical Cavity,” Thesis Advisor: J. Meyer

Queen’s University: B.Sc., Mathematical Physics (1975)

- Recipient of Alumni National Scholarship and Queen’s graduation medals for top grades in Mathematics and Physics

Research and Professional Experience

Lodestar Research Corporation, (1987 – present)

- Senior Scientist, and President, 2016 – present
- Senior Scientist, and Vice-President, 2003 – 2016
- Senior Scientist, 1987 – 2003
- Technical areas of research: nonlinear interaction of intense ion-cyclotron radio frequency (ICRF) waves with the tokamak edge plasma, wave propagation and resonant heating, high energy particle tails, sheath physics, edge convective cells, fusion ignition physics and runaway electrons. Recent research interests also include: scrape-off-layer turbulence, convective transport by coherent objects, rf-driven sheared-flows, rf propagation in turbulent plasmas, and tokamak physics associated with divertor magnetic geometry.

Science Applications International Corporation, Plasma Research Institute (1979 – 1987)

- Senior Scientist 1983 – 1987
- Staff Scientist, 1979 – 1983
- Technical areas of research: nonlinear plasma waves, linear MHD and micro-stability of tandem mirrors, transport theory and the self-consistent ambipolar potential, the interactions of radio frequency waves with tokamak plasmas for mode stabilization and heating.

Synergistic Activities

- Technical reviewer for numerous plasma physics and fusion energy journals, and research proposals
- PI on several grants with DOE and National Laboratories
- Frequent presenter at national and international conferences
- Edge Coordinating Committee member (2013 - present) and executive secretary (2014 - 2016)
- Sub-panel member, SOL/Divertor Physics FES PMI Workshop (2015)

Biographical Sketch

Recent and selected publications *(from 164 refereed publications and 62 published conf. proceedings)*

"(Review Paper): Recent Theoretical Progress in Understanding Coherent Structures in Edge and SOL Turbulence", S.I. Krasheninnikov, D.A. D'Ippolito, and J.R. Myra, J. Plasma Physics **74**, 679 (2008).

"(Review Paper) Convective transport by intermittent blob-filaments: Comparison of theory and experiment," D.A. D'Ippolito, J.R. Myra and S.J. Zweben, Phys. Plasmas **18**, 060501 (2011).

"Reduced model simulations of the scrape-off-layer heat-flux width and comparison with experiment," J. R. Myra, D. A. Russell, D. A. D'Ippolito, J.-W. Ahn, R. Maingi, R. J. Maqueda, D. P. Lundberg, D. P. Stotler, S. J. Zweben, J. Boedo, M. Umansky, and NSTX Team, Phys. Plasmas **18**, 012305 (2011).

"Turbulent transport regimes and the scrape-off layer heat flux width," J. R. Myra, D. A. D'Ippolito, and D.A. Russell, Phys. Plasmas **22**, 042516 (2015).

"Edge sheared flows and the dynamics of blob-filaments," J.R. Myra, W.M. Davis, D.A. D'Ippolito, B. LaBombard, D.A. Russell, J.L. Terry and S.J. Zweben, Nucl. Fusion **53**, 073013 (2013).

"Eigenvalue Solver for Fluid and Kinetic Plasma Models in Arbitrary Magnetic Topology," D. A. Baver, J. R. Myra and M. V. Umansky, Comm. Comp. Phys. 20, 136 (2016).

"Blob structure and motion in the edge and SOL of NSTX," S. J. Zweben, J. R. Myra, W. M. Davis, D. A. D'Ippolito, T. K. Gray, S. M. Kaye, B. P. LeBlanc, R. J. Maqueda, D. A. Russell, D. P. Stotler and the NSTX-U Team, Plasma Phys. Control. Fusion **58**, 044007 (2016).

"Analytical and numerical study of the transverse Kelvin-Helmholtz instability in tokamak edge plasmas," J. R. Myra, D. A. D'Ippolito, D. A. Russell, M. V. Umansky and D. A. Baver, J. Plasma Phys. **82**, 905820210 (2016).

"Mean flows and blob velocities in scrape-off layer (SOLT) simulations of an L-mode discharge on Alcator C-Mod, " D. A. Russell, J. R. Myra, D. A. D'Ippolito, B. LaBombard, J. W. Hughes, J. L. Terry, and S. J. Zweben, Phys. Plasmas **23**, 062305 (2016).

"Theory based scaling of edge turbulence and implications for the scrape-off layer width," J. R. Myra, D. A. Russell, and S. J. Zweben, Phys. Plasmas **23**, 112502 (2016).

Collaborators and Co-editors: D. A. Baver (Lodestar), J. A. Boedo (UCSD), J. M. Canik (ORNL), C.-S. Chang (PPPL), R. M. Churchill (PPPL), W. M. Davis (PPPL), T. K. Gray (ORNL), B. Gui (IPP Hefei), S. M. Kaye (PPPL), I. Keramidas-Charidakos (Univ. Colorado), H. Kohno (Kyushu), B. LaBombard (MIT), R. Ochoukov (Max-Planck), S. E. Parker (Univ. Colorado), M. L. Reinke (ORNL), D. A. Russell (Lodestar), D. N. Smithe (Tech-X), D. P. Stotler (PPPL), J. L. Terry (MIT), M. V. Umansky (LLNL), D. G. Whyte (MIT), X. Q. Xu (LLNL), S. J. Zweben (PPPL).

Graduate and Postdoctoral Advisors: J. Meyer (Univ. British Columbia - retired), C.S. Liu (U. Maryland - retired)

Graduate and Postdoctoral Advisees: (none)

<u>*Two-Page Curriculum Vitae*</u>*:* **Scott E. Parker**

Current Position

Professor, Department of Physics
Campus Box 390
University of Colorado
Boulder, CO 80309

Phone: 303-492-3292 Fax: 303-492-0642 email: sparker@colorado.edu

Education

5/90 Ph.D. Engineering Science
University of California, Berkeley
Major fields: Plasma Physics, Numerical Methods, Nuclear Engineering
Research Advisor: Professor C. K. Birdsall

5/85 B.S. Mathematics and B.S. Nuclear Engineering
University of Wisconsin, Madison

Professional Experience

8/2008-present Professor: Department of Physics, University of Colorado, Boulder. Research in computational plasma physics, plasma turbulence and transport, kinetic-MHD modeling, and magnetospheric plasmas.

1/07-7/09 Director: Center for Integrated Plasma Studies University of Colorado, Boulder. Manage Center, stewardship of plasma physics research and education on campus.

9/92-8/96 Staff Research Physicist: Theoretical Division, Princeton Plasma Physics Laboratory, Princeton University. Research in gyrokinetic theory and simulation, kinetic-MHD hybrid simulation, massively-parallel computing and scientific visualization.

Awards and Fellowships

Oscar Buneman Award for Scientific Visualization of Plasmas (2015)
Boulder Faculty Asssembly Faculty Recognition Award (2014)
Fellow, American Physical Society (2008)
Department of Energy Plasma Physics Junior Faculty Development Award (1997-2000)
Department of Energy Fusion Postdoctoral Research Fellowship (1990-1992)
University of California Regents Fellowship (1985-1986)
Kaiser Engineers Quadrex Fellowship (1985-1986)
Graduation with Distinction (top 15% of class), University of Wisconsin, Madison (1985)
Engineering Scholars Program, University of Wisconsin, Madison (1983-1985)
Deans Honors List, College of Engineering, University of Wisconsin, Madison (1982-1985)

Memberships

American Physical Society
Tau Beta Pi Engineering Honor Society

Recent Published Journal Articles *(76 total published journal articles)*

1. “Low frequency fully kinetic simulation of the toroidal ion temperature gradient instability,” B. J.

Sturdevant, Y. Chen, S. E. Parker, *in press* Phys. Plasmas (2017).

2. “Particle-in-cell δf gyrokinetic simulations of the microtearing mode,” J. Chowdhury, Y. Chen, W. Wan, S.E. Parker, W. Guttenfelder and J.M. Canik, Phys. Plasmas **23** 012513 (2016).
3. “An implicit delta-f particle-in-cell method with sub-cycling and orbit averaging,” B. J. Sturdevant, S. E. Parker, Y. Chen, B. B. Hause, Journal of Computational Physics **316** 519-533 (2016).
4. “Finite time step and spatial grid effects in δf simulation of warm plasmas,” B. J. Sturdevant, S. E. Parker, Journal of Computational Physics **305**, 647–663 (2016).
5. “Effects of the magnetic equilibrium on gyrokinetic simulations of tokamak microinstabilities,” W. Wan Y. Chen, S. Parker, R. Groebner, Phys. Plasmas **22** 063502 (2015).
6. “Finite Larmor radius effects on the (m=2, n=1) cylindrical tearing mode,” Y. Chen, J. Chowdhury, S. Parker, W. Wan, **22** 063502 Phys. Plasmas 22 04211 (2015).
7. “Study of the L-mode tokamak plasma “shortfall” with local and global nonlinear gyrokinetic delta-f Particle-in-cell simulation,” J. Chowdhury, W. Wan, Y. Chen, S. Parker, R. Groebner, C. Holland, N. Howard, “” Phys. Plasmas **21** 112403 (2014).
8. “Comparison of kinetic and extended magnetohydrodynamic computational models for the linear ion temperature gradient instability in slab geometry,” D. D. Schnack, J. Cheng, D. C. Barnes and S. E. Parker, Phys. Plasmas **20** 062106 (2013).
9. “Gyrokinetic simulations of reverse shear Alfvén eigenmodes in DIII-D plasmas, Y. Chen, T. Munsat,” S. E. Parker, W. W. Heidbrink, M. A. Van Zeeland, B. J. Tobias and C. W. Domier, Phys. Plasmas **20** 012109 (2013).
10. “A verification of the gyrokinetic microstability codes GEM, GYRO, and GS2,” R. V. Bravenec, Y. Chen, J. Candy, W. Wan and S. Parker, Phys. Plasmas **20** 104506 (2013).

Recent Published Proceedings, Invited Talks

1. “Gyrokinetic study of edge blobs and divertor heat-load footprint,” S. Parker (Invited Speaker), C. Chang, J. Boedo, R. Hager, S. Ku, J. Lang R. Maingi, D. Stotler, S. Zweben, 25th International Atomic Energy Agency (IAEA) Fusion Energy Conference, 10/13-10/18/2014, St. Petersburg, Russia. Proceedings published by IAEA, Paper TH/2 -3.
2. “Nonlinear gyrokinetic simulations of the tokamak edge pedestal,” S. Parker (Invited Speaker), W. Wan, Y. Chen, J. Chowdhury International Sherwood Fusion Theory Conference, 3/23-3/26/2014, San Diego, CA.
3. “Global Gyrokinetic Simulations of the Dominant High-n and Intermediate-n Instabilities in the H-Mode Tokamak Edge Pedestal,” (Invited Speaker), American Physical Society – Division of Plasma Physics Meeting, Providence, RI, Bull. Am. Phys. Soc. 57 372 (2012).
4. “Bootstrap current destabilization of the kinetic ballooning mode in the tokamak edge pedestal,” Scott Parker (Invited Speaker), W. Wan, Y. Chen, Plenary Talk, U.S. Transport Task Force Workshop, Annapolis, MD, April 10-13, 2012.
5.

Collaborators, Graduate and Postdoctoral Advisors and Advisees

W. Lee, C.S. Chang, S. Ku, R. Hager, PPPL; P; C. Kim Far-Tech; R. Groebner, GA, J. Chowdhury, W. Wan, Y. Chen, I. Keramidas Univ. of Colorado, Boulder, S. Jones, American University of Antigua, S. Vadlamiani, Paratools, Inc., J. Lang, Intel Corp., J. Cheng, Brion Inc., J. Myra, Lodestar Corp.

Synergistic Activities

Executive Committee, American Physical Society Division of Computational Physics (2012-2014)Chair Elect, Edge Coordinating Committee, Office of Fusion Energy Sciences, U.S. DOE (2015-2017)Chair, Executive Committee, International Conference on the Numerical Simulation of Plasmas (2014-2017)Co-Editor, J. of Computational Physics, Special Issue, “Advances in Numerical Simulation of Plasmas” (2016)Co-Guest Editor, Physics of Plasmas, Special Topic Issue, “Gyrokinetic Particle Simulation” (2016/2017)

Curriculum Vita
David Arthur Russell

Education and Training

Undergraduate: Yale College, Mathematics and Physics, B.S. 1975

Graduate: Cornell University, Electrical Engineering, Ph.D. 1981

Research Associate:	Department of Astro-Geophysics University of Colorado, Boulder CO 1980 – 1984
Postdoctoral Fellow:	Theoretical Division, Applied Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos NM 1984 - 1987

Research and Professional Experience

1989 – *present*:	Scientist Lodestar Research Corporation, Boulder CO; Theoretical and computational studies of plasma turbulence in the contexts of magnetic fusion energy, laser-plasma interactions and ionospheric heating experiments
1987 – 1989:	Consultant Theoretical Division, LANL, Los Alamos NM *and* Mathematics Department, U. of Arizona, Tucson AZ; Nonlinear-wave equation studies

Synergistic Activities

Manuscript reviewer for *Physics of Plasmas* and *Nuclear Fusion*
Contributor and presenter at plasma physics and fusion energy conferences
Developer of turbulence models in the context of laser-plasma interactions

Publications

Blob structure and motion in the edge and SOL of NSTX, S. J. Zweben, J. R. Myra, W. M. Davis, D. A. D'Ippolito, T. K. Gray, S. M. Kaye, B. P. LeBlanc, R. J. Maqueda, D. A. Russell, D. P. Stotler and the NSTX-U Team, Plasma Phys. Control. Fusion **58**, 044007 (2016).

Theory based scaling of edge turbulence and implications for the scrape-off layer width, J. R. Myra, D. A. Russell and S. J. Zweben, Phys. Plasmas **23**, 112502 (2016).

Analytical and numerical study of the transverse Kelvin-Helmholtz instability in tokamak edge plasmas, J. R. Myra, D. A. D'Ippolito, D. A. Russell, M. V. Umansky and D. A. Baver, J. Plasma Phys. **82**, 905820210 (2016).

Mean flows and blob velocities in scrape-off layer (SOLT) simulations of an L-mode discharge *on Alcator C-Mod*, D. A. Russell, J. R. Myra, D. A. D'Ippolito, B. LaBombard, J. W. Hughes, J. L. Terry and S. J. Zweben, Phys. Plasmas **23**, 062305 (2016).

Modeling the effect of lithium-induced pedestal profiles on scrape-off-layer turbulence and the heat flux width, D. A. Russell, D. A. D'Ippolito, J. R. Myra, J. M. Canik, T. K. Gray, and S. J. Zweben, Phys. Plasmas **22**, 092311 (2015).

Edge sheared flows and blob dynamics, J. R. Myra, W.M. Davis, D. A. D'Ippolito, B. LaBombard, D. A. Russell, J. L. Terry, and S. J. Zweben, Nucl. Fusion **53**, 073013 (2013).

Effect of parallel currents on drift-interchange turbulence: Comparison of simulation and experiment, D. A. D'Ippolito, D. A. Russell, J. R. Myra, S. C. Thakur, G. R. Tynan and C. Holland, Phys. Plasmas **19**, 102301 (2012).

Numerical investigation of edge plasma phenomena in an enhanced D-alpha discharge at Alcator C-Mod: Parallel heat flux and quasi-coherent edge oscillations, D. A. Russell, D. A. D'Ippolito, J. R. Myra, B. LaBombard, J. L. Terry and S. J. Zweben, Phys. Plasmas **19**, 082311 (2012).

Diffusive-convective transition for scrape-off layer transport and the heat-flux width, J.R. Myra, D. A. Russell and D. A. D'Ippolito, Plasma Phys. Control. Fusion **54**, 055008 (2012).

Identification of Potential Conflicts of Interest or Bias in Selection of Reviewers

Collaborators and Co-editors:

J. M. Canik, Oak Ridge National Laboratory, Oak Ridge, TN 37831
W. M. Davis, Princeton Plasma Physics Laboratory, Princeton, NJ 08543
D. A. D'Ippolito, Lodestar Research Corporation, Boulder, CO 80301
D. F. DuBois, Los Alamos National Laboratory, Los Alamos, NM 87545
T. K. Gray, Oak Ridge National Laboratory, Oak Ridge, TN 37831
C. Holland, Center for Momentum Transport and Flow Organization, San Diego, CA 92093
J. W. Hughes, Plasma Science and Fusion Center, Cambridge, MA 02139
S. M. Kaye, Princeton Plasma Physics Laboratory, Princeton, NJ 08543
B. LaBombard, Plasma Science and Fusion Center, Cambridge, MA 02139
B. P. LeBlanc, Princeton Plasma Physics Laboratory, Princeton, NJ 08543
R. Maingi, Oak Ridge National Laboratory, Oak Ridge, TN 37831
A. V. Maximov, Laboratory for Laser Energetics, Rochester, NY 14623
R. J. Maqueda, Princeton Plasma Physics Laboratory, Princeton, NJ 08543
J. F. Myatt, Laboratory for Laser Energetics, Rochester, NY 14623
J. R. Myra, Lodestar Research Corporation, Boulder, CO 80301
R. W. Short, Laboratory for Laser Energetics, Rochester, NY 14623
D. P. Stotler, Princeton Plasma Physics Laboratory, Princeton, NJ 08543
J. L. Terry, Plasma Science and Fusion Center, Cambridge, MA 02139
S. C. Thakur, Center for Momentum Transport and Flow Organization, San Diego, CA 92093
G. R. Tynan, Center for Momentum Transport and Flow Organization, San Diego, CA 92093

M. Umansky, Lawrence Livermore National Laboratory, Livermore, CA 94550
H. X. Vu, University of California at San Diego, La Jolla, CA 92093
J. Zhang, Laboratory for Laser Energetics, Rochester, NY 14623
S. J. Zweben, Princeton Plasma Physics Laboratory, Princeton, NJ 08543

Graduate and Postdoctoral Advisors:

Edward Ott, University of Maryland, College Park, MD
Martin V. Goldman, University of Colorado, Boulder, CO
Donald F. DuBois, Los Alamos National Laboratory (ret.), Los Alamos, NM

MARK S. SHEPHARD
Samuel A. and Elisabeth C. Johnson, Jr. Professor of Engineering
Scientific Computation Research Center
Rensselaer Polytechnic Institute, Troy, NY 12180-3590
518-276-8044, shephard@rpi.edu

Education and Training:
Clarkson College, Civil Engineering, B.S., 1974
Cornell University, Structural Engineering, Ph.D., 1979

Research and Professional Experience:

1996-present	Professor of Computer Science, Rensselaer Polytechnic Institute
1993-present	Samuel A. and Elisabeth C. Johnson, Jr. Professor of Engineering
1990-present	Director, Scientific Computation Research Center, Rensselaer
1989, 1991	Acting Chairman (while Chairman on sabbatical leave), Civil Engng., RPI
1987-present	Professor, Civil Engineering, Rensselaer Polytechnic Institute
1987-present	Professor, Mechanical Engng, Aeronautical Engng. & Mechanics, RPI
1986-1988	Acting Director, Center for Interactive Computer Graphics, RPI
1986-1987	Associate Professor, Mechanical Engng., Aero. Engng. & Mechanics, RPI
1985	Visiting Research Fellow, General Electric Corporate R&D
1984-1987	Associate Professor, Civil Engineering, Rensselaer Polytechnic Institute
1979-1984	Assistant Professor, Civil Engineering, Rensselaer Polytechnic Institute

Ten Recent Relevant Publications:
1. F. Zhang, R. Hager, S.-H. Ku, C.-S. Chang, S.C. Jardin, N.M. Ferraro, E. S. Seol, E. Yoon and M.S. Shephard, "Mesh Generation for Confined Fusion Plasma Simulation", *Engineering with Computers*, 32:285-293, 2016.
2. Ferraro, N.M., Jardin, S. C., Lao, L.L., Shephard, M., Zhang, F., "Multi-Region Approach to Free-Boundary Three-Dimensional Tokamak Equilibria and Resistive Wall Instabilities", *Physics of Plasmas*, 23:056114 (13 pages), 2016
3. D.A. Ibanez, I. Dunn, and M.S. Shephard, "Hybrid MPI-thread parallelization of adaptive mesh operations", *Parallel Computing,* 55:133-143, 2016.
4. E. Ban, V.H. Barocas, M.S. Shephard and R.C. Picu, "Softening in Random Networks of Non-Identical Beams", *Journal of Mechanics Physics Solids*, 87:38-50, 2016.
5. E. Ban, V.H. Barocas, M.S. Shephard and R.C. Picu, "Effect of fiber crimp on the elasticity of random fiber networks with and without embedding matrices", *Journal of Applied Mechanics*, 83:041008 (7 pages), 2016.
6. D.A. Ibanez, E.S. Seol, C.W. Smith and M.S. Shephard, "PUMI: Parallel Unstructured Mesh Infrastructure", *ACM Transactions on Mathematical Software*, 42(3): Article 17 (28 pages), 2016.
7. Xu, X.G., Liu, T., Su, L., Du., X., Riblett, M., Wei J., Gu, D., Carothers, C.D.; Shephard, M.S., Brown, F.B., Kalra, M.K., Liu, B, "ARCHER, a new Monte Carlo software tool for emerging heterogeneous computing environments", *Annals of Nuclear Engineering*, 82:2-9, Aug. 2015. DOI 10.1016/j.anucene.2014.08.062

8. K.C. Chitale, O. Sahni, M.S. Shephard, S. Tendulkar and K.E. Jansen, "Anisotropic adaptation for transonic flows with turbulent boundary layers", *AIAA Journal*, 53(2):277-295, 2015.
9. M.S. Shephard, C.W. Smith, D.A. Ibanez, B. Granzow, M.W. Beall, and S. Tendulkar, "Developing scalable components for massively parallel adaptive simulations", *Proc. NAFEMS World Congress,* San Diego, CA, 19 pages, 2015.
10. M. Rasquin, C. Smith, K. Chitale, E.S. Seol, B. Matthews, J. Martin, O. Sahni, R. Loy, M.S. Shephard and K.E. Jansen, "Scalable fully implicit finite element flow solver with application to high-fidelity flow control simulations on a realistic wing design", *Computing in Science and Engineering*, 16(6):13-21, 2014.

Synergistic Activities

Technology Development and Transfer: Rensselaer's Scientific Computation Research Center (SCOREC) has a long history of developing and transferring advanced automated, adaptive and parallel simulation technologies to government laboratories, industry and universities. Forty-six companies have supported the development of automated adaptive finite element software. Several have commercialized component of technologies. SCOREC graduates formed Simmetrix Inc. that provides software components for simulation-based design that are being used by CAD, CAE and manufacturing companies.

Educational: Developed three graduate courses on finite element methods and a project level interdisciplinary undergraduate/graduate course in computational science.

Editor: Engineering with Computers

Editorial Board: Computer Methods in Applied Mechanics and Engineering, Int. J. for Numerical Methods in Engineering, J. of Multiscale Computational Engineering, Computers & Structures, Integrated Computer-Aided Engineering

Professional Activities: U.S. Association for Computational Mechanics, Fellow and Past President and winner of the John von Neumann Metal and Computational Science Award; Int. Association for Computational Mechanics, Fellow; ASME, Fellow; AIAA, Associate Fellow; American Academy of Mechanics, Member; SIAM, Member

Collaborators (Non-RPI)

V.H. Barocas, U. Minn.	M.W. Beall, Simmetrix	C.S. Chang, PPPL
K. Devine, Sandia National Labs.	L. Diachin, LLNL	N. Ferraro, PPPL
T. Furlani, U. at Buffalo	R. Hager, PPPL	G.A. Hansen, Sandia Nat. Labs.
K.E. Jansen, U. Colorado	S. Jardin, PPPL	C. Kees; US Army ERDC
O. Klaas, Simmetrix	T. Kolev, LLNL	S.-H. Ku, PPPL
F. Streitz, LLNL	S. Tendulkar, Simmetrix	

Graduate Students and Postdoctoral Scholars

D. Ibanez, Sandia Nat. Labs.	Q. Lu, Altair	M. Rasquin, Cenaero
D. Zaide; Synopsys	F. Zhang; ANSYS	M. Zhou; Simulia

Dr. Daren Stotler
Princeton Plasma Physics Laboratory, Princeton University
Princeton NJ 08543-0451
Phone: 609-243-2063, Email: dstotler@pppl.gov

Education

- Ph.D., Applied Physics, University of Texas at Austin, Austin, TX, 1986
- B.A. (Summa cum Laude), Physics / Materials Science, Rice University, Houston, TX, 1981

Professional Experience

- Research Staff, Princeton Plasma Physics Laboratory, Princeton University, Princeton, NJ, 1986-present (currently Principal Research Physicist)

Synergistic Activities

- Co-developer and maintainer of DEGAS 2 neutral gas transport code
- Member of the Partnership for Edge Physics Simulation (EPSI) SciDAC project (C. S. Chang, P.I.), 2012-present
- Member of Center for Plasma Edge Simulation (CPES) proto-FSP SciDAC project (C. S. Chang, P.I.), 2006-2011
- Member, Edge Coordinating Committee, 2004-2014
- Member, U. S. Burning Plasma Organization task group on verification and validation, 2006-2008

Selected Publications

D. P. Stotler, D. J. Battaglia, R. Hager, K. Kim, T. Koskela, G. Park, and M.L. Reinke, "Kinetic Neoclassical Calculations of Impurity Radiation Profiles", *Nucl. Mater. Energy* (in press, 2017) [doi: 10.1016/j.nme.2016.12.021].

