Thank you for coming!
Odds present 8:00-9:30am.  
Evens present 10:00-11:30am.  
Some presenters will stay for both shifts.

1. PuSH  
2. About ESTSC  
3. FACTS  
4. ORNLReady  
5. IMPACT  
6. STARS  
7. SCALE  
8. HPAC/NFAC  
9. SNAPSHOT  
10. AMIE  
11. n/a  
12. Ubuntu Airplay  
13. RAVEN  
14. Allinea DDT  
15. Memory Measurement and Visualization Using Score-P and Vampir  
16. GlProf  
17. HERCULES  
18. CCI  
19. STCI  
20. xSim  
21. Pegasus  
22. Modular Ecosystem Software Design and Virtual Observation System  
23. LIVV  
24. Eclipse PTP  
25. ICE: MOOSE  
26. ICE: Embedded Visualizations  
27. ICE: AQC  
28. ICE: 3D Modeling  

53. Travis Humble (CSMD, Complex Systems)  
QITKAT—the Quantum Information Toolkit for Application Testing is a software-defined quantum communication library that supports experimental demonstrations of novel quantum protocols. The software framework is based on the GNU Radio project and leverages custom quantum optical hardware.

54. Steven Hahn (NDAVD, Scientific Data Analysis)  
SpinWaveGenie is a C++ software library that facilitates the modeling of spin-wave excitations so that an instrument can convolute four-dimensional scattering data with sophisticated models faster and more efficiently. The source code, installation instructions, and usage examples are available at https://github.com/SpinWaveGenie/SpinWaveGenie.

55. Keith Britt (CSMD, Complex Systems)  
PauliD implements quantum computing Pauli gates, most often associated with the circuit model of quantum computing, on a commercial adiabatic model quantum computer. The software illustrates the ease at which such models can be implemented and the transition between the circuit and adiabatic models.

56. Vickie Lynch (NDAVD, Scientific Data Analysis)  
CAMM Workflow—Center for Accelerating Materials Modeling workflow for Spallation Neutron Source Data enables refinement of model parameters such as force fields and allows researchers to compare model and experimental results in near real time. See camm.ornl.gov for more details.

57. Stuart Campbell & Peter Peterson (NDAVD, Scientific Data Analysis)  
Mantid is data reduction and analysis software for neutron scattering data, written in C++/Python, with a Qt user interface. Additionally, Mantid leverages Paraview for advanced visualization.

58. Mathieu Doucet (NDAVD, Scientific Data Analysis)  
The SNS Web Monitor lets facility scientists and users monitor the progress of their experiments and view the results of automated data processing.

59. Mariano Ruiz-Rodriguez (RAD, Instrumentation)  
The Automated Sample Changer controls an automatic powder sample changer for the SNS Powgen Beam Line.
48. Christopher Smith (PD, Theoretical Physics)

CINA—The Computational Infrastructure for Nuclear Astrophysics is a cloud computing system that enables users to robustly simulate, share, store, analyze, and visualize explosive nucleosynthesis events such as novae, X-ray bursts, and core-collapse supernovae via a web-deliverable, easy-to-use, Java application. Users can also upload, modify, merge, store, and share the complex input data required by these simulations. In addition to the capabilities offered by CINA, the nucastrodata.org website provides the scientific community a comprehensive list of continuously updated, categorized links to all online nuclear astrophysics datasets. It also provides sample investigations using CINA that are appropriate for high school, college, and graduate school students.

49. Michael Smith (PD, Experimental Astrophysics)

bigbangonline.org is a cloud computing system that enables users to robustly simulate, share, store, analyze, and visualize the creation of elements in the early Universe. It also allows comparison to observations and the resulting constraints on cosmological parameters. The system is a web-deliverable, easy-to-use, Java application that enables users to upload, modify, store, and share the complex input data required by these simulations. In addition to the capabilities offered by this tool, the bigbangonline.org website provides the scientific community with detailed information about scientific research into the early Universe. This system is an example of our robust approach for getting science codes online for researchers to easily setup, run, visualize, and share with colleagues.