D. P. Stotler, F. Scotti, R. E. Bell, A. Diallo, B. P. LeBlanc, M. Podesta, A.L. Roquemore, and P.W. Ross, Phys. Plasmas 22, 082506 (2015) [doi: 10.1063/1.4928372].

D. P. Stotler, C. S. Chang, S. H. Ku, J. Lang and G. Park, "Energy Conservation Tests of a Coupled Kinetic Plasma-Kinetic Neutral Transport Code", *Comput. Sci.Disc.* **6**, 015006 (2013) [doi: 10.1088/1749-4699/6/1/015006].

D. P. Stotler, C. S. Chang, S. H. Ku, J. Lang and G. Y. Park, "Pedestal Fueling Simulations with a Coupled Kinetic Plasma-Kinetic Neutral Transport Code", *J. Nucl. Mater.* **438**, S1275 (2013) [doi: 10.1016/j.jnucmat.2013.01.046].

B. Cao, D.P. Stotler, S.J. Zweben, M. Bell, A. Diallo and B. Leblanc, "Comparison of Gas Puff Imaging Data in NSTX with the DEGAS 2 Simulation", *Fusion Sci. Tech.* **64**, 29 (2013).

D. P. Stotler, J. Boedo, B. LeBlanc, R. J. Maqueda, and S. J. Zweben, "Progress Towards the Validation of Models of the Behavior of Neutral Helium in Gas Puff Imaging Experiments", *J. Nucl. Mater.* **363-365**, 686 (2007) [doi:10.1016/j.jnucmat.2007.01.276].

D. P. Stotler, C. S. Pitcher, C. J. Boswell, T. K. Chung, B. LaBombard, B. Lipschultz, J. L. Terry, and R. J. Kanzleiter, "Modeling of Alcator C-Mod Divertor Baffling Experiments", J. Nucl. Mater. 290-293, 967 (2001) [doi: http://dx.doi.org/10.1016/S0022-3115(00)00542-0].

D. P. Stotler, C. F. F. Karney, M. E. Rensink, and T. D. Rognlien, "Coupling of Parallelized DEGAS 2 and UEDGE Codes", *Contrib. Plasma Phys.* **40**, 221 (2000) [doi: 10.1002/1521-3986(200006)40:3/4<221::AID-CTPP221>3.0.CO;2-L].

Collaborators

S. Baek (MIT), D. Battaglia (PPPL), R. Bell (PPPL), B. Cao (Institute of Plasma Physics, Hefei, China), C. S. Chang (PPPL), R. M. Churchill (PPPL), A. Diallo (PPPL), R. Dey (IPR), A. Dimits (LLNL), E. Granstedt (TAE), B. Grierson (PPPL), R. Hager (PPPL), M. Jaworski (PPPL), I. Joseph (LLNL), K. Kim (KAIST), T. Koskela (LBNL), P. Krstic (Stony Brook), S. Ku (PPPL), J. Lang (Intel), B. LeBlanc (PPPL), L. LoDestro (LLNL), R. J. Maqueda (X Science, Princeton, NJ), J. R. Myra (Lodestar Research Corp.), G. Park (NFRI), S. E. Parker (U. of Colorado, Boulder), R. Raman (U. of Washington), M. Reinke (ORNL), M. Rensink (LLNL), D. A. Russell (Lodestar Research Corp.), F. Scotti (LLNL), Y. Sechrest (Nova Photonics), J. L. Terry (MIT), M. Umansky (LLNL), W. Wan (U. of Colorado, Boulder), S. J. Zweben (PPPL)

Students & Advisors

H. L. Berk (U. of Texas), T. Abrams (GA), M. Buttolph (Cornell U.), E. Granstedt (TAE), J. B. Kallmann (LLNL), J. Nichols (PPPL), J. Schwartz (PPPL)

George R. Tynan, PhD
Professor of Engineering Science
Department of Mechanical and Aerospace Engineering
University of California San Diego
9500 Gilman Drive
La Jolla CA 92093 USA
office: +1.858.534.9724
email: gtynan@ucsd.edu

i. Education and Training

1991 PhD, Engineering Science, Department of Mechanical, Aerospace and Nuclear Engineering, UCLA
1987 MS, Engineering UCLA
1983 BS Aerospace Engineering, California State Polytechnic Universit

ii. Research and Professional Experience

2004-Present	*Professor of Engineering Science*, UCSD MAE Department
2001-2004	Associate Professor, UCSD MAE Department
1999-2001	Assistant Professor, UCSD MAE Department
1998-1999	Research Scientist, UCSD
1996-1998	Member of Technical Staff, Trikon Technologies
1991-1995	Assistant Research Engineer, UCLA

iii. Publications

1. Xu, G. S.; Wan, B. N.; Wang, H. Q.; Guo, H. Y.; Zhao, H. L.; Liu, A. D.; Naulin, V.; Diamond, P. H.; Tynan, G. R.; Xu, M.; Chen, R.; Jiang, M.; Liu, P.; Yan, N.; Zhang, W.; Wang, L.; Liu, S. C.; Ding, S. Y., First Evidence of the Role of Zonal Flows for the L-H Transition at Marginal Input Power in the EAST Tokamak. Physical Review Letters **2011,** *107* (12).
2. Xu, M.; Tynan, G. R.; Diamond, P. H.; Manz, P.; Holland, C.; Fedorczak, N.; Thakur, S. C.; Yu, J. H.; Zhao, K. J.; Dong, J. Q.; Cheng, J.; Hong, W. Y.; Yan, L. W.; Yang, Q. W.; Song, X. M.; Huang, Y.; Cai, L. Z.; Zhong, W. L.; Shi, Z. B.; Ding, X. T.; Duan, X. R.; Liu, Y.; Team, H.-A., Frequency-Resolved Nonlinear Turbulent Energy Transfer into Zonal Flows in Strongly Heated L-Mode Plasmas in the HL-2A Tokamak. Physical Review Letters **2012,** *108* (24).
3. Xu, M.; Tynan, G. R.; Diamond, P. H.; Holland, C.; Yu, J. H.; Yan, Z., Generation of a Sheared Plasma Rotation by Emission, Propagation, and Absorption of Drift Wave Packets. Physical Review Letters **2011,** *107* (5).
4. Yan, Z.; Xu, M.; Diamond, P. H.; Holland, C.; Muller, S. H.; Tynan, G. R.; Yu, J. H., Intrinsic Rotation from a Residual Stress at the Boundary of a Cylindrical Laboratory Plasma. Physical Review Letters **2010,** *104* (6).
5. Holland, C.; Yu, J. H.; James, A.; Nishijima, D.; Shimada, M.; Taheri, N.; Tynan, G. R., Observation of turbulent-driven shear flow in a cylindrical laboratory plasma device. Physical Review Letters **2006,** *96* (19).

Synergistic & Community Activities

Chair, US Transport Task Force, 2012-2014

Member, Fusion Energy Sciences Advisory Committee Subpanels – Materials Science & International Collaborations, Sept 2011-Jan 2012
President, University Fusion Associates President (2008-2010)
Panel Leader, Research Needs Workshop, US DOE Office of Science, 2009
Vice-President, University Fusion Associates (2007-2008)

Identification of Potential Conflict of Interests/Bias in Selection of Reviewers

Former Students, Postdocs & their Current Affiliation
Eugenio Schuster, Professor, Lehigh University; M. Burin, Professor, Cal State San Marcos Dept of Physics; K. Taylor, Industry; M. Shimada, Ph.D. Current position: Member of Technical Staff, Idaho National Laboratory, Idaho USA. ; L. Cai, Ph.D. Staff Scientist, Southwestern Institute of Physics, Chengdu, China, ; Z. Yan, Ph.D. Research Scientist, Univ. Wisconsin Madison, Min. Xu, Ph.D. *postdoctoral researcher, UCSD*, J. Steven Ross, PhD. Research Staff Scientist, LLNL, Alex N. James, Ph.D., Facebook.com, Bradley Pollock, Ph.D, *Lawrence Postdoctoral Fellow, LLNL*, Dr. Sung Min Yun, Lam Research Corporation; Nael Crocker, PhD, UCLA, Jonathan Yu, Ph.D., Project Scientist, UCSD, C.H. Holland, Ph.D., UCSD; Jeremy Hanna, Ph.D., NRL, Washington DC, Stefan Mueller, Ph.D. BMW Corporation
Nicolas Fedorczak, IFRM-CEA, France, Peter Manz, Ph.D., IPP-Garching, Germany
Min Xu, Southwestern Inst. Of Physics, Chengdu, CHINA, Istvan Cziegler Ph.d., UCSD Postdoc

Current & Recent (last 4 years) Collaborators
Professor Dennis Whyte, MIT
Dr. Lothar Schmitz, UCLA
Dr. Christopher Holland, UC San Diego
Dr. George McKee, UW Madison
Professor Patrick Diamond, UCSD
Dr. Akihida Fujisawa, Kyushu University, Japan
Dr. Siegfried Glenzer, LLNL
Dr. Kimitaka Itoh, Nat. Inst. Fusion Science, Japan
Dr. Dustin Froula, LLE, Univ. of Rochester
Dr. Uli Stroth, IPP, Garching, Germany
Dr. Hantao Ji, PPPL,
Dr. Garrard Conway, IPP, Garching, Germany
Dr. John Rice, MIT
Professor Nasr Ghoniem, UCLA
Professor Cary Forest, UW Madison
Professor Chan Joshi, UCLA
Professor Paul W. Terry, UW Madison
Professor Michael Mauel, Columbia University
Professor Gerald Navratil, Columbia University
Professor Zhihong Lin, UC Irvine
Professor Nic Brummell, UC Santa Cruz
Professor Tobin Munsat, University of Colorado, Boulder

Graduate Advisor: Professor Robert W. Conn (Emeritus)
Awards:
1985 TRW Graduate Fellowship, UCLA
1999 DOE Plasma Physics Junior Faculty Research Award
2010 APS Fellow
2014: Global Expert in Magnetic Fusion, 1000 Talents Program, People's Republic of China

Patrick H. Worley

High Performance Computing Researcher and Computer Performance Engineer

PHWorley Consulting
116 Porter Road
Oak Ridge, TN 37830 USA

Phone: +1 865 386 4813
E-mail: worleyph@gmail.com

Patrick Worley is a computer scientist with over 30 years experience working with high performance computing systems. Dr. Worley's research interests and expertise include (a) parallel algorithm design, implementation, and optimization, (b) performance evaluation of parallel applications and computer systems, including performance data collection and analysis, benchmarking and benchmarking methodology, and performance modeling and prediction, and (c) software and performance engineering, especially empirical methodology and software infrastructure that enables performance portability. He has been the computer performance lead for the XGC plasma microturbulence simulation codes since 2005.

Education and Training

Ph.D.	Computer Science, Stanford University, Stanford, California, 1988
M.S.	Computer Science, Stanford University, Stanford, California, 1983
B.A.	Computer Science and Mathematics, Indiana University, Bloomington, Indiana, 1980

Research and Professional Experience

2016-present	PHWorley Consulting (self-employed)	
1987-2016	Research and Development Staff, Oak Ridge National Laboratory (ORNL)	
	- Distinguished Research and Development Staff	(2014-2016)
	- Senior Research and Development Staff	(2002-2014)
	- Research Staff Member II	(1990-2002)
	- Research Staff Member I	(1987-1990)

Selected Publications

1. P. Worley, E. D'Azevedo, R. Hager, S-H. Ku, E. Yoon, and C-S. Chang. "Balancing Particle and Mesh Computation in a Particle-In-Cell Code," in *Proc. of the 2016 Cray User Group Meeting*, London, UK, May 8 - 12, 2016.
2. R. Hager, E. Yoon, S-H. Ku, E. D'Azevedo, P. Worley, and C-S. Chang. "A fully non-linear multi-species Fokker-Planck-Landau collision operator for simulation of fusion plasmas," *J. of Comp. Phys.,* **315**, pp. 644-660 (2016).
3. D. Bernholdt, R. Lucas, J. Cary, M. Dorr, A. Koniges, O. Meneghini, B. Norris, F. Poli, B. Van Straalen, and P. Worley, "Software Integration and Performance," Section 5.4 in Report of the Workshop on Integrated Simulations for Magnetic Fusion Energy Sciences, eds. P. Bonoli and L. Mcinnes, Department of Energy, pp. 120–130. (https://www.burningplasma.org/resources/ ref/ Workshops2015/IS/ISFusionWorkshopReport.11.12.2015.pdf)
4. A. Mirin and P. Worley, "Improving the Performance Scalability of the Community Atmosphere Model," International Journal for High Performance Computer Applications, Vol. 26 (1), p. 17–30 (2012), first published on July 7, 2011, doi:10.1177/1094342011412630.
5. P. Worley, A. Craig, J. Dennis, A. Mirin, M. Taylor and M. Vertenstein, "Performance of the Community Earth System Model," in *Proceedings of the ACM/IEEE Intl. Conf. for High Performance Computing, Networking, Storage and Analysis (SC11)*, Seattle, WA, November 12-18, 2011.
6. P. Worley, M. Vertenstein, and A. Craig, "Community Climate System Model," in Encyclopedia of Parallel Computing, ed. D. Padua, Springer, p. 342–351 (2011), doi:10.1007/9780387097664376.

7. P. Worley, “The Community Climate System Model,” Ch. 15 in *Performance Tuning of Scientific Applications*, ed. D. Bailey, R. Lucas and S. Williams, Chapman & Hall / CRC Press, Taylor and Francis Group, 2010, pp. 315-338.
8. M. Adams, S. Ku, P. Worley, E. D’Azevedo, J. Cummings and C-S. Chang, “Scaling to 150K cores: recent algorithm and performance engineering developments enabling XGC1 to run at scale,” *Journal of Physics: Conference Series*, **180** (2009) 012036. (*Proc. of SciDAC 2009*, San Diego, CA, July 14-18, 2009.)
9. P. Colella, D. Keyes, P. Worley, J. Candy, L. Chacon, G. Fann, W. Gropp, C. Kamath, V. Pascucci, R. Samtaney, and J. Shalf, “Mathematical and Computational Enabling Technologies,” Chapter 5 in 2007 DOE Fusion Simulation Project Workshop Report, eds. A. Kritz and D. Keyes, Department of Energy, pp. 71–94. (http://www.science.doe.gov/ofes/programdocuments/reports/FSPWorkshopReport.pdf)
10. J. Drake, P. Jones, M. Vertenstein, J. White III, and P. Worley, “Software Design for Petascale Climate Science,” Chapter 7 in Petascale Computing: Algorithms and Applications, ed. D. Bader, Taylor and Francis Group, LLC, December 2007, pp. 125–146.

Selected Synergistic Activities

- Computer Performance Lead for the SciDAC3 project *Center for Edge Physics Simulation* (2012-2016) and the SciDAC2 Fusion Simulation Prototype Center project *Center for Plasma Edge Simulation* (2005-2011)
- Application Engagement Lead for the SciDAC3 *Institute for Sustained Performance, Energy, and Resilience* (2011-2016) and the SciDAC2 *Performance Engineering Research Institute* (2006-2011)
- Lead Principal Investigator for Performance Evaluation and Analysis Consortium (PEAC) End Station INCITE project, 2005-2012; co-PI for PEAC, 2013-2016
- *Parallel Computing*: Subject Area Editor (2006-2009); Associate Editor (2009-2014)

Selected Awards

- Appreciation Award, Office of Science, U.S. Department of Energy (for sustained technical leadership), 2016
- Association for Computing Machinery (ACM) Distinguished Engineer, 2013
- Outstanding Mentor Award, Office of Science, U.S. Department of Energy, 2010

Collaborators and Co-Editors
S. Abbott[9], M. Adams[4], V. Anantharaj[9], R. Archibald[9], D. Bader[5], A. Bennett[9], D. Bernholdt[9], A. Boghozian[16], M. Branstetter[9], G. Brook[19], P. Caldwell[5], P. Cameron-Smith[5], C-S Chang[11], J. Choi[9], E. D'Azevedo[9], S. Ethier[11], K. Evans[9], J. Foucar[14], J. Fyke[6], A. Gaddis[8], S. Ghan[10], C. Golaz[5], L. Grigori[2], J. Hack[9], R. Hager[11], F. Hoffman[9], M. Hoffman[6], R. Jacob[1], D. Jacobsen[3], H. Johansen[4], P. Jones[6], N. Keen[4], J. Kennedy[9], S. Klasky[9], T. Koskela[4], J. Krishna[1], S-H Ku[11], J. Lang[3], L-Y. Leung[10], W. Lipscomb[6], D. Lu[9], R. Lucas[18], M. Maltrud[6], A. Mametjanov[1], S. Mahajan[9], D. Maxwell[9], B. Mayer[9], J. McClean[15], E. Ng[4], M. Norman[9], L. Oliker[4], M. Parashar[13], S. Parker[17], N. Podhorszki[9], S. Price[6], P. Rasch[10], T. Ringler[6], P. Roth[9], A. Salinger[14], J. Sanseverino[9], A. Sarje[4], M. Shepard[12], S. Sreepathi[9], M. Taylor[14], P. Thornton[9], M. Vertenstein[7], J. Vetter[9], D. Wang[9], J. Wolfe[6], S. Xie[11], E. Yoon[12]

[1]Argonne Natl. Lab., [2]INRIA, [3]Intel, [4]Lawrence Berkeley Natl. Lab., [5]Lawrence Livermore Natl. Lab., [6]Los Alamos Natl. Lab., [7]Natl. Center for Atmos. Res., [8]NSI, [9]Oak Ridge Natl. Lab., [10]Pacific Northwest Natl. Lab., [11]Princeton Plasma Physics Lab., [12]Rensselaer Polytechnic Institute, [13]Rutger Univ., [14]Sandia Natl. Lab., [15]Scripps Institute of Oceanography, [16]Stanford Law School, [17]Univ. of Colorado, [18]Univ. of Southern California, [19]Univ. of Tenn.

Graduate and Postdoctoral Advisors:
Joseph Oliger, Stanford University, Ph.D. Advisor (deceased)
Undergraduate and Graduate Advisees: none

Appendix 2 Current and Pending Support

In alphabetical order by name after lead PI:

1. C. S. Chang
2. M. F. Adams
3. V. Carey
4. L. Chacon
5. Y. Chen
6. J. Y. Choi
7. D. Curreli
8. E. D'Azevedo
9. S. Ethier
10. N. M. Ferraro
11. M. Greenwald
12. G. W. Hammett
13. D. R. Hatch
14. C. D. Hauck
15. J. A. F. Hittinger
16. B. Hoffman
17. S. A. Klasky
18. S. Ku
19. R. Maingi
20. R. D. Moser
21. J. R. Myra / D. A. Russell
22. S. E. Parker
23. M. S. Shephard
24. D. P. Stotler
25. G. R. Tynan
26. P. H. Worley

Choong-Seock Chang

Current Support

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES) and Office of Advanced Scientific Computing Research (OASCR)
Project: SciDAC-3 Center for Edge Physics Simulation (EPSI)
Award Amount: $2,090K from FES and $590K from ASCR
Period of Performance: October 1, 2010 – September 30, 2016. Operating on carryover in FY2017.
Annual Level of Effort: 6 months

Sponsor: Department of Energy, Office of Advanced Scientific Computing Research (OASCR) via ORNL
Project: Exascale Computing: High Fidelity Whole Device Modeling
Award Amount: $5,774K
Period of Performance: September 15, 2016 – September 30, 2020
Annual Level of Effort: 3 months

Sponsor: Department of Energy, Office of Advanced Scientific Computing Research (OASCR) via ORNL
Project: Exascale Computing: Co-Design for Particle-in-Cell Technologies
Award Amount: $1,255K
Period of Performance: November 23, 2016 – September 30, 2020
Annual Level of Effort: 1.2 months

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: National Spherical Torus Experiment Upgrade (NSTX-U) – Science
Award Amount: $15,884K Expected in FY2017
Period of Performance: Funded annually
Annual Level of Effort: 0.5 months

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: DIII-D Science
Award Amount: $3,768K Expected in FY2017
Period of Performance: Funded annually
Annual Level of Effort: 0.5 months

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: Advancing the Frontiers of Magnetic Confinement Theory and Simulation
Award Amount: $4,667K Expected in FY2017
Period of Performance: Funded annually
Annual Level of Effort: 0.8 months

Pending Support

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES) and Office of Advanced Scientific Computing Research (OASCR)
Project: Partnership Center for High-Fidelity Boundary Plasma Simulation
Award Amount: $6,250K from FES and $1,650K from ASCR
Period of Performance: August 1, 2017 – July 31, 2022
Annual Level of Effort: 6 months

Current Funding for Mark Adams

- DOE SciDAC Institute: Frameworks, Algorithms, and Scalable Technologies for Mathematics (FASTMath). PI: Lori Diachin. Duration: 10/01/2011 to 09/30/2016 (extended). $150,000 (30% effort).
- DOE ASCR base program grant “Extending PETSc's Composable Hierarchically Nested Linear Solvers”. PI: Lois Curfman-McInnes. Duration: 10/01/2015 to 09/30/2018. $150,000 per year (30% effort).
- DOE SciDAC Partnership “Partnership for Edge Physics Simulation (EPSI)”. PI: C.S. Chang. Duration: 2/1/2012 - 1/31/2017 (extended). $100,000/year (20% effort).
- DOE: “Simulation Center for Runaway Electron Avoidance and Mitigation”, PI: Dylan Brennan, Duration: 7/01/2016 to 06/30/2018. $100,000 per year (20% effort).

Pending Funding for Mark Adams

- DOE SciDAC Partnership supplement to “Partnership Center for High-fidelity Boundary Plasma Simulation”. PI: C.S. Chang. Duration: 8/1/2017 - 7/31/2022. $100,000 (20% effort).
- DOE SciDAC Partnership supplement to “First Principles Based Transport and Equilibrium Module for Whole Device Modeling and Optimization”. PI: W.W. Lee. Duration: 8/1/2017 - 7/31/2022. $50,000 (10% effort).

Varis Carey

Support: Pending
Proposal Title: Gradient Enhanced Surrogates for Uncertainty Quantification of Chemically Reacting Flows
Source of Support: NSF
Total award amount: 211,115
Total award period: 8/1/17-7/31/20
Person-months per year commited to project: 1.0

Support: Pending
Proposal Title: Partnership Center for High-fidelity Boundary Plasma Simulation
Source of support: DOE
Total award amount: $1,427,937
Total award period covered: 8/1/17-7/31/22
Location of project: University of Colorado -Denver
Person-months per year committed to project: 1.0

Current and Pending Support for Luis Chacón

- Simulation Center for Runaway Electron Avoidance and Mitigation
  DOE-FES-ASCR SCIDAC
  2.5 months
  08/16 - 07/18
- A Multiscale, Non-stochastic Approach to Model Collisions in Particle Systems
  LANL Laboratory Directed Research & Development Program
  2.5 months
  10/15 - 9/18
- LANL Thermonuclear Burn Initiative Program
  4 months
  10/17 - 9/18
- Pending: Enabling Multiphysics Extended MHD Simulations by the Development of Stable, Accurate and Scalable Computational Formulations and Solution Methods
  DOE Office of Science ASCR AMR Program
  3.5 months
  10/17 - 9/20
- Pending: Tokamak Disruption Simulation
  DOE-FES-ASCR SCIDAC
  2 months
  10/17 - 9/20
- Pending this proposal: Partnership Center for High-fidelity Boundary Plasma Simulation
  DOE-FES-ASCR SCIDAC
  4 months
  10/17 - 9/20

Yang Chen

Current and Pending Support: Yang Chen

Current Support:

Source of Support: DOE
Title, P.I.: [Extension Year] Center for Nonlinear Simulation of Energetic Particles in Burning Plasmas, Yang Chen
Person months per year committed to Project: 7.2 months
Total Award Amount: $140,000
Period of Performance: 9/1/2016 – 8/30/2017

Pending Support:

Source of Support: General Atomics
Title, P.I.: AToM: Advanced Tokamak Modeling Environment , Yang Chen
Person months per year committed to Project: 6 months
Total Award Amount: $750,526
Period of Performance: 8/1/2017 – 7/31/2022

Source of Support: DOE
Title, P.I.: Gyrokinetic Simulation of Turbulent Transport, S. Parker
Person months per year committed to Project: 4.2/4.8/4.6 months
Total Award Amount: $570,000
Period of Performance: 2/1/2017 – 1/31/2020

This Proposal
Source of Support: DOE
Title, P.I.: Partnership Center for High-fidelity Boundary Plasma Simulation, S. Parker
Person months per year committed to Project: 6.0/6.0/6.0/5.4/4.8 months
Total Award Amount: $1,650,000
Period of Performance: 8/1/2017 – 7/31/2022

Current and Pending Support

Jong Youl Choi

Current

Project Name: CODAR: Co-Design Center for Online Data Analysis and Reduction at the Exascale
Sponsor: Department of Energy
P.I.: Ian Foster, ANL
Person Months: 6 (50%)

Project Name: EPSI: Edge Physics Simulation
Sponsor: Department of Energy ASCR
P.I.: Choong-Seock Chang, PPPL
Award Period: 6/1/12 – 1/30/17
Person Months: 6 (50%)

Pending

Title: Partnership Center for High-Fidelity Boundary Plasma Simulation
Sponsor: Department of Energy, Office of Advanced Scientific Computing Research
P.I.: Choong-Seock Chang, PPPL
Period of Performance: August 1, 2017 – July 31, 2022
Person Months: 6 (50%)

Davide Curreli (UIUC)

Pending Support

Title	*Sponsor*	*Period of Performance*	*Requested Annual Funding*	*Effort*
Theoretical Assessment of the Role of Charge Exchange in Microscopic Erosion of Plasma Facing Components	US DOE/FES Theory	01/01/2017 – 12/31/2018	$85K	PI (0.5 su. mo.)
An in-situ ex-tempore plasma-material interface (PMI) diagnostic system to study high heat-flux, magnetic-sheath effects on erosion/re-deposition of mixed material and fuel	US DOE	09/01/2017 – 08/31/2020	$350K	Co-PD/PI (1.0 su. mo.)
Self Organization in Cold Magnetized Plasmas	NSF (Natl Science Fdn)	08/16/2017 - 08/15/2020	$140K	Co-PD/PI (0.5 su. mo.)
Manipulating directed plasma nanosynthesis surface interactions to tailor asymmetric surface ultra hydrophobicity	DOE SBIR/STTR	06/12/2017 – 03/11/2018	To be finalized	Co-PD/PI (0.5 su. mo.)
Center for Integrated Simulation of Fusion Relevant RF Actuators	DOE OFES & ASCR	7/1/2017 – 6/30/2022	To be finalized	Co-PD/PI (0.00 su. mo.)
Plasma Surface Interactions: Predicting the Performance and Impact of Dynamic PFC Surfaces	DOE OFES & ASCR	9/1/2017 – 8/31/2022	$4,050K (To be finalized)	Co-PD/PI (1.0 su. mo.)
Partnership Center for High-fidelity Boundary Plasma Simulation (This Proposal)	DOE OFES & ASCR	8/1/2017 – 7/31/2022	To be finalized	Co-PD/PI (0.75 su. mo.)

Current Support

Title	*Sponsor*	*Period of Performance*	*Requested Annual Funding*	*Effort*
Investigation of Uranium Molecular Species Formation Using Laser Ablation	US DoD-DTRA (Defense Threat Reduction Agency)	03/24/2016 – 03/27/2019	$350K	PI (1 su. mo.)
Development of Coupling Methodologies Between Plasma SOL/ Edge Physics and Material Physics	US DOE Labs (ORNL)	10/01/2016 – 09/30/2017	$50K	PI (0 su. mo.)
Atomized Dielectric-Based Electric Discharge Machining for Sustainable Manufacturing	NSF (Natl Science Fdn)	04/01/2016 – 03/31/2019	$300K	Co-PD/PI (0.3 cal. mo.)
Development of an HPC platform for Plasma-Material Interactions and Nanostructuring	University of Illinois NCSA (National Center for Supercomputing Applications)	7/01/16 – 6/30/17	$0	PI (project extension)
An enhanced Materials Analysis Particle Probe (MAPP) for a multi-spatial study of the impact of lithium-based surfaces on plasma behavior	US Dept of Energy	9/15/2016 – 09/14/2019	$500K	Co-PD/PI (1.0 su. mo.)

Ed D’Azevedo

Current Support (ORNL)

Sponsor: Unspecified Federal Agency
Project: 10-ZEUS-R (classified)
Total award Amount:$4,250,000.00
Period of Performance: Oct 1, 2016 – Sept/30/2017
Annual Level of Effort for Ed D’Azevedo: 3 months (0.25FTE)

Sponsor: Department of Energy, Office of Advanced Scientific Computing Research
Project: OLCF-4 Application Code Base
Total Award Amount:$61,500,000.00
Period of Performance: Oct 1, 2016 – Sept/30/2017
Annual Level of Effort for Ed D’Azevedo: 2.4 months (0.2FTE)

Sponsor: Department of Energy, Office of Advanced Scientific Computing Research
Project: Center for Edge Physics Simulation (EPSI)
Total Award Amount:$2,000,000.00
Period of Performance: Oct 1, 2016 – Sept/30/2017
Annual Level of Effort for Ed D’Azevedo: 2.4 months (0.2FTE)

Sponsor: Department of Energy, Office of Advanced Scientific Computing Research
Project: Exascale Computing Project Fusion Application
Total Award Amount:$247,514,000.00
Period of Performance: Oct 1, 2016 – Sept/30/2021
Annual Level of Effort for Ed D’Azevedo: 2.4 months (0.2FTE)

Sponsor: Laboratory Directed Research & Development (LDRD)
Project: Bringing the DMRG++ Scientific App
Total Award Amount:$309,600.00
Period of Performance: Oct 1, 2016 – Sept/30/2017
Annual Level of Effort for Ed D’Azevedo: 1.8 months (0.15FTE)

Pending Support (ORNL)

Sponsor: Department of Energy, Office of Advanced Scientific Computing Research
Project: SciDAC: Center for Integrated Simulation of RF Actuators
Period of Performance: July 1, 2017 – June 30, 2022
Annual Level of Effort for Ed D’Azevedo: 4 months (0.33FTE)

Sponsor: Department of Energy, Office of Advanced Scientific Computing Research
Project: Partnership Center for High-fidelity Boundary Plasma Simulation
Period of Performance: July 1, 2017 – June 30, 2022
Annual Level of Effort for Ed D’Azevedo: 3 months (0.25FTE)

Stephane Ethier

Current Support

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: Advancing the Frontiers of Magnetic Confinement Theory and Simulation
Award Amount: $4,667K Expected in FY2017
Period of Performance: Funded annually
Annual Level of Effort: 3.2 months

Sponsor: Department of Energy, Office of Advanced Scientific Computing Research (OASCR) via ORNL
Project: Exascale Computing: High Fidelity Whole Device Modeling
Award Amount: $5,774K
Period of Performance: September 15, 2016 – September 30, 2020
Annual Level of Effort: 3.2 months

Sponsor: Department of Energy, Office of Advanced Scientific Computing Research (OASCR) via ORNL
Project: Exascale Computing: Co-Design for Particle-in-Cell Technologies
Award Amount: $1,255K
Period of Performance: November 23, 2016 – September 30, 2020
Annual Level of Effort: 3.2 months

Sponsor: Department of Energy, Office of Advanced Scientific Computing Research (OASCR) via ORNL
Project: Performance Understanding and Analysis for Exascale Data Management Workflows
Award Amount: ~$128K
Period of Performance: November 6, 2014 – July 31, 2017
Level of Effort: 2.4 months

Pending Support

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES) and Office of Advanced Scientific Computing Research (OASCR)
Project: SciDAC: Partnership Center for High-Fidelity Boundary Plasma Simulation
Award Amount: $6,250K from FES and $1,650K from ASCR
Period of Performance: August 1, 2017 – July 31, 2022
Annual Level of Effort: 1.8 months in Year 1; 1.7 months in Years 2 and 3; 1.6 months in Years 4 and 5

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: SciDAC: Whole Device Modeling at the Center for Effective Research in Fusion
Award Amount: $4,250K
Period of Performance: August 1, 2017 – July 31, 2022
Annual Level of Effort: 3.5 months in Year 1; 3.2 months in Year 2; 3 months in Year 3; 2.8 months in year 4; 2.5 months in Year 5

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: SciDAC: First Principles Based Transport and Equilibrium Module for Whole Device Modeling and Optimization
Award Amount: $3,365K
Period of Performance: July 1, 2017 – June 30, 2022
Annual Level of Effort: 2.3 months

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: SciDAC: Center for Advanced Simulations of Plasma-Liquid Metal Interactions
Award Amount: $6,700K
Period of Performance: July 1, 2017 – June 30, 2022
Annual Level of Effort: 5.6 months

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: SciDAC: Tokamak Disruption Simulation
Award Amount: $2,500K
Period of Performance: September 1, 2017 – August 31, 2022
Annual Level of Effort: 2.5 months in Year 1; 2.4 months in Year 2; 2.3 months in Year 3; 2.2 months in Year 4; 1.9 months in Year 5

Nathaniel Ferraro

Current Support

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: National Spherical Torus Experiment Upgrade (NSTX-U) – Science
Award Amount: $15,884K Expected in FY2017
Period of Performance: Funded annually
Annual Level of Effort: 6 months

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: Advancing the Frontiers of Magnetic Confinement Theory and Simulation
Award Amount: $4,667K Expected in FY2017
Period of Performance: Funded annually
Annual Level of Effort: 6 months

Pending Support

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES) and Office of Advanced Scientific Computing Research (OASCR)
Project: Partnership Center for High-Fidelity Boundary Plasma Simulation
Award Amount: $6,250K from FES and $1,650K from ASCR
Period of Performance: August 1, 2017 – July 31, 2022
Annual Level of Effort: 1.9 months in Year 1; 1.8 months in Years 2-4; 1.7 months in Year 5

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: Center for Tokamak Transients Simulations
Award Amount: $3,860K
Period of Performance: June 15, 2017 – June 14, 2022
Level of Effort: 4.9 months in Years 1; 4.7 months in Year 2; 4.3 months in Year 3; 3.8 months in Year 4; 3.4 months in Year 5

APPENDIX 2: Current and Pending Support
Investigator: Martin Greenwald

Support: ☐ Current ☒ Pending
Project/Proposal Title: Partnership Center for High -fidelity Boundary Plasma Simulation
Source of Support: DOE DE- FOA-0001670 (THIS PROPOSAL)
Total Award Amount: $200,000 Award Period Covered: 8/01/17-7/31/22
Location of Project: Massachusetts Institute of Technology
Person-Months Per Year Committed to the Project. Cal: 0.73 months

Support: ☒ Current ☐ Pending
Project/Proposal Title: CIF21 DIBBs: PD: Metadata Toolkits for Building Multi-faceted Data-relationship Models
Source of Support: ACI-1640829
Total Award Amount: $ 500,000 Award Period Covered: 10/1/16-9/30/19
Location of Project: Massachusetts Institute of Technology
Person-Months Per Year Committed to the Project. Cal: 1 month

Support: ☒ Current ☐ Pending
Project/Proposal Title: MIT Plasma Science and Fusion Center Magnetic Confinement Fusion Experiment Research Related Activities Source of Support: DOE DE-SC0014264
Total Award Amount: $45,825,571 Award Period Covered: 9/01/15-8/31/20
Location of Project: Massachusetts Institute of Technology
Person-Months Per Year Committed to the Project. Cal: 0 months

Support: ☒ Current ☐ Pending
Project/Proposal Title: MDSplus Development and Support:
Source of Support: DOE DE-SC0012470
Total Award Amount: $1,747,870 Award Period Covered: 9/01/14-8/31/17
Location of Project: Massachusetts Institute of Technology
Person-Months Per Year Committed to the Project. Cal: 2.4 months

Support: ☒ Current ☐ Pending
Project/Proposal Title: Partnership for Edge Physics Simulation
Source of Support: DOE DE-SC0008737
Total Award Amount: $ 500,000 Award Period Covered: 8/1/12-7/31/17
Location of Project: Massachusetts Institute of Technology
Person-Months Per Year Committed to the Project. Cal: .6 months

Support: ☒ Current ☐ Pending
Project/Proposal Title: Alcator C-Mod
Source of Support: DOE DE-FCO2-99ER54512
Annual Award Amount: $14,475,000 NCE Award Period Covered: 1/01/16-06/30/17
Location of Project: Massachusetts Institute of Technology
Person-Months Per Year Committed to the Project. Cal: 2.6 months

Support: ☒ Current ☐ Pending
Title: Head, Office of Computer Services, Plasma Science and Fusion Center
Source of Support: Massachusetts Institute of Technology
Location of Project: Massachusetts Institute of Technology
Person-Months Per Year Committed to the Project. Cal: .6 months

Support: ☒ Current ☐ Pending
Title: Deputy Director, Plasma Science and Fusion Center
Source of Support: Massachusetts Institute of Technology
Location of Project: Massachusetts Institute of Technology
Person-Months Per Year Committed to the Project. Cal: 4.8 months

Gregory Hammett

Current Support

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: Advancing the Frontiers of Magnetic Confinement Theory and Simulation
Award Amount: $4,667K Expected in FY2017
Period of Performance: Funded annually
Annual Level of Effort: 5.6 months

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES) and Office of Advanced Scientific Computing Research (OASCR)
Project: SciDAC-3 Center for Edge Physics Simulation (EPSI)
Award Amount: $2,090K from FES and $590K from ASCR
Period of Performance: October 1, 2010 – September 30, 2016
Annual Level of Effort: 1.6 months

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: SciDAC - Center for the Study of Plasma Microturbulence (CSPM)
Award Amount: $1,078K
Period of Performance: October 1, 2010 – September 30, 2016. Operating on carryover in FY17.
Annual Level of Effort: 1 month

Sponsor: Department of Energy, PPPL Laboratory Directed Research and Development (LDRD)
Project: Simulations of Plasma Turbulence with Lithium or Other Walls
Award Amount: $200K
Period of Performance: February 1, 2015 – January 31, 2018
Annual Level of Effort: 0.4 months

Princeton University supports approximately one month of Dr. Hammett's time to teach a half semester course each academic year.

Pending Support

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES) and Office of Advanced Scientific Computing Research (OASCR)
Project: Partnership Center for High-Fidelity Boundary Plasma Simulation
Award Amount: $6,250K from FES and $1,650K from ASCR
Period of Performance: August 1, 2017 – July 31, 2022
Annual Level of Effort: 1.8 months in Years 1 and 2; 1.7 months in Years 3 and 4; 1.6 months in Year 5

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: Partnership for Multiscale Gyrokinetic (MGK) Turbulence
Award Amount: $1,250K
Period of Performance: July 1, 2017 – June 30, 2022
Level of Effort: 1.2 months

David Hatch
Support: Current
Project/Proposal Title: Establishment of an Institute for Fusion Studies
Source of support: DOE
Total award amount: $6,750,000
Total award period covered: 11/1/15-10/31/18
Location of project: The University of Texas at Austin
Person-months per year committed to project: 9.5

Support: Pending
Proposal Title: Partnership for Multiscale Gyrokinetic (MGK) Turbulence
Source of support: DOE
Total award amount: $2,262,003
Total award period covered: 8/1/17-7/31/22
Location of project: The University of Texas at Austin
Person-months per year committed to project: 2.1

Support: Pending
Proposal Title: Partnership Center for High-fidelity Boundary Plasma Simulation
Source of support: DOE
Total award amount: $1,427,937
Total award period covered: 8/1/17-7/31/22
Location of project: The University of Texas at Austin
Person-months per year committed to project: 0.4

C&P support for Cory D. Hauck

1. *Hybrid Methods for Complex Particle Systems*
   Status: Active
   Role: Principal investigator
   Sponsor: DOE - Office of Science, Early Career Research Program
   Dates: 10/2015–09/2020
   Effort: 6 months/yr.
   1 postdoctoral fellow for PI C. D. Hauck
   2 Ph.D. students for PI C. D. Hauck
   Total award: $2,500,000 (5 years)

2. *Moment Methods for Kinetic Equations*
   Status: Active
   Role: Principal investigator
   Sponsor: DOE - Office of Science, Early Career Research Program
   Dates: 04/2014–03/2017
   Effort: 4 months/yr.
   1 postdoctoral fellow for PI C. D. Hauck
   Total award: $825,000 (3 years)

3. *Sparse Recovery for Scientific Data*
   Status: Pending
   Role: Principal investigator
   Sponsor: DOE - Advanced Scientific Computing Research, Applied Mathematics
   Dates: 04/2015–03/2018
   Effort: 1 months/yr.
   1 postdoctoral fellow for PI C. D. Hauck
   1 Ph.D. students for PI C. D. Hauck
   Total award: 750,000 (3 years)

4. *NSF Research Network: Kinetic Description of Emerging Challenges in Multiscale Problems of Natural Sciences*
   Status: Active
   Role: Director and Principal investigator
   Sponsor: NSF - Division of Mathematical Sciences
   Dates: 03/2012 – 02/2018
   Effort: 0 months/yr.
   Funding for conferences, travel, and visitors
   Total award: $5,000,000 (6 years, estimated)

5. *Optimization-Based Moment Methods for Multi-scale Kinetic Equations*
   Status: Active
   Role: Principal investigator
   Sponsor: NSF - Division of Mathematical Sciences
   Dates: 09/2012-08/2017
   Effort: 1.2 months/yr.
   1 postdoctoral fellow for PI C. D. Hauck
   1 Ph.D. student for PI C. D. Hauck
   Total award: $ 635,680 (3 years, plus 2 year NCE)

6. *Multi-fidelity Models for Uncertainty Quantification of Kinetic Equations and Hyperbolic Balance Laws*

Status:	Pending (Current Proposal)
Role:	Principal investigator
Sponsor:	NSF - Computational Mathematics
Dates:	08/2017 – 08/2020
Effort:	1.2 months/yr.
	1/2 postdoctoral fellow for PI C. D. Hauck
	1 Ph.D. students for PI C. D. Hauck
Total award:	$ 1,109,345

Current and Pending Support for Jeffrey Hittinger

Current Support
Project Title: Variable Precision Computing
Source of Support: LLNL
Total award amount: $5,250,000
Total award period covered: 10/1/16-9/30/19
Location of project: LLNL
Person-months committed to project: 4.0

Project Title: High-Fidelity Whole Device Modeling of Magnetically Confined Fusion Plasmas
Source of Support: DOE Exascale Computing Project
Total award amount: $1,104,000
Total award period covered: 10/19/16-10/18/20
Location of project: LLNL
Person-months committed to project: 3.6

Project Title: High-Resolution Methods for Phase Space Problems in Complex Geometries
Source of Support: DOE ASCR Applied Math Base Program
Total award amount: $1,425,000
Total award period covered: 10/1/14-9/30/17
Location of project: LLNL
Person-months committed to project: 1.2

Pending Support
Proposal Title: High-Resolution Methods for Phase Space Problems in Complex Geometries
Source of Support: DOE ASCR Applied Math Base Program
Total award amount: $1,460,000
Total award period covered: 10/1/17-9/30/20
Location of project: LLNL
Person-months committed to project: 1.2

Proposal Title: Partnership for Multiscale Gyrokinetic (MGK) Turbulence
Source of Support: DOE SciDAC Partnerships
Total award amount: $1,000,000
Total award period covered: 8/1/16-7/31/21
Location of project: LLNL
Person-months committed to project: 1.2

Proposal Title: Partnership Center for High-fidelity Boundary Plasma Simulation
Source of Support: DOE SciDAC Partnerships
Total award amount: $975,000
Total award period covered: 8/1/16-7/31/21
Location of project: LLNL
Person-months committed to project: 1.2

HOFFMAN, BILL

ACTIVE

None.

PENDING

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES) and Office of Advanced Scientific Computing Research (OASCR)
Project: Partnership Center for High-Fidelity Boundary Plasma Simulation
Award Amount: $6,250K from FES and $1,650K from ASCR
Period of Performance: August 1, 2017 – July 31, 2022
Annual Level of Effort: Y1: 0.016 CM; Y2: 0.016 CM; Y3: 0.015 CM; Y4: 0.014 CM; Y5: 0.014CM

OVERLAP

None.