50. Megan Lilly (CSMD, Complex Systems)

CHP—CNOT-Hadamard-Phase is a highly efficient simulator of stabilizer quantum circuits. It can be used to model very large, entangles systems and some of the most interesting quantum effects, as well as the design of quantum error-correction architectures.

51. Anthony Lanzillotta (CSMD, Complex Systems)

Qubit Encoder takes in a picture or file and reads it into 2-bit codes that are used to control a liquid crystal controller. Software will be used to help encode different bell states.

52. Taylor Eisman (CSMD, Computer Science Research)

Quantum Time Distribution Verilog Code—We developed an FPGA designed to read incoming data from a quantum communications platform and use this data to regenerate a GPS time stamp for the smart grid.
1. Ekaterina Danilova (Scientific and Program Services Office, Science & Technology Systems)

PuSH is a new Oracle-based online tool for tracking and archiving information on publications that result from work at HFIR and SNS. PuSH allows linking to the facilities’ proposal system in order to relate publications, experiments, instruments, authors, and proposal team members. PuSH will help scientists and reviewers identify the most productive science being done at our facilities.

2. Leesa Laymance (LPD, Information Security)

About ESTSC — The Energy Science and Technology Software Center is the centralized software management facility for DOE that licenses and distributes scientific and technical software. The Standards-Based Management System defines the policies and procedures required to submit software to the ESTSC, under the Science & Technical (S&T) Software subject area.

3. Ethan Cantrell (CSED, Data System Sciences & Engineering)

FACTS — The Facility Analysis and Chemical Tiering System is a business intelligence product designed to help DHS analyze facilities submitting information to their regulatory program.

4. Daniel Wilson (ETSD, Center for Transportation Analysis)

ORNLReady is an emergency management application that is designed to enable users to maintain situational awareness and coordinate responses in the even of a laboratory emergency. This is accomplished through the use of a GIS platform and using geospatial analysis and tools.

5. Daniel Koch (CSED, Geographic Information Science & Technology)

IMPACT — The Incident Management Preparedness and Coordination Toolkit is a free all-hazards planning tool for first responders sponsored by DHS. Possible uses include: IED, evacuation, and shooter line-of-sight tabletop exercises, search and rescue planning, severe weather monitoring/alerting with geo-fences, hazard impacts to population using built-in population database, use in response vehicles for asset tracking/webcam damage surveys, special event and shelter placement planning, radio communication placement, traffic/security web camera monitoring.

6. Brian Ray (CSED, Data System Sciences & Engineering)

STARS — The Site Security Plan Triage and Reporting System is an extensible, risk-based decision tool that can easily be adopted to any endeavor attempting to provide quantitative answers to qualitative data.

45. Alexandr Sokolov (Isotope Business Office)

NIDC Online Management Toolkit — A new database-driven website, isotopes.gov, has been created for the National Isotope Development Center — the sole government source of isotope products for science. Isotopes.gov hosts the isotope product catalog, the products, online quotation and order generation. A complimentary software system, the NIDC OMT, has also been developed, enabling staff to modify and manage online customer accounts.

46. Suzanne Parete-Koon (NCCSD, User Assistance & Outreach)

Bellerophon is a software support system for automated regression testing of developing application codes, near real-time data analysis via data and 2D renderings of data, and tracking and storage of all data files, metadata, and renderings in a database.

47. Eirik Endeve (CSMD, Computational & Applied Math)

BEAM — The Bellerophon Environment for Analysis of Materials software system enables instrument scientists to leverage the Compute and Data Environment for Science (CADES) large-scale storage system, by providing users with a mechanism to easily manipulate their private remote directories and transmit data files through the Java client directly to CADES. At the core of this new system is a web and data server enabling multiple, concurrent users to securely access uploaded data, execute materials science workflows, and interactively engage analysis artifacts. In addition, BEAM’s multi-tier architecture facilitates user workflow needs by enabling integration of custom data analysis routines (serial and parallel) into the back-end framework.
40. Dmitry Liakh (NCCSD, Scientific Computing)