Current & Pending Support
Scott Klasky
Oak Ridge National Laboratory

Current: (Amount is per year)

Title: Runtime System for I/O staging in support of voluminous in-situ processing of extreme scale data:
Amount: $858,000
Location: Oak Ridge National Laboratory
Sponsor: Department of Energy ASCR
P.I.: Scott Klasky
Award Period: 08/01/13 – 09/30/16
Person Months: 1.0

Project Name: Scalable Data Analysis and Visualization
Amount: $2,403,000
Location: LBNL + Oak Ridge National Laboratory
Sponsor: Department of Energy ASCR
P.I.: Arie Shoshani, LBNL
Award Period: 03/01/12 – 09/30/16
Person Months: 1.0

Title: EPSI: Edge Physics Simulation
Amount: $2,000,000
Location: Oak Ridge National Laboratory
Sponsor: Department of Energy ASCR
P.I.: Choong-Seock Chang, PPPL
Award Period: 6/1/12 – 1/30/17
Person Months: 1.0

Title: Tools to Analyze Morphology and Spatially Mapped Molecular Data
Amount: $ 2,015,673
Location: Oak Ridge National Laboratory
Sponsor: NIH
P.I.: Joel Saltz, Stony Brook University
Award Period: 7/31/14 – 5/31/17
Person Months: 1.0

Title: Project Name: Oak Ridge Leadership Class Facility (PI/ Project Manager: Buddy Bland)
Amount: > $100,000,000
Location: Oak Ridge National Laboratory
Sponsor: Department of Energy, ASCR
Award Period: 10/1/10 - 9/30/18
Person Months: 1.0

Title: Science-driven Data Management for multi-tiered storage
Amount: $1,650,000
Location: Oak Ridge National Laboratory
Sponsor: Department of Energy ASCR
Award Period: 9/1/15 – 9/30/18
Person Months: 1.0

Title: High-Fidelity Whole Device Modeling of Magnetically Confined Fusion Plasmas
Amount: $2,500,000

Location: Oak Ridge National Laboratory
Sponsor: ECP: Department of Energy ASCR
Award Period: 9/1/16 – 9/30/20
Person Months: 2.0

Title: A Co-Design Center for Online Data Analysis and Reduction at the Exascale
Amount: $4,000,000
Location: Oak Ridge National Laboratory
Sponsor: ECP: Department of Energy ASCR
Award Period: 9/1/16 – 9/30/20
Person Months: 2.0

Title: The ADIOS framework for Scientific Data on exascale systems
Amount: $1,500,000
Location: Oak Ridge National Laboratory
Sponsor: ECP: Department of Energy ASCR
Award Period: 9/1/16 – 9/30/20
Person Months: 2.0

Pending

Title: Partnership Center for High-Fidelity Boundary Plasma Simulation
Amount: $3,500,000
P.I.: Choong-Seock Chang
Location: Oak Ridge National Laboratory
Sponsor: Department of Energy FES/ASCR
Award Period: Pending
Person Months: 1.0

Title: ISEP: Integrated Simulation of Energetic Particles in Burning Plasma
Amount: $2,100,000
P.I.: Zhihong Lin
Location: Oak Ridge National Laboratory
Sponsor: Department of Energy FES/ASCR
Award Period: Pending
Person Months: 1.0

Seung Hoe Ku

Current Support

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES) and Office of Advanced Scientific Computing Research (OASCR)
Project: SciDAC-3 Center for Edge Physics Simulation (EPSI)
Award Amount: $2,090K from FES and $590K from ASCR
Period of Performance: October 1, 2010 – September 30, 2016
Annual Level of Effort: 6.6 months

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: National Spherical Torus Experiment Upgrade (NSTX-U) – Science
Award Amount: $15,884K Expected in FY2017
Period of Performance: Funded annually
Annual Level of Effort: 3.6 months

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: Advancing the Frontiers of Magnetic Confinement Theory and Simulation
Award Amount: $4,667K Expected in FY2017
Period of Performance: Funded annually
Annual Level of Effort: 0.6 months

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES) and Office of Advanced Scientific Computing Research (OASCR)
Project: SciDAC: International Collaboration Framework for Extreme Scale Experiments (ICEE)
Award Amount: $270K
Period of Performance: October 1, 2012 – September 30, 2015. Currently operating on carryover.
Annual Level of Effort: 0.6 months

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: PMI for LP Optimization EAST/KSTAR
Award Amount: $2,130K
Period of Performance: August 1, 2016 – July 31, 2019
Annual Level of Effort: 0.6 months

Pending Support

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES) and Office of Advanced Scientific Computing Research (OASCR)
Project: Partnership Center for High-Fidelity Boundary Plasma Simulation
Award Amount: $6,250K from FES and $1,650K from ASCR
Period of Performance: August 1, 2017 – July 31, 2022
Annual Level of Effort: 6 months in Year 1; 5.9 months in Years 2 and 3; 5.8 months in Year 4; 5.4 months in Year 5

Rajesh Maingi

Current Support

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: National Spherical Torus Experiment Upgrade (NSTX-U) – Science
Award Amount: $15,884K Expected in FY2017
Period of Performance: Funded annually
Annual Level of Effort: 6 months

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: DIII-D Science
Award Amount: $3,768K Expected in FY2017
Period of Performance: Funded annually
Annual Level of Effort: 3.2 months

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: PMI for LP Optimization EAST/KSTAR
Award Amount: $2,130K
Period of Performance: August 1, 2016 – July 31, 2019
Annual Level of Effort: 2.4 months

Sponsor: Department of Energy, PPPL Laboratory Directed Research and Development (LDRD)
Project: Lithium Studies in Devices with Metallic Plasma Facing Components
Award Amount: $180K
Period of Performance: February 1, 2015 – January 31, 2018
Annual Level of Effort: 0.4 months

Pending Support

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES) and Office of Advanced Scientific Computing Research (OASCR)
Project: Partnership Center for High-Fidelity Boundary Plasma Simulation
Award Amount: $6,250K from FES and $1,650K from ASCR
Period of Performance: August 1, 2017 – July 31, 2022
Annual Level of Effort: 0.6 months

Current and Pending Support

(See GPG Section II.D.8 for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Other agencies (including NSF) to which this proposal has been/will be submitted.

Investigator: Robert D. Moser

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Integrating Domain Expertise with machine Learning for Turbulence Model Development

Source of Support: Sandia National Labs

Total Award Amount: $675,000 Total Award Period Covered: 03/03/2016-09/30/2018

Location of Project: UT Austin

Person-Months Per Year Committed to the Cal: 0.25 Acad: 0.0 Sumr: 0.0

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: DiaMonD: An Integrated Multifaceted Approach at the Interfaces of Data, Models, and Decisions (PI: Ghattas)

Source of Support: DOE ASCR

Total Award Amount: $5,425,000 Total Award Period Covered: 12/15/2012-2/14/2018

Location of Project: UT Austin

Person-Months Per Year Committed to the Cal: 1.0 Acad: 0.0 Sumr: 0.0

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Inference, Simulation, and Optimization of Complex Systems Under uncertainty: Theory, Algorithms, and Applications to Turbulent Combustion (PI: Ghattas)

Source of Support: DARPA

Total Award Amount: $3,242,180 Total Award Period Covered: 06/1/2015-08/31/2018

Location of Project: UT Austin

Person-Months Per Year Committed to the Cal: 2.0 Acad: 0.0 Sumr: 0.0

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Fundamental Investigations of Film Cooling or Gas Turbine Engines (PI: Bogard)

Source of Support: GE Aviation

Total Award Amount: $500,000 Total Award Period Covered: 01/01/2017-12/31/2017

Location of Project: UT Austin

Person-Months Per Year Committed to the Cal: 0.0 Acad: 0.0 Sumr: 0.0

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Novel Hybrid RANS/LES Models for Aerodynamic Flows

Source of Support: NASA

Total Award Amount: $617,101 Total Award Period Covered: 10/01/2015-09/30/2018

Location of Project: UT Austin

Person-Months Per Year Committed to the Cal: 0.5 Acad: 0.0 Sumr: 0.0

Current and Pending Support

(See GPG Section II.D.8 for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: Robert D. Moser	Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Partnership for Edge Physics Simulation (EPSI)

Source of Support: DOE-SciDAC

Total Award Amount: $700,000 Total Award Period Covered: 08/1/2012-07/31/2017

Location of Project: UT Austin

Person-Months Per Year Committed to the Cal: 0.5 Acad: 0.0 Sumr: 0.0

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Extreme-scale Bayesian Inference for Uncertainty Quantification of Complex Simulations-EUREKA (PI: Biros)

Source of Support: DOE

Total Award Amount: $2,442,858 Total Award Period Covered: 09/1/2013-08/31/2017

Location of Project: UT Austin

Person-Months Per Year Committed to the Cal: 0.45 Acad: 0.0 Sumr: 0.0

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: PREEVENT TRACK2: A Multiscale Computational Framework for Predicting Extreme Wildfire (PI: Ezekoye)

Source of Support: NSF

Total Award Amount: $1,381,732 Total Award Period Covered: 06/2017-05/2020

Location of Project: UT Austin

Person-Months Per Year Committed to the Cal: 0.0 Acad: 0.0 Sumr: 0.01

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Partnership Center for High-fidelity Boundary Plasma Simulation (PI: C.S. Chang)

Source of Support: DOE

Total Award Amount: $675,000 Total Award Period Covered: 8/1/2017-7/31/2022

Location of Project: UT Austin

Person-Months Per Year Committed to the Cal: 0.5 Acad: 0.0 Sumr: 0.0

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: AToM: Advanced Tokamak Modeling Environment (PI: Jeff Candy)

Source of Support: DOE

Total Award Amount: $750,000 Total Award Period Covered: 08/01/2017-07/31/2022

Location of Project: UT Austin

Person-Months Per Year Committed to the Cal: 0.5 Acad: 0.0 Sumr: 0.0

Current and Pending Support

(See GPG Section II.D.8 for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: Robert D. Moser

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Partnership for Multiscale Gyrokinetic Turbulence (PI: David Hatch)

Source of Support: DOE

Total Award Amount: $1,250,000 Total Award Period Covered: 08/01/2017-07/31/2022

Location of Project: UT Austin

Person-Months Per Year Committed to the Cal: 0.5 Acad: 0.0 Sumr: 0.0

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Center for Tokamak Transients Simulations (PI: Stephen Jardin)

Source of Support: DOE

Total Award Amount: $1,000,000 Total Award Period Covered: 6/15/2017-6/14/2022

Location of Project: UT Austin

Person-Months Per Year Committed to the Cal: 0.5 Acad: 0.0 Sumr: 0.0

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:

Total Award Amount: $ Total Award Period Covered:

Location of Project: UT Austin

Person-Months Per Year Committed to the Cal: 0.0 Acad: 0.0 Sumr: 0.0

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:

Total Award Amount: $ Total Award Period Covered:

Location of Project: UT Austin

Person-Months Per Year Committed to the Cal: 0.0 Acad: 0.0 Sumr: 0.0

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:

Total Award Amount: $ Total Award Period Covered:

Location of Project: UT Austin

Person-Months Per Year Committed to the Cal: 0.0 Acad: 0.0 Sumr: 0.0

Lodestar Research Corporation: Current and Pending Support

James R. Myra

- OFES theory (DE-FG02-97ER54392) 11/1/2014 - 10/31/2017, $1530k/3-yr, 7.9 mo/yr
- NSTX-U (DE-FG02-02ER54678) 8/15/2014 - 8/14/2018, $293k/4-yr, 1.4 mo/yr
- RF CSWPI-SciDAC (DE-FC02-05ER54823) 4/1/2016 - 3/31/2017, $72k/1-yr, 2.6 mo/yr
- RF SciDAC-4 (pending) 07/01/2017 - 06/30/2022, $775k/5-yr, 5.5 mo/yr
- HBPS SciDAC-4 (pending) 08/01/2017 - 07/31/2022, $500k/5-yr, 2.3 mo/yr

David A. Russell

- OFES theory (DE-FG02-97ER54392) 11/1/2014 - 10/31/2017, $1530k/3-yr, 12 mo/yr
- HBPS SciDAC-4 (pending) 08/01/2017 - 07/31/2022, $500k/5-yr, 2.3 mo/yr

Person-months per year are based on 2016 loaded rates. For current active grants, actual 2016 person-month charges are given; for pending applications, estimated future commitments in 2017 are given.

Scott E. Parker

Current Support:

Source of Support: DOE
Title, P.I.: Partnership for Edge Physics Simulation, S. Parker
Person months per year committed to Project: 1.0 mo. summer
Total Award Amount: $1,100,000
Period of Performance: 8/1/2012 – 7/31/2017

Source of Support: Princeton Plasma Physics Lab
Title, P.I.: Exascale Computing Project, A. Bhattacharjee
Person months per year committed to Project: 1.0 mo. summer
Total Award Amount: $627,543 (Univ. of Colorado portion only)
Period of Performance: 10/1/2016 – 9/30/2020

Pending Support:

Source of Support: DOE
Title, P.I.: Gyrokinetic Simulation of Tokamak Fusion Plasmas, S. Parker
Person months per year committed to Project: 1.0 mo. summer
Total Award Amount: $570,000
Period of Performance: 2/1/2017 – 1/31/2020

This Proposal
Source of Support: DOE
Title, P.I.: Partnership Center for High-fidelity Boundary Plasma Simulation, S. Parker
Person months per year committed to Project: 1.0 mo. summer
Total Award Amount: $1,650,000
Period of Performance: 8/1/2017 – 7/31/2022

Current and Pending Support

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: Mark S. Shephard

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: S12-SSE: Fast Dynamic Load Balancing Tools for Extreme Scale Systems (Principal Investigator)

Source of Support: NSF

Total Award Amount: $500,000 Total Award Period Covered: 10/01/15 – 09/30/18

Location of Project: Rensselaer Polytechnic Institute

Person-Months Per Year Committed to the Project. Cal: Acad: 0.00 Sumr: 0.63

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: High Technology Matching Grant – High Performance Computing (Co-Principal Investigator)

Source of Support: ESD/NYSTAR

Total Award Amount: $3,000,000 Total Award Period Covered: 09/01/13 – 08/31/17

Location of Project: Rensselaer Polytechnic Institute

Person-Months Per Year Committed to the Project. Cal: Acad: 0.00 Sumr: 0.50

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Component-Based Technologies for the Massively Parallel Simulation of Integrated Circuit Physics (Principal Investigator)

Source of Support: IBM Corp

Total Award Amount: $500,000 Total Award Period Covered: 08/15/15 – 08/14/17

Location of Project: Rensselaer Polytechnic Institute

Person-Months Per Year Committed to the Project. Cal: Acad: 0.00 Sumr: 0.00

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Methods for Reliable Simulation of Multiphase Processes (Co-Principal Investigator)

Source of Support: ARO

Total Award Amount: $1,019,053 Total Award Period Covered: 09/16/14 – 09/15/19

Location of Project: Rensselaer Polytechnic Institute

Person-Months Per Year Committed to the Project. Cal: Acad: 0.00 Sumr: 0.25

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Collaborative Research: Frameworks, Algorithms, and Scalable Technologies for Mathematics (FASTMath) SciDAC Institute (Principal Investigator)

Source of Support: Lawrence Livermore National Lab/DOE

Total Award Amount: $2,500,000 Total Award Period Covered: 09/01/11 - 08/31/17

Location of Project: Rensselaer Polytechnic Institute

Person-Months Per Year Committed to the Project. Cal: Acad: 0.72 Sumr: 1.00

Current and Pending Support

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: Mark S. Shephard	Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: Center for Extended Magnetohydrodynamic Modeling (CEMM) (Collaboration) (Principal Investigator)
Source of Support: DOE
Total Award Amount: $352,000 Total Award Period Covered: 09/01/11 - 08/31/17
Location of Project: Rensselaer Polytechnic Institute
Person-Months Per Year Committed to the Project. Cal: Acad: 0.09 Sumr: 0.13

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: ECP Co-Design: Center for Efficient Exascale Discretizations (CEED) (Principal Investigator)
Source of Support: Lawrence Livermore National Laboratory
Total Award Amount: $700,000 Total Award Period Covered: 01/01/17 – 12/31/20
Location of Project: Rensselaer Polytechnic Institute
Person-Months Per Year Committed to the Project. Cal: Acad: 0.09 Sumr: 0.38

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: Community Project for Accelerator Science and Simulation 3 ($ComPASS_3$) (Principal Investigator)
Source of Support: DOE
Total Award Amount: $130,000 Total Award Period Covered: 09/01/15 – 08/31/17
Location of Project: Rensselaer Polytechnic Institute
Person-Months Per Year Committed to the Project. Cal: Acad: 0.00 Sumr: 0.25

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: Partnership for Edge Plasma Physics Computation (PEPPC) (Principal Investigator)
Source of Support: DOE/PPPL
Total Award Amount: $500,000 Total Award Period Covered: 08/01/12 - 07/31/17
Location of Project: Rensselaer Polytechnic Institute
Person-Months Per Year Committed to the Project. Cal: Acad: 0.23 Sumr: 0.50

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: MSM: Multiscale Mechanics of Bioengineered Tissue (Principal Investigator)
Source of Support: University of Minnesota (NIH)
Total Award Amount: $422,253 Total Award Period Covered: 06/01/13 – 05/31/17
Location of Project: Rensselaer Polytechnic Institute
Person-Months Per Year Committed to the Project. Cal: Acad: 0.36 Sumr: 0.00

Current and Pending Support

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: Mark S. Shepherd

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Multiscale Modeling of Facet Capsule Mechanobiology (Co-Principal Investigator)

Source of Support: University of Minnesota (NIH)

Total Award Amount: $352,777 Total Award Period Covered: 07/15/13 – 06/30/18

Location of Project: Rensselaer Polytechnic Institute

Person-Months Per Year Committed to the Project. Cal: Acad: 0.14 Sumr: 0.00

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Parallel Adaptive Mesh Control for Large Deformation Simulations (Principal Investigator)

Source of Support: Sandia National Laboratory

Total Award Amount: $143,649 Total Award Period Covered: 07/01/16 – 06/30/17

Location of Project: Rensselaer Polytechnic Institute

Person-Months Per Year Committed to the Project. Cal: Acad: 0.00 Sumr: 0.25

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Unstructured Mesh Technologies for Massively Parallel Simulation and Data Analysis of Magnetically Confined Plasmas (Principal Investigator)

Source of Support: Simmetrix, Inc.

Total Award Amount: $398,907 Total Award Period Covered: 08/01/16 – 07/31/18

Location of Project: Rensselaer Polytechnic Institute

Person-Months Per Year Committed to the Project. Cal: Acad: 0.00 Sumr: 0.50

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Tools for Parallel Adaptive Simulation of Multiphase Ballistic Flows (Principal Investigator)

Source of Support: Simmetrix, Inc.

Total Award Amount: $398,005 Total Award Period Covered: 10/01/16 – 09/27/18

Location of Project: Rensselaer Polytechnic Institute

Person-Months Per Year Committed to the Project. Cal: Acad: 0.18 Sumr: 0.50

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: EFRC Supplement to RPI for the Center for Hierarchical Waste Form Materials (Principal Investigator)

Source of Support: Lawrence Livermore National Laboratory

Total Award Amount: $50,000 Total Award Period Covered: 11/15/16 – 09/15/17

Location of Project: Rensselaer Polytechnic Institute

Person-Months Per Year Committed to the Project. Cal: Acad: 0.00 Sumr: 0.00

Current and Pending Support

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: Mark S. Shephard	Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: MRI: Acquisition of a Next Generation Data-Centric Supercomputer (Co-Principal Investigator)

Source of Support: NSF

Total Award Amount: $2,467,496 Total Award Period Covered: 09/01/17 – 08/31/20

Location of Project: Rensselaer Polytechnic Institute

Person-Months Per Year Committed to the Project. Cal: Acad: 0.00 Sumr: 0.00

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Computational Workflow for Elastography and Biomechanical Imaging (Co-Principal Investigator)

Source of Support: NIH

Total Award Amount: $3,704,360 Total Award Period Covered: 07/01/17 – 06/30/22

Location of Project: Rensselaer Polytechnic Institute

Person-Months Per Year Committed to the Project. Cal: Acad: 0.45 Sumr: 0.00

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Plasma Surface Interactions: Predicting the Performance and Impact of Dynamic PFC Surfaces (Principal Investigator)

Source of Support: DOE

Total Award Amount: $750,000 Total Award Period Covered: 09/01/17 – 08/31/22

Location of Project: Rensselaer Polytechnic Institute

Person-Months Per Year Committed to the Project. Cal: Acad: 0.00 Sumr: 0.50

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Partnership Center for High-fidelity Boundary Plasma Simulation (Principal Investigator)

Source of Support: DOE / Princeton Plasma Physics Lab

Total Award Amount: $750,000 Total Award Period Covered: 09/01/17 – 08/31/22

Location of Project: Rensselaer Polytechnic Institute

Person-Months Per Year Committed to the Project. Cal: Acad: 0.00 Sumr: 0.50

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Center for Tokamak Transient Simulations (Principal Investigator)

Source of Support: DOE / Princeton Plasma Physics Lab

Total Award Amount: $1,375,000 Total Award Period Covered: 06/15/17 – 06/14/22

Location of Project: Rensselaer Polytechnic Institute

Person-Months Per Year Committed to the Project. Cal: Acad: 0.09 Sumr: 0.50

Current and Pending Support

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: Mark S. Shephard

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: Center for Integrated Simulation of Fusion Relevant RF Actuators (Co-Principal Investigator)

Source of Support: DOE / MIT

Total Award Amount: $750,000 Total Award Period Covered: 0701/17 – 06/30/22

Location of Project: Rensselaer Polytechnic Institute

Person-Months Per Year Committed to the Project. Cal: Acad: 0.00 Sumr: 0.50

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:

Total Award Amount: Total Award Period Covered:

Location of Project:

Person-Months Per Year Committed to the Project. Cal: Acad: 0.00 Sumr: 0.00

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:

Total Award Amount: Total Award Period Covered:

Location of Project:

Person-Months Per Year Committed to the Project. Cal: Acad: 0.00 Sumr: 0.00

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:

Total Award Amount: Total Award Period Covered:

Location of Project:

Person-Months Per Year Committed to the Project. Cal: Acad: 0.00 Sumr: 0.00

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:

Total Award Amount: Total Award Period Covered:

Location of Project:

Person-Months Per Year Committed to the Project. Cal: Acad: 0.00 Sumr: 0.00

Daren Stotler

Current Support

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: National Spherical Torus Experiment Upgrade (NSTX-U) – Science
Award Amount: $15,884K Expected in FY2017
Period of Performance: Funded annually
Annual Level of Effort: 6 months

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: Advancing the Frontiers of Magnetic Confinement Theory and Simulation
Award Amount: $4,667K Expected in FY2017
Period of Performance: Funded annually
Annual Level of Effort: 3.6 months

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES)
Project: C-Mod Science
Award Amount: Funded through September 30, 2016. Operating on carryover in FY17.
Period of Performance: October 1, 2009 – September 30, 2017
Annual Level of Effort: 1.2 months

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES) and Office of Advanced Scientific Computing Research (OASCR)
Project: SciDAC-3 Center for Edge Physics Simulation (EPSI)
Award Amount: $2,090K from FES and $590K from ASCR
Period of Performance: October 1, 2010 – September 30, 2016
Annual Level of Effort: 1.2 months

Pending Support

Sponsor: Department of Energy, Office of Fusion Energy Sciences (OFES) and Office of Advanced Scientific Computing Research (OASCR)
Project: Partnership Center for High-Fidelity Boundary Plasma Simulation
Award Amount: $6,250K from FES and $1,650K from ASCR
Period of Performance: August 1, 2017 – July 31, 2022
Annual Level of Effort: 2.4 months in Years 1 and 2; 2.3 months in Years 3 and 4; 2.2 months in Year 5

CURRENT AND PENDING

Investigator: George Tynan

Current:

Agency: DOE –DE-FG02-06ER54871
Project Title: : Muliti-Machine Validation of Fluids and Gyrokinetic Plasma Turbulence Models
Percent Effort: 1 Summer Months @1% / 0 per mo
PI: C. Holland   CO PI: G. Tynan
Total Award Amount: $2,828,925
Total Award Period Covered: 6/01/06 – 5/31/17
Location of Project: General Atomics

Agency: DOE –DE-FG02-07ER54912
Project Title: Plasma Boundary Science, Materials Interactions & Collaborative Fusion
Percent Effort: 1 Summer Month @ 100% /   1. per mo
PI: G. Tynan   CO PI: R. Doerner
Total Award Amount: $22,338,380
Total Award Period Covered: 12/15/06 – 12/14/18
Location of Project: University of California, San Diego

Agency: DOE –DE-FG02-02-07ER54917
Project Title: DIII-D Edge Physics Disruptions, & Radioactive Processes
Percent Effort: 0 Summer Month @ 0% / 0 per mo
PI: E. Hollmann, CO PI: G. Tynan, R. Moyer & J. Boedo
Total Award Amount: $12,245,190
Total Award Period Covered: 1/15/07 – 2/28/19
Location of Project: General Atomics

Agency: DOE –DE-SC0008689
Project Title: Partnership for Edge Physics Simulation (ESPI) UCSD subtask: XGC Validation Studies Using the L-H Transition
Percent Effort: 1 summer month @ 5% /   0.1 per mo
PI: G. Tynan / CO-PI Diamond
Total Award Amount: $573,081
Total Award Period Covered: 08/1/12 – 07/31/17
Location of Project: University of California, San Diego

Agency: DOE –DE-SC0010593
Project Title: Development of Long-Pulse Heating & Current Drive Actuators & Operational Techiques Compatible with a High-Z Divertor & First Wall
Effort: 0.5 per months/ cal
PI: G. Tynan / CO-PI: R. Doerner
Total Award Amount: $539,000
Total Award Period Covered: 08/15/13 – 08/14/17
Location of Project: MIT / University of California, San Diego

Agency: California Clean Energy / Cal Seed – 300-15-007
Project Title: Cal SEED Technical Advisory Committee
Percent Effort: 3 Summer Month @ 12.24% / 0.4 per mo
PI: G. Tynan
Total Award Amount: $99,500
Total Award Period Covered: 09/07/16 – 03/01/23
Location of Project: CalCEF

Pending:

Agency DOE – ePD 5427 / UCID 2017-1450
Project Title: Measurement of thermos-mechanical properties of plasma-facing material surfaces subjected to plasma and/or ion beam exposure
Effort: 1. per months
PI: G. Tynan / CO-PI R. Chen
Total Award Amount: $1,134,279
Total Award Period Covered: 04/01/17 – 03/31/20
Location of Project: University of California, San Diego

Agency NSF – ePD 5531 / 2017-1404
Project Title: Mesoscale Pattern Competition in Turbulent Plasma
Effort: 1. per months
PI: G. Tynan / CO-PI P. Diamond
Total Award Amount: $1,044,932
Total Award Period Covered: 04/01/17 – 03/31/20
Location of Project: University of California, San Diego

Agency: DOE – ePD 6573 / UCID 2017-2247 / DE-FG02-07ER54912
Project Title: Plasma Boundary Science, Materials Interactions & Collaborative Fusion
Percent Effort: 1 Summer Month @ 100% / 1. per mo
PI: G. Tynan CO PI: R. Doerner
Total Award Amount: $700,000
Total Award Period Covered: 12/15/16 – 12/14/18
Location of Project: University of California, San Diego

Patrick H. Worley - PHWorley Consulting
Current and Pending Funding (February 2017)

Dr. Worley is currently funded by two subcontracts, one from Sandia National Laboratories and one from Princeton Plasma Physics Laboratory, as documented below. His work contributes to two DOE-funded projects, at the indicated commitment level, but this is at the direction of the subcontract technical managers.

Current:

1) Subcontract #S015397-F with Princeton Plasma Physics Laboratory (PPPL):

Subcontract Title: XGC and SciDAC-3 EPSI Project Performance Engineering Services
Period: 12/1/2016 -- 11/30/2017
Annual Funding: $80,500.00
Person-months/year: 3

Source: DOE SciDAC (ASCR and OFES) via PPPL
Project Title: Center for Edge Physics Simulation (EPSI)
Period Covered: 7/2012 - 6/2017

2) Subcontract #1730267 with Sandia National Laboratories (SNL):

Subcontract Title: ACME Model Development Professional Services
Period: 09/15/2016 -- 09/14/2017
Annual Funding: $149,100.00
Person-months/year: 5.4

Source: DOE (BER) via SNL
Project Title: Accelerated Climate Modeling for Energy
Period Covered: 5/2014 – 4/2017

Pending:

1) If this proposal:

Source: DOE SciDAC (ASCR and OFES) via PPPL
Project Title: Partnership Center for High-fidelity Boundary Plasma Simulation
Period: 7/2017 -- 6/2022

is funded, then a new year subcontract with PPPL will likely start in 12/2017, for a similar annual funding and number of person-months per year, and renewed yearly for the duration of the SciDAC project.

2) If the ACME project is renewed, then a new year subcontract with SNL will likely start in 9/2017, for a similar annual funding and number of person-months per year.

Source: DOE (BER) via SNL
Project Title: Accelerated Climate Modeling for Energy
Period Covered: 5/2017 – 4/2019

Appendix 3 Bibliography and References Cited

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Appendix 4 Facilities and Other Resources

1. Princeton Plasma Physics Laboratory
2. Oak Ridge National Laboratory
3. University of Colorado, Boulder
4. The University of Texas at Austin, ICES
5. Los Alamos National Laboratory
6. Lawrence Livermore National Laboratory
7. University of Illinois at Urbana-Champaign
8. Lawrence Berkeley National Laboratory
9. Rensselaer Polytechnic Institute
10. Lodestar Research Corporation
11. PHWorley Consulting
12. Kitware Inc.
13. University of California San Diego
14. University of Colorado-Denver
15. Massachusetts Institute of Technology, PSFC

PPPL Facilities

Computational Resources

PPPL provides a robust, enterprise quality computing environment in support of the Lab's mission. Its computing resources are primarily housed in the PPL Computing Center (PPLCC). This data center contains the core switches of the PPPL network, business and general purpose servers, networked storage, and high performance research computing clusters.

The center has 4704 sq. ft. of raised floor space. A recent consolidation project freed half the space used for equipment racks (see drawing attached), realizing significant energy efficiency gains. The center also contains a dedicated network engineering lab, a tape vault for long term secure storage of tapes, and a store room for the staging of new equipment and excessing of old. UPS power is provided to critical switches, servers, and storage, and a backup 300KW generator is operational.

Approximately 2000 sq. ft. is free for additional computing capabilities, translating into a build out of ~60 racks. Given the current densities of server and storage systems, the center is capable of physically housing an additional 25,000 CPUs (a 450% increase) and multiple petabytes of storage.

In addition, bandwidth utilization on the two 10Gb ESnet connections has considerable headroom, with utilization rates typically in the 2-8% range. An increase to 50% utilization could be achieved with no negative effect upon network edge performance, but at that level, traffic profiling would be needed to identify internal destinations, so some upgrades to 10Gb may be required internally. The ESnet router to which we connect is capable of 100Gb operation.

Network Infrastructure

PPPL utilizes the Energy Sciences Network (ESnet) for its connection to the Internet. ESnet provides PPPL with two 10Gb circuits, one to a main ESnet router in Vienna, VA, and another to an ESnet router in New York, NY. Traffic is routed based on the shortest distance to the destination.

PPPL also has a dedicated 1Gb circuit to Princeton University main campus, and a closed secure network linking ORNL and ITER (Cadarache, FR) used for the transfer of ITER engineering data.

There are 28 network closets on the PPPL campus, each containing one or more high performance switches. These provide network services to offices and labs throughout PPPL's campus with 100Mb connections to the desktop. 1Gb connections are available upon request. All closets have a 1Gb downlink to the core switch in the PPLCC.

A robust indoor and outdoor network using b/g/n channels provides full wireless coverage.

Dedicated high speed connections are made to the NSTX Control Room and Test Cell. These connections were upgraded to 10Gb in 2015.

A dedicated 10Gb filesystem network is implemented for the Research Computing Clusters, allowing excellent throughput for file system access and transmission of data to/from collaborators offsite. A Globus Online system provides easy to use interfaces for data transfer to/from other research institutions.

Phone services are provided by an internal phone system linking ~2000 phones throughout the lab. This system provides both analog and digital phone lines, as well as VoIP phone service for new construction.

Storage

PPPL provides networked storage via a Storage Area Network, a dedicated fiber optic network linking disk storage arrays with high performance servers. The network operates at 8Gbps. Virtual disk storage arrays serve ~1.3PB of storage, with enterprise reliability, availability, and performance. These arrays can survive multi disk failures with no loss of data.

Server data is backed up to a set of tape libraries, with restoration available up to 6 years after the deletion of data. Copies of these tapes are stored offsite.

Research Computing Clusters

Approximately 7500 processors are available to researchers, both at PPPL and in the fusion research community. These processors are contained in multiple high performance clusters with either 10Gb ethernet or 40Gb Infiniband network meshes connecting nodes in the cluster.

The clusters provide computing resources for the small to mid size jobs (1-256 processors) not favored by the leadership computing sites (like NERSC or ORNL). The PPPL clusters provide quick turnaround, ease of use, high reliability, long runs times, and architectures that allow scaling portability to larger clusters.

Some clusters are application specific. For example, there is a dedicated cluster for TRANSP computing, the tokomak transport code whose use increases substantially each year. These application specific clusters are tuned to the unique characteristics of the codes which they run.

There are also several Symmetrical Multiprocessing (SMP) systems with very large memory sizes (16GB/core) that are utilized by large models.

Experimental Facilities

PPPL is home to the National Spherical Torus Experiment Upgrade (NSTX-U, http://nstx-u.pppl.gov), an innovative magnetic plasma confinement device designed to explore the properties of low aspect ratio (spherical) plasmas. That serves as a principal advantage of NSTX-U, providing data on plasma confinement and turbulence at smaller aspect ratio and magnetic fields than the bulk of the existing tokamak database. Moreover, the values of plasma "beta" (ratio of plasma to magnetic field pressure) attained are significantly higher than those of conventional tokamaks. Relative to the predecessor NSTX, NSTX-U has a new central solenoid and a second neutral beam. The resulting increases in magnetic field, plasma current, and heating power will yield insight into the scaling of the H-mode pedestal and edge plasma turbulence with those parameters. Diagnostics available for studying plasma turbulence include Gas Puff Imaging and Beam Emission Spectroscopy. Numerous other edge, as well as core, diagnostics make NSTX-U a highly qualified validation target for this project.

Description of Facilities and Resources

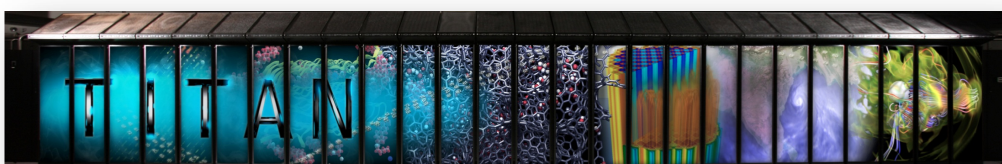
Oak Ridge National Laboratory
and the
UT-ORNL Joint Institute for Computational Sciences

1. Oak Ridge National Laboratory

Computer Facilities. The Oak Ridge National Laboratory (ORNL) hosts three petascale computing facilities: the Oak Ridge Leadership Computing Facility (OLCF), managed for DOE; the National Institute for Computational Sciences (NICS), operated for the National Science Foundation (NSF); and the National Climate-Computing Research Center (NCRC), formed as collaboration between ORNL and the National Oceanographic and Atmospheric Administration (NOAA) to explore a variety of research topics in climate sciences. Each of these facilities has an experienced operational and engineering staff comprising groups in high-performance computing (HPC) operations, technology integration, user services, scientific computing, and application performance tools. The ORNL computer facility staff provides continuous operation of the centers and immediate problem resolution. On evenings and weekends, computer room operators provide front-line problem resolution for users with additional user support and system administrators on-call for problems that require escalation.

Other Facilities. The Oak Ridge Science and Technology Park at ORNL was the nation's first technology park on the campus of a national laboratory. The technology park is available for private sector companies that are collaborating with research scientists. This facility is used to establish new companies from emerging technologies developed at ORNL.

1.1 Primary Systems



Titan is a Cray XK7 system consisting of 18,688 AMD sixteen-core Opteron™ processors providing a peak performance of more than 3.3 petaflops (PF) and 600 terabytes (TB) of memory. A total of 512 service input/output (I/O) nodes provide access to the 32 petabytes (PB) "Spider II" Lustre parallel file system at more than 1 terabyte (TB/s). External login nodes provide a powerful compilation and interactive environment using dual-socket, twelve-core AMD Opteron processors and 256 GB of memory. Each of the 18,688 Titan compute nodes is paired with an NVIDIA Kepler graphics processing unit (GPU) designed to accelerate calculations. With a peak performance per Kepler accelerator of more than 1TF, the aggregate performance of Titan exceeds 27PF. Titan is the Department of Energy's most powerful open science computer system and is available to the international science community through the INCITE program, jointly managed by DOE's Leadership Computing Facilities at Argonne and Oak Ridge National Laboratories and through the DOE Office of Science's ALCC program.

Gaea is a Cray XC40 system consisting of 2,992 compute socket R3 Intel 16-core Haswell processors, providing 47,872 (95,744 logical, when using Intel Hyper-Threading) compute cores, 93.5 TB of double data rate 4 (DDR4) memory, and a peak performance of 1.76 petaflops (PF) all within a small fraction of the footprint of the previously decommissioned XE6 systems. The XC40 uses the Cray Aries Interconnect with the Dragonfly network topology. This provides a higher bandwidth and lower latency interconnect than that of previous systems.

Gaea is supported by a series of external login nodes and a single Lustre file system. The F1 file system is based on more than 2,000 Nearline-SAS drives and provides just under 6 PB (formatted) space to Gaea as well as data transfer capability to the NOAA archive. Gaea is one of NOAA's most powerful computer systems and is available to the climate research community through the Department of Commerce/NOAA allocation mechanisms.

The ORNL Institutional Cluster (OIC) consists of two phases. The original OIC consists of a bladed architecture from Ciara Technologies called VXRACK. Each VXRACK contains two login nodes, three storage nodes, and 80 compute nodes. Each compute node has dual Intel 3.4 GHz Xeon EM64T processors, 4 GB of memory, and dual gigabit Ethernet interconnects. Each VXRACK and its associated login and storage nodes are called a block. There are a total of nine blocks of this type. Phase 2 blocks were acquired and brought online in 2008. They are SGI Altix machines. There are two types of blocks in this family.

- Thin nodes (3 blocks). Each Altix contains 1 login node, 1 storage node, and 28 compute nodes within 14 chassis. Each node has eight cores and 16 GB of memory. The login and storage nodes are XE240 boxes from SGI. The compute nodes are XE310 boxes from SGI.
- Fat nodes (2 blocks). Each Altix contains 1 login node, 1 storage node, and 20 compute nodes within 20 separate chassis. Each node has eight cores and 16 GB of memory. These XE240 nodes from SGI contain larger node-local scratch space and a much higher I/O to this scratch space because the space is a volume from four disks.

EOS is a 744-node Cray XC30 cluster with a total of 47.6 TB of memory. The processor is the Intel® Xeon® E5-2670. Eos uses Cray's Aries interconnect in a network topology called Dragonfly. Aries provides a higher bandwidth and lower latency interconnect than Gemini. Support for I/O on Eos is provided by (16) I/O service nodes. The system has (2) external login nodes.

The compute nodes are organized in blades. Each blade contains (4) nodes connected to a single Aries interconnect. Every node has (64) GB of DDR3 SDRAM and (2) sockets with (8) physical cores each. Intel's Hyper-threading (HT) technology allows each physical core to work as two logical cores so each node can functions as if it has (32) cores. Each of the two logical cores can store a program state, but they share most of their execution resources. Each application should be tested to see how HT impacts performance before HT is used. The best candidates for a performance boost with HT are codes that are heavily memory-bound. The default setting on Eos is to execute without HT, so users must invoke HT with the -j2 option to aprun.

In total, the Eos compute partition contains 11,904 traditional processor cores (23,808 logical cores with Intel Hyper-Threading enabled), and 47.6 TB of memory.

Rhea is a (196)-node commodity-type Linux cluster. The primary purpose of Rhea is to provide a conduit for large-scale scientific discovery via pre- and post-processing of simulation data generated on Titan. Users with accounts on INCITE- or ALCC-supported projects are automatically given an account on Rhea. Director's Discretion (DD) projects may request access to Rhea.

Each of Rhea's nodes contains two 8-core 2.0 GHz Intel Xeon processors with Hyper-Threading and 128GB of main memory. Nine GPU nodes complement the processing power each adding 1TB of main memory and two NVIDIA K80 GPU's, similar to what is in production on Titan. Rhea is connected to the OLCF's 32PB high performance Lustre filesystem "Atlas".

CADES (Compute and Data Environment for Science) facility has been developed as a capability that builds upon ORNL's key strengths in data system infrastructure and delivery of new capabilities through data intensive science to meet the mission needs of R&D projects at ORNL and beyond to address big data analytics and science needs. The technical objective of the CADES facility is to provide a data intensive infrastructure that support the mission needs of key projects at ORNL and external users. The hardware infrastructure will comprise a multi-petabyte data storage environment coupled with a multi-teraop data intensive HPC compute environment and a multi-node cloud compute infrastructure. This system will include the necessary software to apply the system to important data intensive problems at ORNL.

1.2 The Joint Institute for Computational Sciences

The University of Tennessee Knoxville (UTK) and Oak Ridge National Laboratory (ORNL) established the Joint Institute for Computational Sciences (JICS) in 1991 to encourage and facilitate the use of high-performance computing in the state of Tennessee and later expanding to encompass a world-class center for research, education, and training in computational science and engineering. JICS contains a national supercomputing user facility, the National Institute for Computational Sciences (NICS) that has delivered more than 4 billion core hours to the National Science Foundations' (NSF's) open science and engineering community as a founding partner in NSF's national cyberinfrastructure, the eXtreme Science and Engineering Discovery Environment (XSEDE). NICS has supported over 6,500 users in 54 fields of science and engineering. The center's high-bandwidth connectivity up to 100 Gbps ensures seamless access and use of data from multiple sources including UTK and remote sites via Internet2.

JICS advances scientific discovery and state-of-the-art engineering by enhancing knowledge of computational modeling and simulation through educating a new generation of scientists and engineers that are well versed in the application of computational modeling and simulation to solve the world's most challenging scientific and engineering problems. To fulfil these roles in the advancement of computational science and education JICS has a professional and experienced operational and engineering staff comprising group in HPC operations, technology integration, user services, and scientific computing. JICS also employs professional research staff, joint faculty, postdoctoral fellows and students, and administrative staff. UTK/ORNL joint faculty hold dual appointments as faculty members in departments at UTK and as staff members in ORNL research groups. The following items describe the relevant resources JICS and NICS currently operate or have available.

The JICS facility, Figure 1, represents a large investment by the state of Tennessee and features a state-of-the-art interactive distance learning center with seating for 66 people, conference rooms, informal and open meeting space, executive offices for distinguished scientists and directors, and incubator suites for students and visiting staff.

Figure 1 Joint Institute for Computational Sciences building

The JICS facility is a hub of computational and engineering interactions. Joint faculty, postdocs, students, and research staff shares the building, which is designed specifically to provide intellectual and practical stimulation. The auditorium serves as the venue for invited lectures and seminars by representatives from academia, industry, and other laboratories The open lobby doubles as casual meeting space and the site for informal presentations and poster sessions, including an annual student poster session with over 200 presenters.

JICS employs professional research staff, joint faculty, postdoctoral fellows and students, and administrative staff. The joint faculty holds dual appointments as faculty members in departments at UT and as staff members in ORNL research groups.

One of JICS' main projects is the National Institute for Computational Sciences (NICS), originally founded in 2007. The mission of NICS is to enable the scientific discoveries of researchers nationwide by providing leading-edge computational resources and education, outreach, and training. NICS has a professional, experienced operational and engineering staff comprising groups in HPC operations, technology integration, user services, scientific computing, and application performance tools.

1.2.1. JICS Resources

JICS has various resources that are the result of National Science Foundation (NSF) awards, UTK investments, and/or strategic partnerships. These resources are available, based on funding and award status, to researchers at the University of Tennessee, Oak Ridge National Laboratory, JICS partners, and the national science and engineering community through director's discretionary allocations, open calls for proposals, and through the NSF funded Extreme Science and Engineering Discovery Environment (XSEDE) program. Resource allocations are made to researchers based on the discretion of resource or institute directors, internal review, or peer-review. The following sections describe the resources that JICS currently operates.

Darter

Darter is a Cray XC30 system funded from UT investments and NSF award ACI:0711134. This system has 1,448 compute sockets each with an Intel Sandy Bridge processor (8 cores/socket.) In total, the machine provides 240.9 TFlops of compute, 11,584 compute cores, and 23.2 TB of memory. This compute resource is a highly integrated computational platform with a high performance interconnect and Dragonfly network topology. This machine was purchased to provide computational cycles to UTK and other academic institutions. The machine is located in the OLCF computer facility.

Beacon

Beacon is an existing JICS cluster, funded from UT investments and NSF awards OCI:1137907 and ACI:0711134. Beacon is an energy efficient Cray cluster that utilizes Intel Xeon Phi coprocessors. Beacon consists of 48 compute nodes and 6 I/O nodes connected with FDR InfiniBand. Beacon has 768 conventional cores and 11,520 accelerator cores that provide more than 210 TFLOP/s of combined computational performance, 12 TB of system memory, 1.5 TB of coprocessor memory, and over 73 TB of SSD storage. The configuration of Beacon's compute nodes makes it an ideal and versatile platform with 256 GB of RAM, 1 TB of SSD storage, and 16 conventional processor cores per node. Using 36 of these compute nodes, a Green500 run was performed that demonstrated a new world record for power efficiency delivering just under 2.5 GFlops per Watt in November of 2012.

High-Performance Storage

JICS currently supports two Lustre file systems located in the OLCF computer facility. A direct attached scratch file system (connected to Darter) is available and comprised of two couplets of Cray Sonexion 1600 storage controllers and back end disk, accessed through an FDR InfiniBand storage area network (SAN). The Sonexion scratch file system provides approximately 350 TB of short-term, high-performance storage to users, with a peak I/O rate of 11 GB/s. The Medusa file system is a multi-cluster file system implemented as a site-wide file system at NICS. Medusa is currently running as three couplets of DDN 10K controllers and their back-end disks, and is accessed through a QDR InfiniBand storage area network (SAN). The Medusa file system provides approximately a 1.3 PB of capacity with a peak I/O rate of 30 GB/s.

1.3 Computer Facilities

In June 2004, JICS moved into the then brand new 52,000 ft^2 building next door to the ORNL OLCF computer facility. The JICS building has a 1,500 ft^2 computer room, which is home to Beacon. The OLCF computer facility, located on the ORNL campus, is among the nation's most modern facilities for scientific computing and currently is home to Darter and the JICS high-performance file systems. The OLCF facility has 40,000 ft^2 divided equally into two rooms with 9 x 2.5MVA transformers, and another 27,000 ft^2 divided over two rooms in a recently added expansion building with 1 x 2.5 MVA transformer and the ability to expand; and finally 6,600 tons of chilled water – all of which is designed specifically for high-end computing systems. Finally, the UTK campus has a 2,116 ft^2 computer room. ORNL and JICS utilize staff who provide continuous monitoring and immediate problem resolution in all of the computing facilities except UTK, where the UTK Office of Information Technology is responsible. On-site Operators and Tier-1 System Administrators provide front-line problem resolution for users 24x7x265. Additional user support and system administration services are available for issues that require further escalation.

2. Infrastructure

Physical and Cyber Security. ORNL has a comprehensive physical security strategy including fenced perimeters, patrolled facilities, and authorization checks for physical access. An integrated cyber security plan encompasses all aspects of computing. Cyber security plans are risk-based. Separate systems of differing security requirements allow the appropriate level of protection for each system, while not hindering the science needs of the projects.

Network Connectivity. ORNL has access to all major research and education (R&E) networks around the world. Connectivity to these networks is provided via the Department of Energy (DOE) Energy Sciences Network (ESnet), the Southern Crossroads (SoX) southeastern regional R&E exchange, and the ORNL optical network operated by UT-Battelle. ORNL connects to diverse ESnet hubs at 100Gbps and SoX at 10Gbps. The ORNL optical network uses leased fiber-optic cable and connects the OLCF to major networking hubs in Atlanta, Nashville, and Chattanooga.

ORNL network connectivity to university, national laboratory, and industry partners.

The EVEREST laboratory has been upgraded with dual power walls and 3-D capability.

Visualization and Collaboration. ORNL has state-of-the-art visualization facilities that can be used on site or accessed remotely.

ORNL's **E**xploratory **V**isualization **E**nvironment for **RE**search in **S**cience and **T**echnology (EVEREST) facility is a scientific laboratory deployed and managed by the Oak Ridge Leadership Computing Facility (OLCF). The primary mission of this laboratory is to provide tools to be leveraged by scientists for analysis and visualization of simulation data generated on the OLCF supercomputers.

Three computing systems are currently provided in the laboratory. These consist of a distributed memory Linux cluster, a shared memory Linux node, and a shared memory Windows node. Access to the Linux computing resources requires an EVEREST account and an RSA Secure ID. Access to the Windows computing resources requires a standard ORNL UCAMS account and does not require a specific EVEREST account.

Two tiled display walls are provided. The primary display wall spans 30.5' x 8.5' and consists of eighteen 1920×1080 stereoscopic Barco projection displays arranged in a 6 x 3 configuration. The secondary display wall consists of sixteen 1920×1080 Planar displays arrange in a 4 x 4 configuration providing a standard 16:9 aspect ratio.

There are four additional peripheral video inputs located on pop-out boxes in the conference table. Each input supports both digital DVI and analog VGA. Users of the laboratory are welcome to control either wall using personal hardware that is brought into the laboratory. Power outlets are provided at the conference table.

The laboratory instruments are controlled using a touch panel interface located at the control desk. All computing resources can be routed to any available display wall. User hardware using the video input ports on the conference table can also be routed via the touch panel.

High Performance Storage and Archival Systems. To meet the needs of ORNL's diverse computational platforms, a shared parallel file system capable of meeting the performance and scalability requirements of these platforms has been successfully deployed. This shared file system, based on Lustre, Data Direct Networks (DDN), and InfiniBand technologies, is known as Spider and provides centralized access to petascale datasets from all major on-site computational platforms. Delivering more than 1 TB/s of aggregate performance, scalability to more than 20,000 file system clients, and 30-petabyte (PB) storage ca-pacity, Spider is one of the world's largest scale Lustre file system. Spider consists of 36 DDN SFA12KX storage arrays managing 20,160 2-TB Nearline-SAS drives served by 288 Dell dual-socket, quad-core I/O servers Metadata are stored on a NetApp EF560 storage array and are served by eight Dell single-socket, eight-core systems with an aggregate of over 2 Terabytes of memory. ORNL systems are interconnected to Spider II via an InfiniBand system area network, which consists of 3 Mellanox SX6506 Director Class IB switches, and 36 Mellanox SX6036 IB switches; with more than 3 miles of optical cables. Archival data are stored on the center's High Performance Storage System (HPSS), developed and operated by ORNL. HPSS is capable of archiving hundreds of petabytes of data and can be accessed by all major leadership computing platforms. Incoming data are written to disk and later migrated to tape for long term archiving. This hierarchical infrastructure provides high-performance data transfers while leveraging cost effective tape technologies. Robotic tape libraries provide tape storage. The center has six SL8500 tape libraries each holding up to 10,000 cartridges. The libraries house 72 T-10K-D tape drives (8 terabyte cartridges, uncompressed). Several generations of media exist, but all new data is being written to T10K-D. Each drive delivers a bandwidth in excess of 200 MB/s. ORNL's HPSS disk storage is provided by DDN and NetApp storage arrays with nearly 20 petabytes of capacity and over 200 GB/s of bandwidth. This infrastructure has allowed the archival system to scale to meet increasingly demanding capacity and bandwidth requirements with more than 53 PB of data stored as of January 2016.