ExaTensor—Tensor (multi-linear) algebra provides the computational basis for quantum many-body theory, in particular for coupled-cluster formalism, which is heavily used in quantum chemistry, atomic, and nuclear physics. The TAL-SH library implements basic tensor algebra operations (a multi-linear analogue of BLAS) for use on multicore CPU, NVIDIA GPU, and Intel Xeon Phi. This library will form a lower-level layer in larger software project ExaTensor, a virtual tensor algebra processor for large-scale heterogeneous HPC systems. It is expected to facilitate an adaptive multiscale description of the electron correlation effects in simulations of the soft matter and large molecular aggregates of interest to nano- and biochemistry.

41. Markus Eisenbach (NCCSD, Group)

LSMS—The Linear Scaling Multiple Scattering code is a software package to solve the Schrödinger or Dirac equation for electrons in solids in the Density Functional Theory (DFT) framework; it can be used on computers ranging from desktop machines to HPS supercomputers such as Titan. Unlike most DFT codes that scale cubically, LSMS scales linearly in the number of atoms. The main strength of the code lies in first principles materials calculations for magnetic materials and alloys. By combining the code with Wang-Landau Monte Carlo method, it is possible to use HPC resources to calculate thermodynamic properties such as phase transitions in alloys and magnets from first principles without the need to resort to fitting of model parameters.

42. Stuart Slattery (CSMD, Computational Engineering & Energy Sciences)

DTK—DataTransferKit is a library providing parallel data transfer services for multi-physics problems. The library is designed to provide scalable algorithms to exchange fields in coupled physics simulations.

43. Christian Cardall (PD, Theoretical Physics)

GenASiS Basics—Aside from numerical algorithms and problem setup, large-scale physics simulations on distributed-memory supercomputers require more basic utilitarian functionality, such as physical units and constants; display to the screen or standard output device; message passing; I/O to disk; and runtime parameter management and usage statistics. Here we describe and make available Fortran 2003 classes furnishing extensible object-oriented implementations of this sort of rudimentary functionality, along with individual ‘unit test’ programs and larger example problems demonstrating their use. These classes compose the Basics division of our developing astrophysics simulation code GenASiS (General Astrophysical Simulation System), but their fundamental nature makes them useful for physics simulations in many fields.

7. Bradley Rearden (RNSD)

SCALE Code System is a widely-used suite of computational tools and simulation that provides comprehensive capabilities for criticality safety, reactor physics, and uncertainty analysis. SCALE’s framework implements the Monte Carlo radiation transport solvers that are at the heart of the solution. SCALE includes the latest nuclear data group radiation transport as well as activation, decay, and shielding calculations; SCALE’s graphical user interfaces assist with analysis, visualization, and convenient access to desired results.

8. Ronald Lee (CSED, Data Systems Sciences)

HPAC / NFAC—ORNL develops and maintains Nuclear Facility Accident Model (NFAC) in Hazard Prediction and Assessment Code System (HMS) for supporting in situ nondestructive assay (NDA) measurements of nuclear facility accident scenarios as well as emergency management and material release objectives. NFAC uses the HPAC incident source model (ISM), NFAC uses atmospheric transport and dispersion and environmental fate as well as visualization, and convenient access to desired results.

9. Nathan Rowe (NSITD, Safeguards & Security)

SNAPSHOT aims to develop a modern, long-term sustainable Holdup Measurement System (HMS) for supporting nondestructive assay of fissionable materials for nuclear criticality safety analysis.

10. Alain Giorla (FMNSD, Light Water Reactor Safety)

AMIE—The Automated Mechanics Integrated Environment is a C++ finite element library designed for multi-scale analysis of coupled physics models, several advanced numerical techniques such as implicit full-field time finite elements. Degradation is simulated with a local continuum damage algorithm which ensures the path dependent evolution of damage naturally be coupled with plasticity or visco-elastic microstructure generator able to represent heterogeneous composites with a wide variety of shapes and strains, including alkali-silica reaction, radiation-induced microcracking, and age shrinkage in a hydrating cement paste.
12. Ben Klein (NCCSD)

Ubuntu Airplay is an open-source project aiming to provide near-native performance airplay (including photo, presentation, desktop, audio, and video streaming) to proprietary Airplay Receivers.