OLCF tape archive.

Appendix 5: University of Colorado, Boulder Facilities and Other Resources

The University of Colorado, Boulder campus provides a rich environment for research in basic plasma physics. It is the home of the Center for Integrated Plasma Studies, which has active research in theoretical and experimental plasma physics and is well supported by DOE, NSF and NASA. The plasma physics faculty includes five theorists S. Parker, D. Uzdensky, and M. Goldman, J. Cary and M. Horanyi and three experimentalists
T. Munsat, S. Robertson (Emeritus) and S. Kempf. Prof. Munsat is an expert in fluctuation measurements in tokamak plasmas and provides a valuable experimental contact and resource. Prof. Uzdensky is a well-established expert magnetic reconnection and plasma astrophysics. Prof. Cary is an expert on nonlinear dynamics applied to accelerators and transport in toroidal plasmas. Prof. Goldman is an expert in kinetic theory with research primarily on high-frequency nonlinear plasma turbulence in the ionosphere and magnetosphere, as well as kinetic processes during reconnection. An important local resource is the Laboratory for Space Physics (LASP) and the Department of Astrophysical and Planetary Sciences, both of which have many researchers who are very active in space and astrophysical plasma physics. Plasma physics related research is also performed at NCAR, NIST and NOAA laboratories in Boulder. Researchers with expertise in plasma physics in Boulder, both on campus and at the institutes, include Drs. D. Baker, R. Ergun, F. Bagenal, R. Ergun, J. Meiss, D. Newman, G. Lapenta, J. Bollinger, A. Kiplinger and Z. Sternovsky. Additionally, fusion research is performed at Lodestar Research Corporation and Tech-X Corporation, including research physicists Drs. J. Myra, J. Cary and S. Kruger.

Kinetic simulation requires large-scale computing. We have excellent access and computer time allocations at both the Oak Ridge Leadership Computing Facility (OLCF) and the National Energy Research Supercomputer Center (NERSC) at Lawrence Berkeley Laboratory. The University of Colorado computing networks provide the necessary access and bandwidth to the national computer centers across the country. Local computing resources include a broad mix of UNIX workstations. We utilize local cluster computing locally for smaller scale particle simulation research and scientific visualization. The Center for Integrated Plasma studies has a rack-mount Linux cluster for in-house medium-scale computation. We utilize MATLAB and VISIT for simulation data analysis and visualization using low-cost high-performance Linux workstations. We have been quite successful at utilizing high-performance gaming workstations for scientific computing, which is extremely economical.

ICES/POB Facilities and Equipment

ICES and the POB Building

The Institute for Computational Engineering and Sciences (ICES) is located in the O'Donnell Building for Applied Computational Engineering and Sciences (POB) on The University of Texas at Austin main campus. This facility has offices and work areas equipped with desktop computers, printers and copiers, mini-clusters, computational visualization facilities, and extensive network access for faculty, staff, students, and visitors. Several machine rooms distributed throughout the POB house supercomputers, servers, and large-scale storage devices. The building has a 196-seat auditorium with Ethernet ports at each seat. The auditorium also furnishes wireless networking, video conferencing and remote learning capabilities. There are fifteen networked seminar rooms with high-resolution audio visual systems, some with video conferencing and video taping facilities.

POB Building

Networking Infrastructure. The POB building networks are designed to support both bandwidth-intensive computational research and to accommodate new technology when available. The networks are built around high-performance, multilayer Cisco 6509, 2960 and 4003 network switches, with Lucent Gigaspeed copper Ethernet and Multimode Fiberoptic to each desktop and work area. Wireless networking is available throughout the building and courtyard area.

Workstation Environment. The ICES workstation environment encompasses all offices, cubicles, work areas, and laboratories. Over 300 general-purpose workstations are available, including Linux-based PCs, Macs, and Windows PCs. Several color printers and scanners are available. File and email service is provided by a number of Linux servers with over 40 TB of disk storage. Other Mac and Linux-based computers function as web servers, LDAP authentication servers, domain name servers, directory servers, application servers, and compute servers.

On-site Linux-Based Clusters. ICES systems and networking team currently supports nine Linux-based Clusters with others in the planning and design stages. These include the following:

- Bevo3, a 180-core cluster,
- Deanston, a 16-node compute cluster,
- Euclid, a 184-core compute cluster.
- Junior, a 184-core compute cluster,
- Muskoka an 80-processor AMD Opteron Cluster

- Prism2, a 64-core rendering cluster,
- Reynolds, a 256-core compute cluster,
- Ronaldo, a 120-core compute cluster, and
- Stampede_1, a 512-core compute cluster.

Off-site Supercomputing Facilities. ICES has access to supercomputing facilities via high-speed networking at the Texas Advanced Computing Center (TACC) at the J. J. Pickle Research Center, eight miles north of the main campus. At TACC, the two primary HPC production systems include:

- the Lonestar cluster, with 1,888 Dell M610 PowerEdge blade servers, and peak performance of 302 Tflop/s; and
- the Dell-Intel supercomputer, Stampede, which has 102,400 processing cores, 272 TB of total memory, 14 PB of on-line disk storage, and a peak performance of approximately 9.6 Pflop/s. This system was place in production mode in the first quarter of 2013.

As part of the Lonestar system described above, ICES researchers have priority access to approximately 27 million CPU hours in a separate queue at TACC. Compute cycles in this queue are managed by the Institute with allocations awarded weekly.

The long-term storage solution at TACC is an Oracle Mass Storage Facility, called Ranch. Ranch utilizes Oracle's Storage Archive Manager Filesystem for migrating files to/from a tape archival system with a current storage capacity of 60 PB. A 640-TB disk cache enables users to move files between compute resources and tape. Two Oracle SL8500 Automated Tape Library devices house all of the off-line archival storage. Each SL8500 library contains 10,000 tape slots and 64 tape drive slots. Two types of tape media are available, capable of holding 1 terabyte and 5 terabytes of compressed data per tape.

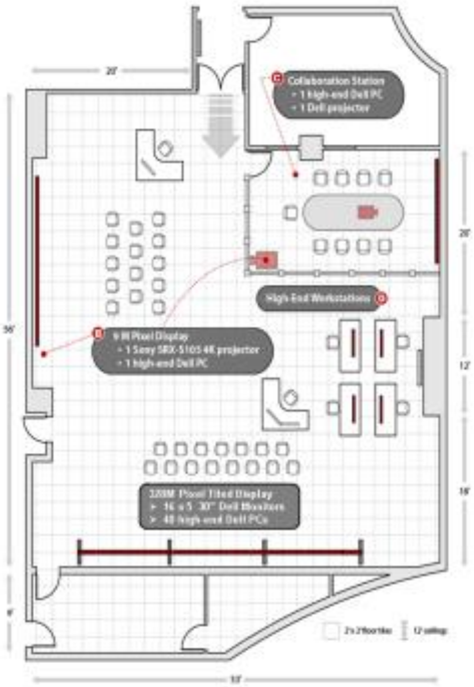
Facilities at TACC also include Corral, a storage system designed to support data-centric science. Corral consists of 5 PB of replicated online disk and a number of servers providing high-performance storage for all types of digital data. The system supports MySQL and Postgres databases, a high-performance parallel file system, web-based access, and other network protocols for storage and retrieval of data to and from sophisticated instruments, HPC simulations, and visualization laboratories.

In FY12-13 Corral was expanded to include 10 PB of raw storage capacity, split between the TACC facility and the Arlington Data Center, which provides geographical replication and high-availability accesses to research data. This repository provides research data storage and access services to researchers at all 15 University of Texas academic and health campuses.

POB Visualization Laboratory:

The POB Visualization Laboratory, managed by TACC, provides an end-to-end infrastructure for data-intensive and display-intensive computing and is available to all UTA investigators as well as UT System users. The lab includes a Dell visualization cluster, *Stallion*, with a 16 x 5 - 328 megapixel tiled display; *Bronco* a Sony 9M pixel flat projection system driven by a high-end Dell workstation; Lasso, a 12.4-megapixel touch sensitive display screen; and *Mustang*, a 55-inch LED display with active 3D stereo capabilities. These systems provide a unique environment for interactive and immersive visual exploration.

Brief descriptions of these systems are given below.



POB Visualization Laboratory

Dell Visualization Cluster and 328 Megapixel Tiled Display (Stallion).

The Stallion cluster provides users with the ability to perform visualizations on a large 16 x 5 tiled display of Dell 30-inch flat panel monitors, for 328 megapixel resolution. This configuration allows for exploration of visualizations at an extremely high level of detail and quality. The cluster allows users to access to over 80GB of graphics memory, 1.2TB of system memory, and 240 processing cores. This configuration enables the processing of datasets of a massive scale, and the interactive visualization of substantial geometries.

Sony SRX-S105 (9M Pixel) Projection System (Bronco).

The Sony projection system, Bronco, features a 20 ft. x 11 ft., 4096 x 2160 resolution flat-screen display, driven by a Sony SRX-S105 overhead projector and a high-end Dell workstation. This configuration provides users with the added flexibility to run a wide variety of applications, as only one workstation is required to drive the display. The projector gives exceptional brightness and a high resolution, 9M pixel viewing area. In addition, Bronco may be configured to accept inputs from up to four simultaneous video sources, allowing for a hybrid display of multiple systems.

12-Megapixel Touch Display System (Lasso).

Lasso is a touch display system consisting of six - 46 inch HD thin-bezel displays driven by a single compute node. The compute node features AMD Eyefinity technology for a seamless display surface, allowing for a tiled-display environment without the need to write parallel graphics applications. The display surface is supplemented by an infrared touch-sensitive perimeter with 5mm touch precision and the capability to detect 32 touch points simultaneously. Lasso is also augmented with a Microsoft Kinect for touchless interactions.

Collaboration Room (Saddle).

The collaboration room offers the opportunity for small groups to work together on developing and exploring visualizations. The display is provided by a high resolution projector with many possible input combinations. The room also includes a 5.1 theater stereo system with Blu-Ray capability. Users may develop their visualizations in the room, and then easily transition them to one of the two larger display systems in the main lab area at a later time.

Stereoscopic 3D Visualization System (Mustang).

The Vislab also includes Mustang, a Stereoscopic 3D system that can be used in visualization to render depth as a result of parallax generated by active and passive stereoscopic technologies. Mustang is equipped with the latest active stereoscopic technology, using Samsung's 240 Hz stereo output modes in conjunction with a 55-inch LED display panel.

TACC Facilities, Equipment, and Other Resources

Texas Advanced Computing Center

The Texas Advanced Computing Center (TACC) at The University of Texas at Austin (UT Austin) develops and deploys an integrated cyberinfrastructure of advanced computing resources to enhance the research and education activities of the faculty, staff, and students at UT Austin, and in Texas and across the US through its involvement in various state and national programs. This infrastructure includes high performance computing (HPC) systems, advanced scientific visualization systems, data analytics systems, cloud computing systems, data servers and storage/archival systems, IT systems, high-bandwidth networks, and a comprehensive software environment comprising applications, tools, libraries, and databases. Services include documentation, consulting, and training in a wide variety of advanced computing topics.

Data Center Facilities

TACC's storage, visualization, and computing systems are housed in the TACC data center located in the Research Office Complex Building on the J. J. Pickle Research Campus of The University of Texas at Austin. This 15,000ft^2 raised-floor facility is served by a dedicated chilling plant capable of producing 3750 tons of chilled-water cooling capacity and 10MW of highly reliable power supplied by the City of Austin. The datacenter is set up with In-Row Chillers (IRCs) in an enclosed hot aisle configuration, which brings chilled water next to each compute rack. All storage, critical management and switch infrastructure will be backed up via a 400kVA UPS providing several hours of battery power. Individual blade chasses will employ a redundant power supply configuration using two separate 415V, 3-phase circuits provided to each rack to mitigate the effect of a single circuit failure. In the event of a chilled-water system failure, each node and chassis, as well as the servers and disk arrays, in the system will automatically shut down if the internal temperature exceeds a preset safety threshold. The data center is monitored 24x7 by TACC operations staff and UT facilities personnel. TACC also operates a data center in the Commons Building (CMS), also located on PRC. The CMS date center provides 3,800 square feet of raised floor and a robust power and cooling infrastructure that was upgraded in 2010. TACC also uses UT Arlington's data center for a replicated data storage system.

Advanced Computing Systems

Stampede, a large-scale supercomputing resource, was deployed in January 2013 with 10 PFlops of theoretical peak performance. Stampede is a Dell Linux cluster with Dell DCS servers using Intel Xeon E5 8-core processors for a total of 102,400 2.7 GHz cores connected via FDR InfiniBand through Mellanox core switches. Stampede has more than 270 TB of memory and 14 PB of disk storage. Stampede is equipped with 6,880 of the 61-core 1.1 GHz Intel Xeon Phi SE10P Co-Processor cards each offering ~1 TFlops of peak computational capability and 8 GB of GDDR5 memory. This innovative capability offers enhanced computing with a familiar MPI or OpenMP programming model. Stampede is equipped with sixteen 1 TB shared-memory nodes and 128 compute nodes with NVIDIA K20 GPUs. These additional nodes support remote visualization, GPU programming, and large shared-memory parallel programs.

Lonestar contains 23,184 cores within 1,888 Dell PowerEdgeM610 compute blades (nodes), 16 PowerEdge R610 compute-I/Oserver-nodes, and 2 PowerEdge M610 (3.3GHz) login nodes. Each compute node has 24GB of memory, and the login/development nodes have 16GB. The system storage includes a 1 PB parallel (SCRATCH) Lustre file system, and 276 TB of local compute-node disk space (146 GB/node). Lonestar also provides access to five large memory (1 TB) nodes, and eight nodes containing two NVIDIA GPU's, giving users access to high-throughput computing and remote visualization capabilities respectively. A QDR InfiniBand switch fabric interconnects the nodes (I/O and compute) through a fat-tree topology.

Wrangler, the TACC DELL/DSSD Data Analytics system, was deployed in February 2015. This system has a large 10 PB storage system replicated between TACC and Indiana University to provide researchers with storage and services to support the full lifecycle of data, from data capture, translation, integration, analysis, collaboration, and final publication. To support the typically I/O bound workflows that drive this lifecycle, Wrangler features 120 dual core Intel Haswell CPU based servers, each with 128 GB of memory, 96 at TACC and 24 at Indiana University. The 96 nodes at TACC are also connected via PCI to a shared 500 TB flash based storage system capable of delivering I/O rates to the cluster of 1 TB/s and 200 million IOPS. The compute cluster is connected to the 10 PB storage array via non-blocking InfiniBand FDR networking and a 40 Gbps Ethernet network.

Rustler is a data analytics system dedicated to supporting workflows using Hadoop MapReduce and other Hadoop Distributed File System based tools. The system uses 64 Hadoop data nodes, each a Dell R720XD dual socketed Ivy Bridge server with 128 GB of RAM and sixteen 1TB disks, as the compute and HDFS servers. The system is controlled from two Hadoop Name Nodes with identical specifications supporting the YARN job manager. Migration of data in and out of the HDFS file system is supported by the system login node, which has 34 TB of local storage space as a traditional UNIX file system to be used to migrate data to and from the primary HDFS storage system.

Rodeo is a powerful cloud resource that allows for the full customization of computational environments, the ability to archive these environments, and easy access to stored data from any location. Rodeo lets users create virtual machines, host data, and provide services like science Gateways. Rodeo offers researchers the ability to easily conduct a variety of scientific activities including modeling and simulation, visualization, data analytics and management. Rodeo has 80 nodes with 16 TB of total memory, 875 TB of storage, and a 10 Gbps interconnect.

Chameleon is an experimental testbed for cloud software, architecture, and applications. Consisting of a set of standard cloud units (SCUs), 10 at TACC and 2 at the University of Chicago (UC), an SCU is a self-contained rack with all the components for a complete cloud infrastructure, and the capability to combine with other SCUs to form a larger experiment. An SCU rack consists of 42 Dell R630 servers with dual 12-core Intel Haswell processors with 128 GB of RAM; Dell S6000 OpenFlow compliant switches at 10Gbps to enable software-defined networking; 4 Dell FX2 storage servers, each with sixteen 2TB drives, totaling 128 TB of raw disk storage with dual Intel Haswell processors, that can be combined across SCUs to create a significant Hadoop infrastructure with more than a PB of storage. A Fourteen Data Rate (FDR) InfiniBand network is deployed on one SCU at TACC to allow exploration of alternate networks. The

SCUs are supplemented by a set of heterogeneous cloud units (HCUs) that incorporate a wide variety of alternate processor and network technologies within the testbed.

Jetstream, a production cloud computing resource to be deployed in early 2016, is a self-service cloud to increase participation in advanced computing for researchers who need flexible, reproducible, powerful and easy-to-use computing. Jetstream will feature a rich catalog of project- and user-contributed VM "appliances" configured to support varied uses such as 3D image reconstruction, natural language processing, basic software development, and biostatistics. Furthermore, VM images will be sharable outside of Jetstream and can be associated with citable Digital Object Identifiers (DOIs). Thus, all the computational requirements to do an analysis – data, software code, and scripts – can be packaged up in and published to a digital library. Jetstream will provide more than 0.5 PFlops of computing power using Intel Haswell processors, with 1.3 PB of node local storage and 2 PB of secondary storage, distributed equally between TACC and Indiana University.

Network Connectivity and Cybersecurity

TACC maintains a high-speed internal 40/10GigE network using a Juniper EX9214 switch to provide connectivity between each of the production systems, with multiple network paths to commodity networks and to XSEDE via 100GigE connections into a Juniper MX480 core router. A Juniper SRX 3600 redundant firewall protects the systems, and a cluster of servers running the “Bro” intrusion detection system monitors network traffic. TACC is connected to Internet2 (I2) via 100GigE link operated by UT Austin, with additional routing for commodity Internet traffic. TACC’s network connects to the UT Austin network via multiple protected and redundant 10GigE links as well. The external 100GigE and failover 10GigE connections currently run across the Texas high-speed networks to Houston where it connects to the Houston GigaPOP. With these two multiple redundant network paths, connectivity to TACC systems from other locations in the US is maintained even if one of the fiber paths is interrupted. The I2 100GigE connection provides ample bandwidth for users accessing the system from non-XSEDE sites, since most universities and research labs are or will be connecting to I2. TACC is monitoring the development of new 25/50GigE network hardware and will switch to these new standard speed networks should costs merit it.

Global Work File System

TACC maintains a 25 PB Lustre global work file system for all users of TACC resources, which is available to users of of any one of TACC’s data- or compute-intensive HPC systems. This global storage is hosted on a DataDirect Networks (DDN) SFA12K-40 storage solution leveraging 64 OSS servers and 16 LNET Routers to provide more than 100 GB/s throughput to the current Stampede system. The system was designed to support future growth needs, as the current system can handle double the current disk capacity. Further, this system can sustain 256 GB/s throughput with the current hardware.

Archival Storage
TACC provides users a tape-based archival storage system, Ranch, with 160PB maximum capacity and 2PB of RAID-6 disk cache. Ranch has two StorageTek SL8500 modular tape libraries containing 24 StorageTek T10K-D and 16 T10K-C tape drives with an aggregate write speed of 6GB/s. Stampede 2 will have access to six data movers for transfer to Ranch.

Additional Data Systems
Corral, a storage and data management resource, is designed and optimized to support large-scale collections and a collaborative research environment. Corral consists of two replicated 6 PB disk arrays, installed at UT Austin and UT Arlington, along with 24 Dell servers providing high-performance storage and services for all types of digital research data. Corral provides a high performance file system accessible directly or via an iRODS data grid, MySQL and Postgres databases, and web access for data sharing. Various other services are also provided to facilitate storage and retrieval of data from sensor networks, specialized research instruments, and HPC and visualization resources.

Visualization Resources
TACC operates the Visualization Laboratory (VisLab), a 2900 square foot facility located in the Peter O'Donnell Building on the UT Austin main campus. The VisLab currently houses Stallion, which consists of 20 Dell Linux workstations, 20 NVIDIA K5000 GPUs and 80 Dell 30" widescreen displays, increasing the aggregate resolution to ~327M pixels. In addition, the VisLab includes a 9M pixel Sony front-projection system with a 20'x11' screen (Bronco), stereo capability (Mustang), and a 3x2 tiled display with a PQ Labs overlay providing 32point/5mm touch capability (Lasso). The VisLab includes 4 high-end workstations for individual use and a collaboration room with a conferencing and projection system (Saddle). Stereo and immersive capabilities are provided with a ZSpace display and an Occulus Rift.

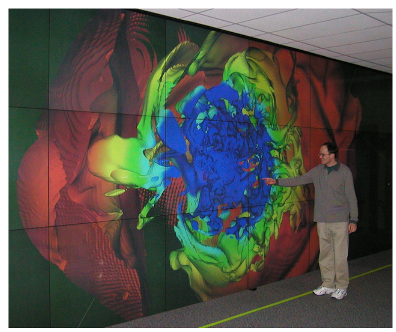
Maverick, the TACC HP/NVIDIA dedicated visualization and data analysis resource, began production in February 2014. This system is a hybrid CPU/GPU system designed for remote, interactive visualization and data analysis. In addition, Maverick supports production, compute-intensive calculations on both the CPUs and GPUs. Maverick consists of 132 dual-socket HP nodes with 10-core Intel Xeon E5-2680 v2 Ivy Bridge CPUs, 265 GB of RAM, and a single NVIDIA Tesla K40 "Atlas" GPU with 12 GB of RAM. The total system has 2640 compute cores, 132 GPUs, and 34.5 TB of aggregate memory all connected via Mellanox FDR InfiniBand. Maverick connects to Stockyard, TACC's 25PB shared Lustre filesystem.

Office Facilities
The main offices are located in the Research Office Complex (ROC) at the UT Austin J. J. Pickle Research Campus (PRC), nine miles northwest of the main campus. The ROC is a joint facility that serves as home to both TACC and the UT Institute for Geophysics (UTIG). The ROC is approximately 90,000 square feet, with about 40,000 square feet

allocated to TACC's first floor and 50,000 square feet to the UTIG second and third floors. TACC's floor includes nearly 100 offices for staff and a workspace for students, as well as 6 conference rooms and two large training/seminar spaces. An expansion is underway that will be completed in early 2016, a 3-story, 38,000 square foot building that will connect to the existing ROC and will add more than 60 offices, a 260-seat auditorium, an additional 50-seat training room, a visualization lab, and more space for students. TACC has several offices on the main UT Austin campus in the Peter O'Donnell Building for Applied Computational Engineering and Sciences for staff and students to operate the VisLab and to collaborate with researchers on the main campus.

Los Alamos National Laboratory Facilities and Resources

Members of the proposed effort will have access to state-of-the-art facilities at Los Alamos National Laboratory (LANL). These resources come in the form of production systems that are part of LANL's Institutional Computing resources and additional testbed systems devoted to supporting active research and development activities.



The current available institutional computing systems that we have access to include:

- **Grizzly**: Based on Penguin Computing's TundraES Family which uses their Relion module. Comprises 1490 nodes, with 36 cores per node using the Intel Xeon Broadwell processor and Intel Omni-Path Interconnect. Aggregate cluster performance is 1.8 PF/s with 191 TB of memory on 53,640 cores.

- **Wolf**: Comprises 616 compute nodes with 16 cores per node, totalling 9856 cores and 205 TFlops. It has 24 I/O nodes. Compute nodes and I/O nodes employ the 8-core Intel Xeon SandyBridge processor. The nodes are connected together with a Qlogic Infiniband (IB) Quad Data Rate (QDR) network in a fat tree topology, using a 7300 Series switch.