13. Byung Park (CSMD, Computer Science Research)

RAVEN—RAS data Analysis through Visually Enhanced Navigation is a system-independent tool for analyzing supercomputer log data. RAVEN is configurable through XML files, uses Qt and Qwt to visualize the logs in a friendly format, and has been used on Cray XT5.

14. Nick Forrington (CSMD, Computer Science Research)

Allinea DDT—Allinea’s Distributed Debugging Tool is scalable and parallel. From small-scale, multi-threaded programs, to full Titan-scale jobs, DDT allows users to quickly and intuitively inspect and control all processing elements in their program simultaneously. DDT supports various languages and communication models, including C/C++, Fortran, CUDA, OpenMP, OpenACC, MPI, OpenSHMEM, and UPC.

15. Frank Winkler, Tomislav Janjusic, & Christos Kartsaklis (CSMD, Computer Science Research)

Memory Measurement and Visualization using Score-P and Vampir—Vampir is a widely successful trace visualization tool for understanding the performance bottlenecks that plague many parallel applications. Recent developments include: 1) the addition of memory tracing features in Score-P and 2) the ability to visualize the memory utilization, using Vampir.

16. Tomislav Janjusic & Christos Kartsaklis (CSMD, Computer Science Research)

GProf is a trace profiling tool specifically aimed to lessen the programmer’s burden of pinpointing heavily involved data structures during an application’s runtime and understanding data structure runtime usage. GProf is built as an extension to our memory-tracing tool, Gleipnir. Inspired by the widely-used Gprof tool, GProf aims to be simple to use and to offer a very detailed, data-centric view of memory-related performance metrics back to the user.

17. Christos Kartsaklis (CSMD, Computer Science Research)

HERCULES is an Open64-based, PROLOG-backed system for program constraint programming and customizable, user-level, transformation formulation. In addition to the core system, it offers a source code base scanner for patterns (hscan) and numerous transformation directives in an F90 compiler (hslf90).

35. Alex Pawlowski (ETSD, Fuels, Engines, Emissions & Research Center)

Interactive 0D Combustion Modeling in R aims at simulating the thermodynamics of engines, with a focus on areas of carbon intensity or energy usage reduction. It is written in R and parallelized for HPC architectures. R is chosen mainly because of its growing popularity and modular framework (Shiny). Although this software is still in its beta phase, it allows us to describe the efficiency limits for applicable technologies that have market-proven and commercially viable. A subsequent analysis will assess the practical limits of engine efficiency and carbon reduction within various engines and operating strategies.

36. Rangan Sukumar (CSED, Computational Data Analytics)

EAGLE is an algorithmic graph library for exploratory analysis. It was developed for Cray’s Urika, this open-source graph store. We have tested EAGLE to work on desktops, laptops and desktops such as Amazon C2. EAGLE can play a critical role in the analysis of heterogeneous graph data (e.g. semantic knowledge stores). With more support and user feedback, we can create a “MATLAB” for LinkedData.

37. George Ostrouchov (CSMD, Scientific Computing)

pbdR—programming in big data R extends the R analytics capability to large clusters. Powered by the same scalable and efficient libraries that are used in simulation science code, pbdR adds high-level R scripting and graphics capabilities.

38. Arnold Tharrington (NCCSD, Scientific Computing)

MSM—The Multilevel Summation Method solves classical and intrusive interactions for typical point particle biological and material systems. It is written in C++ and parallelized for HPC architectures.