The current set of available testbed systems that we have access to include Darwin. **Darwin** is an ASC R&D testbed HPC cluster with 210 nodes. It contains many different server architectures and accelerators. It is designed to facilitate research and development work for ASC and ASCR projects by coalescing cutting-edge hardware and software into a single cluster to leverage common network and storage resources in a unified OS environment. Darwin has over 30 server models in many configurations. The default SLURM partition has nodes with x86_64, ppc64, ppc64le, and arm64 instruction sets, RAM varying from 8GB to 1.5TB, and cores counts from 4 to 72. Many nodes contain GPUs.

Description of Facilities and Resources

Livermore Computing | Lawrence Livermore National Laboratory (LLNL)

LLNL computational scientists are supported by Livermore Computing (LC), which delivers a balanced High Performance Computing (HPC) environment with constantly evolving hardware resources and a wealth of HPC expertise in porting, running, and tuning real-world, large-scale applications. Currently LC delivers multiple petaflops of compute power, massive shared parallel file systems, powerful data analysis platforms, and archival storage capable of storing hundreds of petabytes of data. This balanced hardware environment supports key collaborations between LLNL applications developers and LC experts on the creation, production use, and performance monitoring and analysis of results of HPC parallel applications in a wide variety of scientific disciplines.

Major systems include the 20 PFLOP Sequoia system with a 55 PB file system, the 5 PFLOP Vulcan system, the Jade and Quartz systems at 3 PFLOPs each, the 970 TFLOP Zin system, the 431 TFLOP Cab system, and additional large multi-core, multi-socket Linux clusters with a variety of processor types, ranging from IBM PowerPC to Intel Broadwell processors, and nVidia Graphical Processing Units (GPUs) for some platforms. In total, more than 135,000 nodes with more than 2,300,000 cores and more than 3.2PB of memory are available across the production LC systems on two networks.

Computational scientists may also take advantage of several testbeds for evaluating next generation hardware and software. Researchers use these testbeds to investigate hardware advances in areas such as multi-core processors, neuromorphic computing, networking technologies, I/O, GPUs, memory, and power-aware HPC (via a dedicated power lab), as well as investigations of software technologies. In addition, LC hosts production collaboration environments that facilitate the sharing of scientific data among international research groups, including the Green Data Oasis and the Green Collaboration Environment with a Linux cluster and storage resources available to collaborators worldwide.

Several facilities house the simulation infrastructure at LLNL. The largest (LEED-certified) simulation facility offers 48,000ft^2 and 37.5MW of power for systems and peripherals, and additional power for the associated cooling system. Engineering and facilities staff maintains it in a physically secure environment.

The balanced LLNL simulation environment includes Lustre multi-cluster file systems, HPSS-based archival resources, a Federated Ethernet networking infrastructure, advanced visualization resources, and a rich tool environment, as described below.

Lustre: LLNL contributes to the development of and supports the open source Lustre parallel file systems, which are mounted across multiple compute clusters and delivers high-performance, global access to data.

High Performance Archival Storage: LC provides high-performance archival storage services via High Performance Storage System (HPSS). A world-class array of hardware integrated beneath HPSS includes disk arrays, tape subsystems, mover nodes, networks, robotics, and petabytes of media.

LC Networking: LC's simulation environment includes a Federated Ethernet networking infrastructure as well as Infiniband SANs. LC employs InfiniBand and Omni-Path fabrics for high-speed interconnects. Testbed work includes evaluation of next generation networking equipment.

Visualization facilities: Data analysis resources include the 324-node Max machine with more than 82 TB of memory and the 162-node Surface machine with 41 TB of memory and 316 Kepler K40 GPUs. These interactive data analysis machines are equipped with high-speed access to Lustre and local NFS storage. LC operates several visualization theaters, ranging from auditoriums with PowerWalls to smaller collaboration spaces.

HPC Tool Environment: LC provides a stable, usable, leading-edge parallel application development environment that significantly increases the productivity of applications developers by enabling better scalable performance and enhancing application reliability. The tool environment includes high-performance compilers, debuggers, analyzers, editors, and locally developed custom libraries and application packages for software development. Through collaborations with vendors and other third party software developers, LC ensures a complete environment that meets the needs of today's code developers while steering their code development to exploit emerging technologies.

Primary Production Computing Platforms

Sequoia and Vulcan: Sequoia is a 20 PFLOP system based on IBM BlueGene Q (BG/Q) technology. Rated the most powerful supercomputer in the world in June, 2012 shortly after its arrival, Sequoia has 1.6 petabytes of memory, 96 racks, 98,304 compute nodes, and 1.6 million cores. Vulcan is a BG/Q system one-quarter the size of Sequoia, running on the unclassified network. The BG/Q machines are based on the POWER architecture.

Jade and Quartz: Identically configured Penguin Computing systems, Jade and Quartz each have 2,688 nodes and 343 TB of memory and a peak speed of 3.2 PFLOPs. Each system is a 14 Scalable Unit multiprocessor cluster with Intel Broadwell processors.

Zin: A Cray system with 2,916 nodes and 93.3 TB of memory, Zin has a peak speed of 970 TFLOPs and uses Intel Sandy Bridge processors.

Cab: A Cray system with 1,296 Intel Sandy Bridge nodes and 41.5 TB of memory, Cab has a peak speed of 431 TFLOPs. Cab has Intel Sandy Bridge processors.

Syrah: This Cray system is a multi-core, multi-socket Linux cluster. Syrah has 324 nodes and 20 TB of memory, clocking in at a peak speed of 108 TFLOPs.

Catalyst: A Cray cluster with 304 nodes, 7,776 cores, 41.5 TB of memory and 243 TB of NVRAM this system is part of a partnership between LLNL, Intel and Cray focusing on HPC big data technologies, architectures and applications.

For a complete list of more than 20 production compute platforms supported by LC, see the **Livermore Computing Systems Summary.**

Institutional Resources and Facilities

LLNL researchers benefit from an institutional IT infrastructure that provides desktop support and experts in server technologies. The latter includes virtualization expertise that has been applied to provide multiple operating systems on shared resources and to create a wide variety of virtual machines to leverage resources servers across LLNL. Networking service is also provided by an enterprise team. Connections into LLNL include ESnet and a wide variety of programmatic networks.

UIUC - Facilities and other Resources

University of Illinois at Urbana-Champaign

The College of Engineering at the University of Illinois offers an excellent education to its students, providing a ready source of talented people who are eager to learn and are carry out high-quality research. The University of Illinois at Urbana Champaign is a center for supercomputing applications and maintains excellent computing resources. Several machine shops on the engineering campus provide modern in-house fabrication capability. In addition to these resources, the Center for Plasma Material Interactions (CPMI) offers a stimulating and well-equipped plasma laboratory environment for the preparation of plasma-exposed samples. The CPMI has access to the Center for Microanalysis of Materials (CMM). The CMM is a user-oriented and user-friendly Department of Energy/Basic Energy Sciences user facility that provides the modern analytical capabilities essential to today's materials science. The Center is an integral part of the Frederick Seitz Materials Research Laboratory (MRL) on the campus of the University of Illinois at Urbana-Champaign. By using the CMM center, the members of CPMI can access 30 major instruments in the areas of electron microscopy (SEM, TEM) scanning probes, surface microanalysis (AFM, EBSD, Profilometer, Ellipsometer), X-ray diffraction (XRD), and back-scattering spectroscopies (Raman, RBS, AES, XPS, TOFSIMS). The breadth of instrumentation available through the center enables researchers to find the best combination of analytical techniques for their specific needs.

Blue Waters

Blue Waters is one of the most powerful supercomputers in the world, and is the fastest supercomputer on a university campus. Scientists and engineers across the country use the computing and data power of Blue Waters to tackle a wide range of challenging problems, from predicting the behavior of complex biological systems to simulating the evolution of the cosmos. We use the system for simulations of plasma-material interactions and nano-structuring. The facility provides a sustained-petascale high-performance computing resource and support to researchers at the University of Illinois and across the country. Up to 7% of the computing capacity of Blue Waters, or about 10-13 million node-hours each year, is reserved for faculty and staff at the University of Illinois at Urbana Champaign on a peer-review base.

Illinois Campus Cluster

The shared Illinois Campus Cluster at the University of Illinois Urbana Champaign is a collectively researcher-owned and researcher-controlled computational resource. It is operated on behalf of the campus by the National Center for Supercomputing Applications (NCSA), which has more than 25 years of experience deploying and supporting high-performance computing resources. The first shared system became operational in March 2011, and it has now been greatly expanded.

The infrastructure includes two clusters “Taub” and “Golub”, designed to support up to 512 nodes with QDR Infiniband (Taub) and FDR InfiniBand (Golub) for applications communications and data transport with a Gigabit Ethernet control network. Few technical features are reported in the table below.

More details on the clusters can be found at https://campuscluster.illinois.edu

Taub cluster	**Golub cluster**
Head nodes: DL380 G7 Admin Nodes with: - (2) Intel E5650 2.67GHz Hex Core Proc. 95W - 24 GB RAM via (12) 2GB 2Rx8 PC3-10600E-9 DIMMs - HP P410 Smart Array Controller with 512MB BBWC cache - (2) HP 146GB 6G SAS 10K 2.5in DP ENT HDD - HP IB 4X QDR CX-2 PCI-e G2 Dual Port HCA	*Login Nodes*: (4) Dell PowerEdge R720 Login Nodes each configured with: - Intel E5-2660 2.2GHz 8 Core Processors, 95W - 128 GB RAM via (16) 8GB 1333MT/s RDIMMs - (2) 300GB 6G SAS 10K 2.5in HDD - Mellanox ConnectX-3 FDR IB HCA - (2) NVIDIA TESLA M2090 GPUs
Compute Nodes: maximum count (164) HP s6500 4U Chassis each with: - HP 1200W CS HE Power Supply Kit - (8) HP s6500 Redundant Fan Kit (512) Compute Nodes — HP SL390G7 1U Servers each configured with: - (2) Intel HP X5650 2.66Ghz 6C Processors, 95W 12, 24, 48, or 96GB RAM at customers choice - HP 160GB 3G SATA 7.2K 3.5in QR ETY HDD HP IB Enablement Kit	*Compute Nodes*: maximum count (72) Dell PowerEdge C8000 4U Chassis each with: - (2) 1400W Power Supply Units - (6) 6 x 120mm high-efficiency fans with PWM control (512) Compute Nodes Dell C8220 compute sleds each with: - (2) Intel E5-2670 2.60GHz, 20M Cache, 8C, 115W - 32, 64, 128GB RAM at customers choice - (2) HD 1TB, 7200 RPM, SATA, 3Gbps, 2.5in - (4) Intel Ethernet Controller i350 Compute Node Options: - Mellanox ConnectX-3 FDR IB HCA - (3) NVIDIA TESLA M2090 GPUs

LBNL Facilities & Other Resources

Lawrence Berkeley National Laboratory is the leading provider of computing and networking resources supporting the DOE Office of Science's research mission. Berkeley Lab researchers have access to leading-edge computing platforms and services at the National Energy Research Scientific Computing Center (NERSC) and have 100 Gbps connectivity to other national labs and institutions via ESnet, DOE's Energy Sciences Network, both of which are managed by Berkeley Lab. The lab also manages several departmental clusters.

At the end of 2015, NERSC moved from its facility in Oakland to the newly built Shyh Wang Hall on the main Berkeley Lab campus. The move re-unites NERSC with the staff of ESnet and the Computational Research Division and is expected to lead to more collaboration.

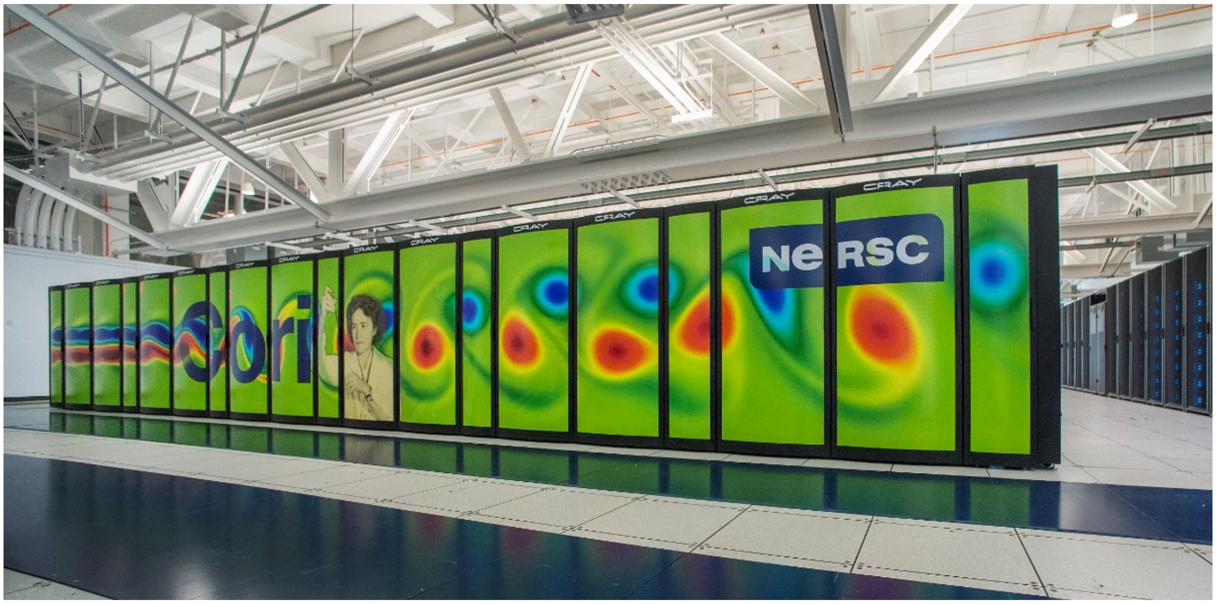
NERSC

In addition to providing world-class supercomputers, NERSC staff provide expert support to ensure users make the most efficient and effective use of the resources. This support has made NERSC one of the most scientifically productive centers in the world – in 2016, NERSC users reported more than 2,000 refereed papers based on work performed at the center and NERSC staff contributed some 120 papers to scientific journals and conferences.

Coinciding with the move was the installation of NERSC's newest supercomputer, an Intel-based Cray XC40 with a theoretical peak performance of 30 petaflop/s and will deliver 10x the sustained computing capability of NERSC's recently retired Hopper system, a Cray XE6 supercomputer. Named "Cori" in honor of biochemist Gerty Cori, the first American woman to receive a Nobel Prize in science, the system has a number of new features that will benefit data-intensive science. Cori was delivered in two phases. The first phase — also known as the Data Partition — was installed in late 2015 and comprises 12 cabinets and more than 1,600 Intel Xeon "Haswell" compute nodes. It was customized to support data-intensive science and the analysis of large datasets through a combination of hardware and software configurations and queue policies..

The second phase of Cori, installed in summer 2016, added another 52 cabinets and more than 9,300 nodes with second-generation Intel Xeon Phi processors (code-named Knights Landing, or KNL for short), making Cori the largest supercomputing system for open science based on KNL processors. With 68 active physical cores on each KNL and 32 on each Haswell processor, Cori has almost 700,000 processor cores. The two phases of Cori are integrated via the Cray Aries interconnect, which has a dragonfly network topology that provides scalable bandwidth.

Cori features a Burst Buffer based on the Cray DataWarp technology. The Burst Buffer, a 1.5 PB layer of NVRAM storage, sits between compute node memory and Cori's 30-petabyte Lustre parallel scratch file system. The burst buffer provides about 1.5 TB/sec of I/O bandwidth, more than twice that of the scratch file system.. . NERSC has also added software defined networking features to Cori to more efficiently move data in and out of the system, giving users end-to-end connectivity and bandwidth for real-time data analysis, and a real-time queue for time-sensitive analyses of data.



NERSC's other large system is Edison, a Cray XC30 supercomputer that is the first Cray supercomputer with Intel processors, a new Aries interconnect and a dragonfly topology. Installed in 2013, Edison was designed to optimize data motion—the primary bottleneck for many of our applications—as opposed to peak speed. It has very high memory bandwidth, interconnect speed and bisection bandwidth. In addition, each node has twice the memory of many leading systems. This combination of fast data motion and large memory per node make it well suited for both our traditional HPC workload and newly emerging data intensive applications. Edison features 124,608 compute cores for running scientific applications, 332 terabytes of memory, and 7.6 petabytes of online disk storage with a peak I/O bandwidth of 144 gigabytes (GB) per second. Edison has a theoretical peak performance of 2.39 petaflops/second.

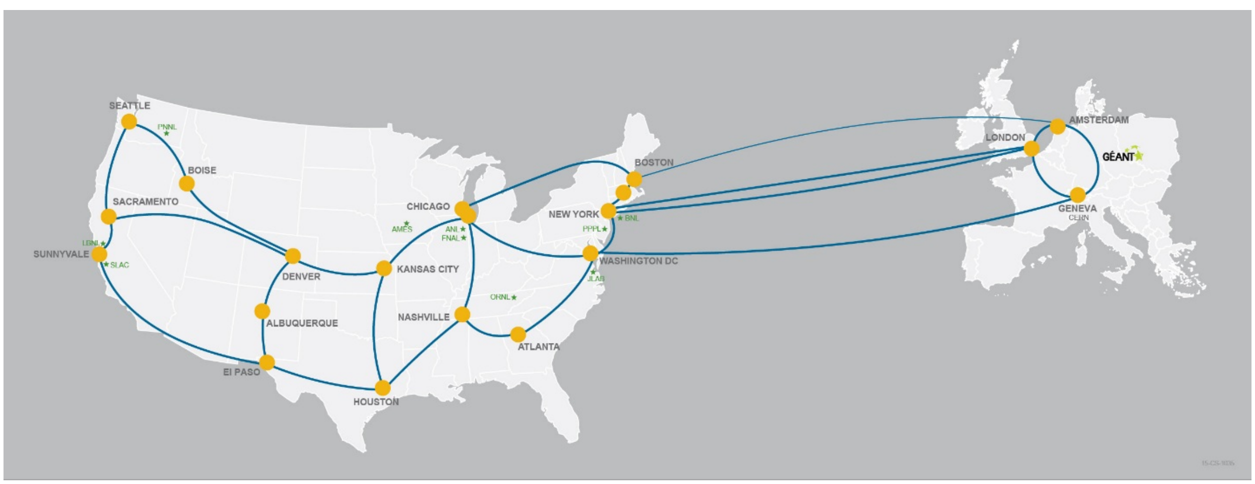
NERSC's research in data-intensive computing is grounded in their operation of a major production facility, the PDSF (Parallel Distributed Systems Facility). PDSF is a networked distributed computing environment used to meet the detector simulation and data analysis requirements of large scale Physics, High Energy Physics and Astrophysics and Nuclear Science investigations.

All NERSC systems are connected to the NERSC Global Filesystem (NGF), a collection of center-wide file systems, based on IBM's GPFS, available on nearly all systems at the facility. The several different file systems comprising NGF, including one providing a common login user environment for all our systems, one for sharing data among collaborators on a science project or team, and one for high bandwidth short term storage across systems at the facility. The main focus of NGF is data sharing, ease of workflow management (i.e., not moving data around or maintaining unnecessary copies of data), and data analysis.

Finally, these systems are connected to a High Performance Storage System (HPSS) for archival storage. NERSC's HPSS system currently contains more than 42 petabytes, making it one of the largest unclassified archival storage systems in the world.

ESnet

Access to Berkeley Lab's computational and experimental facilities from anywhere in the U.S. or the world is available through ESnet, which provides a 100-gigabit Ethernet backbone connection between NERSC, LBNL and other DOE national laboratories. In December 2014, ESnet extended its connectivity to Europe with three 100 Gbps links and one 40 Gbps connection. ESnet also provides major backbone links including peering with hundreds of domestic and international research and education networks.



ESnet
ENERGY SCIENCES NETWORK

★ Department of Energy Office of Science National Labs

Ames	Ames Laboratory (Ames, IA)	LBNL	Lawrence Berkeley National Laboratory (Berkeley, CA)
ANL	Argonne National Laboratory (Argonne, IL)	ORNL	Oak Ridge National Laboratory (Oak Ridge, TN)
BNL	Brookhaven National Laboratory (Upton, NY)	PNNL	Pacific Northwest National Laboratory (Richland, WA)
FNAL	Fermi National Accelerator Laboratory (Batavia, IL)	PPPL	Princeton Plasma Physics Laboratory (Princeton, NJ)
JLAB	Thomas Jefferson National Accelerator Facility (Newport News, VA)	SLAC	SLAC National Accelerator Laboratory (Menlo Park, CA)

Rensselaer Polytechnic Institute

Center for Computational Innovations

The Center for Computational Innovations (CCI) is housed in a 22,000 square foot facility at the Rensselaer Technology Park. It includes a 4,500 square foot machine room, offices and space for industry visitors. The CCI operates heterogeneous supercomputing systems consisting of massively parallel IBM Blue Gene supercomputer and Intel Xeon processor-based clusters. The computational power of the current hardware configuration is rated at over 1 petaflop peak. The CCI system is supported by over a petabyte of disk storage. The CCI has dedicated high-speed connections to the main campus and to the NYSERNet optical infrastructure that provides access to the national and international high-speed networks.

The CCI Computational Facilities:

- Blue Gene/Q: 5 racks (5K nodes, 80Kproc) with 80 TB of RAM total
- Intel Xeon Cluster #1: 32, 8-way Xeon processors with 256 GB of RAM each.
- Intel Xeon Cluster #2: 64, dual 8-way Xeon processors with 128GB of RAM each.
- Parallel Storage: 2.1 Petabytes disk storage over GPFS parallel file system.
- Network: 384-port non-blocking 56Gbps/FDR Infiniband interconnect.

Scientific Computation Research Center Computing Facilities

Rensselaer Scientific Computation Research Center (SCOREC) computing facilities include parallel compute systems, servers and visualization workstations. Linkage to off campus collaborators is supported by a campus connection to Internet 2. The SCOREC equipment list is as follows:

Data Storage: 9.6 TB for home directories; 64 TB for long-term storage of data; and 16 TB of storage for short term storage and specific projects. Home directories are backed up to tape.

Parallel Computational Facilities:

- Atipa / Supermicro cluster with 232 AMD Opteron 2.4GHz processors (8 cpu cores per node), 896GB of DDR3 RAM, ~14 TB local disk (500GB / node) and a 40Gbps Q-Logic Infiniband interconnect.
- 1/3 of the dual 8-way Xeon Cluster #2 located at the CCI is for SCOREC users
- Dell PowerEdge r905 with 16 3.1GHz AMD Opteron cores and 128GB DDR2 RAM.
- Dell PowerEdge r805 with 8 2.3GHz AMD Opteron cores and 64GB DDR2 RAM.

Lab Facilities:

- Various Intel Core i7, AMD Phenom, AMD Athlon 64 hex/quad/dual-core lab workstations with high end video hardware
- Color and B&W printing facilities.
- Linux Thin-Client terminals at every student desk.

Lodestar Research Corporation Facilities and Resources

Lodestar Research is a commercial company incorporated in the State of Colorado in 1987 that specializes in contract research in plasma physics, with an emphasis on fusion energy applications. Lodestar currently has contracts with the U.S. Department of Energy; past contracts have also been completed with Princeton Plasma Physics Laboratory, UCSD, the National Science Foundation, Los Alamos National Laboratory and Oak Ridge National Laboratory. Current contracts support two Ph.D. physicists, one Ph. D. consultant, one sub-contract with the University of Colorado, as well as support personnel. The productivity of Lodestar is aided by state-of-the-art computer and communications systems and strong scientific collaborations with both U.S. and international research groups. Lodestar has access to computational resources at NERSC as well as access to data from relevant experiments.

PHWorley Consulting Facilities and Other Resources

PHWorley Consulting is a home-based sole proprietorship consulting business with a single owner/employee located in Oak Ridge, Tennessee. Dr. Patrick Worley, the owner, is a computer scientist with over 30 years experience working with high performance computing systems. He has been the computer performance lead for the XGC plasma microturbulence simulation codes since 2005.

PHWorley Consulting currently has two contracts, one with Sandia National Laboratories (contributing to the Department of Energy (DOE) project Accelerated Climate Modeling for Energy) and one with Princeton Plasma Physics Laboratory (contributing to the DOE project Center for Edge Physics Simulation). Prior to this, Dr. Worley was Distinguished Research Staff at Oak Ridge National Laboratory (ORNL), retiring from ORNL in August 2016.

By virtue of allocations from the (a) DOE Innovative & Novel Computational Impact on Theory and Experiement (INCITE) program, (b) DOE Advanced Scientific Computing Research (ASCR) Leadership Computing Challenge (ALCC) program, (c) National Energy Research Scientific Computing Center (NERSC) Energy Research Computing Allocations Process (ERCAP), (d) Oak Ridge Leadership Computing Facility (OLCF) Center for Accelerated Application Readiness (CAAR) program, (e) NERSC Exascale Science Applications Program (NESAP), and (f) Argonne Leadership Computing Facility (ALCF) Aurora Early Science Program, Dr. Worley has access to the high performance computing systems at ALCF, NERSC, and OLCF, including prototypes of the next generation systems Summit and Aurora. PHWorley Consulting has reliable local computing and internet connectivity, enabling working on the remote systems at ALCF, NERSC, OLCF, and PPPL as well as project and code development collaboration sites.

Kitware Inc. – Facilities and Equipment

Kitware Inc. headquarters is located just north of Albany, New York in a Clifton Park office complex. Kitware rents approximately 27,000 square feet of office space at this location. Kitware also has offices in Chapel Hill, North Carolina (approximately 6,200 square feet in size) and in Santa Fe, NM. All offices are linked via a common virtual private network and a shared phone system, and share financial and administrative personnel. They also have on-site office managers, lunchrooms, private meeting rooms, and advanced conference facilities including large screen projection systems and whole-room Polycom video conferencing systems.

Computer Hardware and Software: Kitware has a mixed environment of personal and shared computing platforms that are built on top of a secure infrastructure with high redundancy; we have developed an extensive collection of software development and data processing tools; we host software and provide web services to number open-access systems; and we have access to shared resources via our collaborators.

Personal computing: Employees average three computers per person (desktop, laptop, and/or home system), with each computer typically equipped with multiple multi-core processors, a high-performance graphics card, dual monitors, and 8GB or more of main memory. These personal systems run a mix of Windows, Mac OS X and Linux operating systems. Shared resources include compilation and testing farms as well as workstations running a variety of alternative operating systems for testing purposes, e.g., Windows XP, FreeBSD, MacOS, or Vista.

Shared computing: Kitware hosts several special-purpose, high-end workstations, GPU systems, haptic systems, and magnetic and optical trackers. One such workstation is a multi-GPU computer featuring 6 NVidia GPU boards: 5 C2050 Tesla and 1 Quadro 5000 Fermi, as well as a 6-Core X5680 3.33GHz processor. A noteworthy haptic system is a MBP Freedom 7S haptic device, configurable for 6 or 7 degrees of freedom. We also operate clusters that are built using hadoop, condor, and other grid services. These systems are shared with collaborators and among our projects to support our algorithm development, software development, documentation, and communication efforts.

Secure, redundant infrastructure: To support our personal and shared resources, to host our critical services, and to host our public resources, Kitware has developed a VMware high availability cluster. It allows not only for an almost immediate recovery from critical hardware failures, but also allows us to perform upgrades and maintenance with almost zero downtime. Our infrastructure also includes a data center with redundant air conditioning and a backup generator to keep the datacenter functioning during any power issues. Kitware has designed these systems with redundancy in mind. All our servers have redundant power supplies and we utilize RAID disk technology to ensure a low impact to critical operations. On these and on all of our systems, we also strive to ensure security and protection of sensitive data by using firewalls and strict policies for passwords and external access. High encryption VPN tunnels and clients are used extensively for remote access.

Software and data processing tools: Kitware has extensive computer software resources including industry-leading software development tools for code generation, compilation, debugging, and memory testing. Kitware is also the principal developer of CMake, a cross-platform, open-source make system that is used to control the software compilation process using simple platform and compiler independent configuration files (www.cmake.org). It is downloaded over 3000 times per day. It is used in a multitude of projects, including KDE (a Linux Windowing environment and one of the largest open-source projects in the world.) Kitware also has in place an extensive testing environment based on its CDash regression testing tool (www.cdash.org). This cutting-edge system is used by several large-scale software systems including VTK, ITK, CMake, ParaView, KDE, Slicer, VXL, and over 1000 other projects within and beyond Kitware.

Services provide to open-access communities: Kitware maintains numerous servers to provide public access to VTK, ITK, Slicer, CMake, Titan, TubeTK, IGSTK, ParaView and numerous other open-source systems; to host web pages and web services for open source communities such as NA-MIC and Visomics; to operate open-access journals such as the Insight Journal and the Midas journal which has hosted workshop papers for nearly ten years; and to provide access to massive collections of public data for computer vision and medical imaging algorithm evaluation. Access to these systems is provided by a fiber connection to the internet yielding a total of 100 Mbit/second data rate.

Resources available from collaborative research centers: Kitware has also established collaborations with NIH Centers, NSF Resources, and National Labs that provide us access to supercomputing facilities. For example, our North Carolina office is located next to the UNC campus and our NIH-funded work has access to the Biomedical Analysis and Simulation Supercomputer (BASS) as an NIH-shared-resource operated by the Department of Computer Science at UNC. The BASS consists of 452 CPUs tightly coupled to each other and to 180 GPU Computing Processors that function as image and geometry calculation accelerators, providing the equivalent computing power of over thirteen thousand processors for image-intensive applications.

FACILITIES – UC SAN DIEGO (G.R. TYNAN)

The PISCES Laboratory is housed within Engineering Building II, located within the Jacobs School of Engineering suite of building and facilities. The laboratory has approximately 7000 sq ft of floor space, and houses three major devices: The PISCES-B facility, capable of performing mixed material PMI experiments with ITER candidate materials including beryllium, the PISCES-A facility, which is used for student research, divertor and edge turbulence studies, and hardware development and testing for the PISCES-B facility, and finally the CSDX device, which is a linear device that uses an RF helicon plasma source. This facility allows us to study the spontaneous formation of shear flows in turbulent plasmas in a manner that is analogous to what is thought to occur in tokamak devices. Photographs of these experiments are shown in the figures below. We also have a small unmagnetized plasma device that can be used for fundamental PMI studies. Diagnostics for these experiments include numerous fixed and scanning Langmuir probe arrays, visible light emission spectroscopy, mass spectroscopy, fast framing cameras for turbulence studies, and associated signal conditioning and data acquisition equipment. We also have office space, desktop computer, and other support for a staff of about 20 scientists, engineers, post-docs, and graduate students.

As mentioned above, the PISCES-B device sits inside of a beryllium compatible clean room maintained at all times at a negative pressure with respect to the remainder of the PISCES Laboratory. The enclosure is capable of circulating approximately 110 m3/min through redundant HEPA filters before exhausting the air flow to the roof of the building. We have a set of 8 Be-qualified personnel who form the PISCES Beryllium operations team, and who are qualified by UCSD EH&S to carry out experiments in this facility. This capability allows UCSD to make unique contributions to the US and World MFE PMI research program by exploring key issues associated with the ITER candidate PFC materials. This work forms a key element of the on-going US/EU-EFDA collaborative exchange program. The laboratory also has a suite of materials analysis capabilities includes in-situ surface compositional analysis using AES (Auger Electron Spectroscopy) and XPS (X-Ray Photoelectron Spectroscopy). A depth profiling SIMS (Secondary Ion Mass Spectroscopy) system is available for measurements of composition of samples as a function of depth into the surface. Quantitative measurements of surface morphology changes can be made using our JOEL SEM with quantitative compositional analysis provided by EDS (Energy Dispersive Spectroscopy) and WDS (wavelength Dispersive Spectroscopy). The quantity of retained deuterium is determined by using TDS (Thermal Desorption Spectrocopy) ovens capable of monitoring partial pressures of various gasses during controlled vacuum heating of samples. We also have a suite of laser systems including two <1J nanosec pulse length Q-switched Nd:YAG lasers, one short pulse (<100 fsec) low energy (~mJ) Ti:Sapphire laser with CPA pulse compression, a long pulse (0.1-10msec) 50J laser, and a CW 1kW laser for steady-state high heat flux (up to 10 MW/m^2) heat pulses.

Heat transfer laboratory (Co-PI R. Chen)

Co-PI Chen's laboratory is located in the Engineering Building Unit II (Rooms 208, 209, 211, 219, 234). The laboratory is well-equipped with facilities for optical and thermal characterization, materials characterization, as well as computational analysis. Facilities relevant to this project include:

- Optical spectrometers (UV-NIR spectrometer, FTIR, with integration spheres)
- Custom-made *3ω* system for thin-film thermal characterization (housed in Janis Research vacuum cryostat chambers (pressure <10^{-6} torr) within a wide combined temperature range of 20 to 800°K, plus various electronic instruments such as temperature controllers, lock-in

amplifiers, source-meters, current sources, nano-voltmeter, power supplies, thermometry apparatuses, heaters, pressure gauges, and mass flow controllers).

- COMSOL multi-physics simulation software for thermomechanical modeling, with computer clusters (shared with faculty in ECE).
- AFMs (VEECO MultiMode), suitable for nano-indentation based mechanical characterization of samples.
- Thin film sputtering system (Denton) with DC and RF deposition capabilities and an electron-beam evaporator for metal film deposition (Thermonics VE-100 Evaporator);
- Optical microscopes (Zeiss, Olympus, Leitz, Nikon) and metallography lab facilities;

Shared UCSD User Facilities and Equipment

1. Nano3 cleanroom facility. The Nano3 facility at UCSD is a state-of-the-art class 100 and 1000 cleanroom for micro- and nanofabrication. Notable equipment that is housed in the > 7,000 sq ft facility includes metal deposition via electron beam deposition (e.g., Raith50 E-beam writer), photolithography (e.g., EVG620 lithography system, Karl Suss MJB3 mask aligner), and dry etching (e.g., Trion RIE/ICP). The Nano3 facilities also have various characterization instruments that will be used to characterize the plasma/ion irradiated materials including scanning electron microscopes (SEM), focused ion beam (FIB), atomic force microscopy, profilometer, and an ellipsometer.
2. Upper Campus Research Machine Shop (UCRMS) is available to all research groups for precise custom-equipment manufacturing and can be used to manufacture hardware.

3.

FIG. 1: The UCSD PISCES-B device is housed within the beryllium enclosure. A PISCES Beryllium team worker can be seen in the fully enclosed protective gear allowing access to the experiment for maintenance and operations.

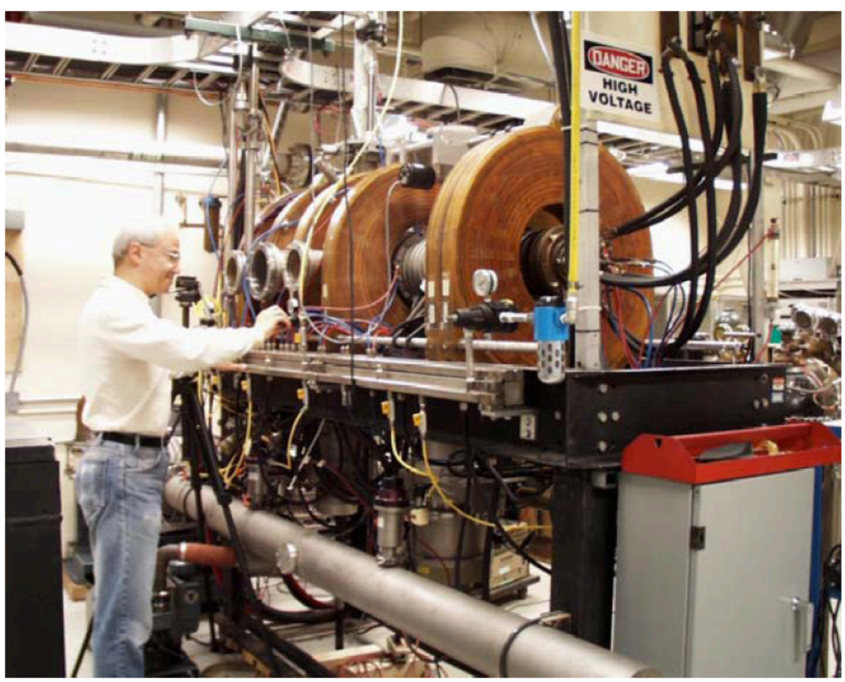


FIG. 2: The UCSD PISCES-A Device allows easy access for student research and for hardware testing and development prior to deployment on PISCES-B.

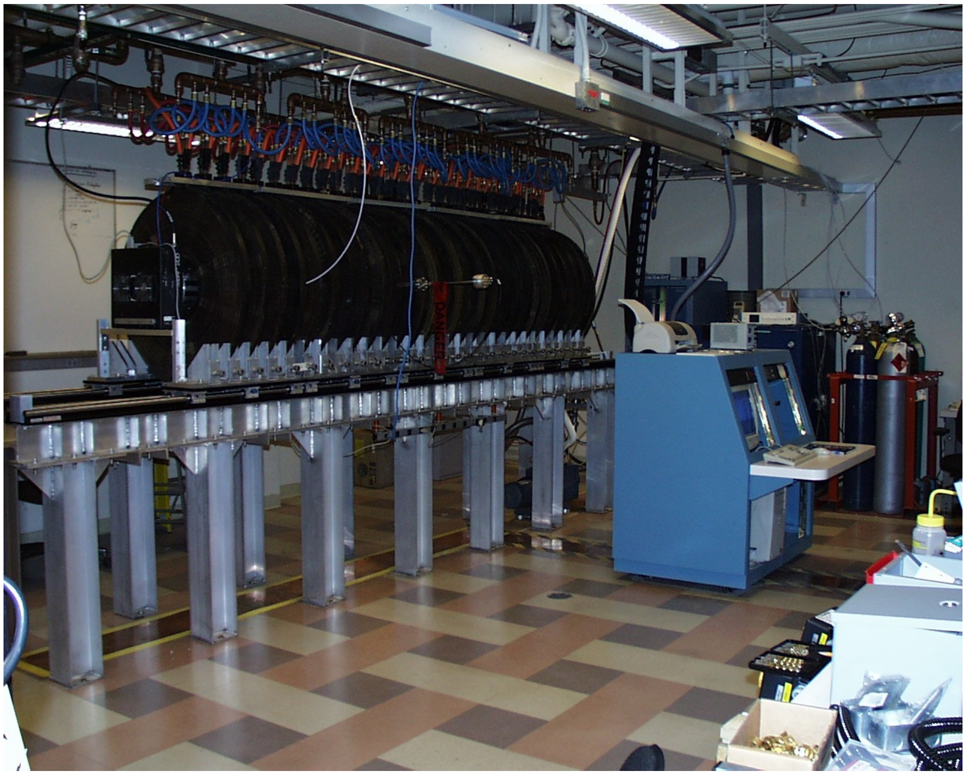


FIG. 3: The Controlled Shear Decorrelation experiment (CSDX) is a linear plasma device that uses an RF helicon plasmas source. This source technology produces plasma without any momentum input, allowing us to study plasma turbulence and spontaneous structure formation in conditions that are relevant to the edge region of a tokamak.

University of Colorado-Denver

1. Center for Computational Mathematics (CCM)

On-Site Computing Facilities

- **<u>Gross</u>**: Linux supercomputing cluster with total 24 Intel Nehalem x5570 CPUs (96 cores) and 288GB memory, additional large memory node with 2 x5070 CPUs, total 144 cores, 144GB memory, 40TB disk array, QDR Infiniband 40Gb/s interconnect
- **<u>Colibri</u>** 24 compute nodes at 2x Intel Xeon E5-2670 Sandy Bridge, and 2x NVIDIA Tesla M2090 total 384 CPU cores and 1536GB CPU memory, CPU theoretical peak 8TFlop/s, GPU peak 32 TFlop/s.
- machine room with independent air-conditioning
- numerous Linux servers with up to 16 Cores and 64 GB RAM
- NVIDIA Tesla S1070 GPU supercomputing system (960 cores) with CUDA developement tools
- gigabit optical fiber backbone
- disk arrays with disk-to-disk backup of users' files

The Center for Computational Mathematics and the Department of Mathematical and Statistical Sciences have a professional full time system administrator.

Off-Site Computing Facilities:

Summit: Computing Research, CU-Boulder

Summit is a heterogeneous supercomputing cluster based primarily on the Intel Xeon "Haswell" CPU, with additional NVidia Tesla K80 and high-memory nodes and, in the future, an Intel Xeon Phi "knights landing" MIC component. It replaces Janus as Research Computing's flagship computational resource. All nodes sit on a first-generation Intel Omni-Path Architecture interconnect which also provides access to an IBM GPFS Parallel scratch file system.

CU-Denver has a 10% share in Summit.

DESCRIPTION OF MIT FACILITIES AND RESOURCES

MIT Plasma Science and Fusion Center (PSFC)

Founded in 1865, MIT is widely known for its excellence in scientific research and technical education. The Plasma Science and Fusion Center is a large, multi-disciplinary facility located on the MIT campus. The PSFC is affiliated with the departments of Physics, Electrical Engineering and Computer Sciences, Nuclear Science and Engineering, Mechanical Engineering, Aeronautic Engineering and Materials Sciences. The primary objective of the center is to provide research and educational opportunities aimed at basic understanding of plasma behavior, and the use of that knowledge to develop useful applications. Occupying over 250,000 square feet of office, shop, and lab space on MIT's Cambridge campus, the center is currently staffed by about 250 faculty, researchers, students, support staff and visiting scientists. Founded in 1976, the Center consolidated plasma physics research carried out in MIT's academic departments, the Francis Bitter Magnet Laboratory, and the Research Lab for Electronics.

MIT-PSFC Computational Infrastructure

The PSFC computer staff supports a diverse collection of computers, storage systems, LAN and wide-area network infrastructure. The center has approximately 1000 network attached devices interconnected by a switched 1Gb/10Gb ethernet backbone and connected to the Internet via a 1Gbps link (upgradable to 10Gbps). Two clusters, one of 3200 cores and one of 600 cores are available for local computing. Data backups are accomplished through local servers and MIT’s Tivoli Storage Manager (TSM), a large enterprise-class automated tape library on campus. Older versions of files are maintained on TSM for 30 days, allowing further redundancy and a path for recovery from short-term data integrity problems. Individual desktop systems in developer or user offices are backed up using MIT’s CrashPlan cloud service.

MIT-PSFC Project Management and Cost Control

The management of research activities, which are financed through contracts with government and industry, is supported by the Office of Sponsored Programs under the Vice President for Research. The Office of the Vice President for Financial Operations is responsible for financial and business policies and procedures for sponsored research, including those designed to meet the requirements of grants and contracts.. The Accounting Office reporting to the Comptroller directs the accounting for all sponsored research projects. The Office of Sponsored Programs (OSP) at MIT has the immediate responsibility for the business administration aspects of research projects sponsored by the government. OSP provides summarized terms and conditions of new and renewed research contracts to the PSFC Principal Investigators and key Office of Resource Management personnel. Other chief management systems MIT provides to its research community include the Comptrollers Accounting Office; Property Office; Travel Office; Payroll Office; Purchasing Department and Accounts Payable. To supplement support from the MIT administration, the PSFC maintains its own headquarters operation for fiscal affairs, budget management and project management. This operation successfully manages numerous grants and cooperative agreements.

Appendix 5 Equipment

Not applicable; see Appendix 4 for equipment relevant to this proposal.

Appendix 6 Data Management Plan

Data Sharing and Preservation The scale of the data generated by the proposed simulations is sufficiently large that the management of those data is an important part of our project's research. That work is spelled out in detail in Sec. 3.2 of the main proposal text. The overall objective is to use ADIOS based technologies to extract and preserve output data of sufficient accuracy to achieve the project's missions. First, our data management team will focus on realizing efficient I/O performance on the LCF platforms; visualization and analysis will be incorporated into the "staging" methods developed for this purpose. Second, ADIOS technology will be exploited to make processed output accessible to users together with the source code and job input. ADIOS based tools will be developed to facilitate the movement, archival, and manipulation of simulation output.

Digital Access to Published Data Public access to the digital data displayed in publications will be governed by policies established by the home institution of each publication's lead author. The procedures are similar for all participants in this project: the required data and descriptive metadata will be archived on a facility prescribed by the home institution and linked with a "Archival Resource Key" (ARK), which will then appear in the published version of the paper, online and in print.

For PPPL authors, these data are available at the the Princeton University Data Repository, called Dataspace. Cross-referencing between these data and the published paper is facilitated by a "Digital Object Identifier" (DOI). MIT authors will be using the Dataverse repository for this purpose.

Publications and theses related to this project written by University of Illinois Urbana-Champaign (UIUC) authors will be deposited in the University of Illinois Library's IDEALS (Illinois Digital Environment for Access to Learning and Scholarship) campus digital repository. IDEALS provides preservation, search, and browsing functions at http://www.ideals.illinois.edu/. IDEALS is designed to collect, disseminate, and provide persistent and reliable access to the research and scholarship of faculty, staff, and students at the University of Illinois. IDEALS provides a direct deposit mechanism for loading digital content and assigning the appropriate metadata for the content. IDEALS will provide the capability of open access for this project. In addition, the Library is developing a trusted digital repository environment that will be compliant with all preservation and archiving standards.

Other institutions will establish their own policies and facilities; some of these policies are linked below in connection with experimental data.

Researchers external to the project wishing to access the underlying data (i.e., the data used to generate the processed or derived data presented in a publication), will be granted such access through the formal establishment of a collaboration between that person and the project member responsible for those data. This agreement may be subject to additional constraints and requirement imposed by the project member's home institution.

Experimental data used in code testing and validation activities are subject to the specific data access and usage policies set out by those facilities. For NSTX and NSTX-U data, see their Data Management Plan. Similar policies have been published by Alcator C-Mod and DIII-D. These policies also cover public access to the digital data appearing in publications resulting from experiments performed on those devices.

Data Management at Office of Science User Facilities This project will make extensive use of Office of Science computational centers, as is discussed in Sec. 3.2 and many other places in the main proposal text. Each of these facilities maintains their own data storage systems and has in place their own policies for accessing data kept there; our physics and data management teams have extensive experience with both.

Data from numerical simulations performed at the National Energy Research Scientific Computing Center (NERSC) can be stored in NERSCâĂŹs data archive in a web-accessible location, which is linked to a particular person or project. NERSC's maintains a data management strategy, with specific guidance for the HPSS file storage system. Similar documents are available for the Oak Ridge Leadership Computing Facility and the Argonne Leadership Computing Facility. URLs to these facilities will be provided in publications when appropriate.

Code Version Control and Access Plans for project code development and version control are described in Sec. 3.2.4 of the main proposal. The XGC source code is maintained in a Git based repository hosted on Bitbucket. The repository will be moved to GitHub as part of this project to utilize its more advanced capabilities; an analogous repository for Gkeyll will be added when needed. Workflows are being constructed for testing code development branches prior to them being merged into the master branch; these workflows will include nightly testing to ensure code stability and performance.

The principal project codes are available to external users under conditions specified by and via facilities provided by the home institutions of their principal developers.

The PPPL codes XGC, M3D-C1, and DEGAS2 are governed by the conditions stipulated in the "Theory Code License Release Form", available on the Theory Department Codes website. Gkeyll will be available in similar fashion when sufficiently mature. External users are encouraged to enter into an official collaboration which must be filled out and signed by the user before access to the code can be granted. The GEM gyrokinetic code is accessible via its web site. The GENE gyrokinetic code also has a web site. Multiple third party libraries are utilized by these codes, including ADIOS and PETSc.

Verification of the project codes is discussed in Sec. 3.1.6 of the main proposal text; the anticipated validation work appears in Sec. 2.6. Information on past code verification and validation activities is also available for XGC, and DEGAS2.

Finally, as required by the Statement on Digital Data Management provided by DOE Office of Science, we will ensure that the saved data protects confidentiality, personal privacy, Personally Identifiable Information, and U.S. national, homeland, and economic security; recognize proprietary interests, business confidential information, and intellectual property rights; avoid significant negative impact on innovation, and U.S. competitiveness; and otherwise be consistent with all applicable laws, regulations, and DOE orders and policies; and proprietary data will not be shared.