39. Miroslav Stoyanov (CSMD, Computational & Applied Math)

ApproximatioN is a collection of algorithms for approximating real-valued functions. The methods are based on Stochastic Collocation/Sparse Grids, where the approximation is constructed from an ensemble of independent realizations of the target functions (i.e. samples). See tasmanian.ornl.gov for more details.
29. Taylor Patterson (CSMD, Computer Science Research)

**Code Quality & Usability Testing** focuses on improving the quality of Eclipse ICE, both from the developer and user perspectives. Through the use of static code analysis, the ICE team has identified and eliminated issues within the ICE code base to improve the source code’s maintainability and mitigate potential future bugs. We have designed formal usability testing experiments to gather objective and subjective data to assess the quality of ICE’s user interface and generate quantitative measures of the software’s usability.

30. Andrew Bennett (CSMD, Computer Science Research)

**VIBE**—The Virtual Integrated Battery Environment within ICE provides a user-friendly environment to manage the workflow of battery simulations. ICE’s VIBE plug-ins cover input generation, job-launching, and post-processing capabilities.

31. Kasper Gammeltoft (CSMD, Computer Science Research)

**Reflectivity Modeling**—ICE has recently implemented a neutron reflectivity simulator that provides Excel-like features and uses GlazedLists to set up generic Material types and improve project support.

32. John Turner (CSMD, Computational Engineering & Energy Sciences)

**VIBE**—The Virtual Integrated Battery Environment for CAEBAT is designed to study a coupled battery system, including its electro-chemistry, thermal transport, and structural dynamics.

33. Sophie Blondel (CSMD, Computer Science Research)

**Xolotl** is an open-source, high-performance plasma-surface interactions simulator that takes a continuum approach and solves the advection-diffusion-reaction equations in order to predict the time evolution of cluster concentrations in the helium irradiated tungsten material near the surface of a tokamak’s diverter. It recently underwent verification through comparison to other simulation results like molecular dynamics.

34. Roland Schulz (BD, Center for Molecular Biophysics)

**Gromacs** is a high-throughput and highly parallel open-source molecular simulation toolkit. Advanced performance and scaling allows modeling of complex bio-molecular interaction and function in a manner directly testable by experiment.

18. Geoffroy Vallée (CSMD, Computer Science Research)

**CCI**—The Common Communication Interface project provides a simple and portable API, high-performance, fault-tolerance, and robustness to the presence and efficiency of high-performance computing (HPC) environments. CCI provides a common network abstraction layer for high-speed gigabit and terabit data transfer over dedicated wide area networks, such as ESNet infrastructure. Visit http://cci-forum.com for more information.

19. Thomas Naughton (CSMD, Computer Science Research)

**STCI**—The Scalable RunTime Component Infrastructure is a modular component-based library for the implementation of customizable run-time systems. The STCI library enables the design and implementation of scalable, resilient, and versatile run-time systems. To illustrate the benefits of STCI, we present how STCI has been used to provide a basis for supporting the following tools and HPC workloads: (i) Message Passing Interface (MPI) programming model, (ii) MPI process fault tolerance, (iii) resilience tools, (iv) many-task workflow.

20. Christian Engelmann & Thomas Naughton (CSMD, Computer Science Research)

**xSim**—The Extreme-scale Simulator is a performance investigation toolkit that permits running native HPC applications or proxy applications in a controlled environment with millions of concurrent executing application processes. The goal is to study application performance and resilience in a simulated environment under extremely complex hardware/software co-design. Using a lightweight parallel discrete event simulation (PDES), xSim executes a Message Passing Interface (MPI) application on a much smaller system in a highly oversubscribed fashion, such that performance data can be extracted from a model with an appropriate simulation scalability/accuracy trade-off. xSim is designed like a traditional performance tool, as an interposition library that sits between the MPI application and the MPI library. It has been run up to 134,217,728(2^27) communicating MPI ranks using a 960-core Linux cluster.
21. **Benjamin Mayer** (CSMD, Computational Earth Sciences)
Pegasus—The BER Accelerated Climate Modeling for Energy (ACME) project will be deploying an end-to-end (experiment to analysis result to data publication) workflow based on the Pegasus workflow management system. This workflow will leverage not only Pegasus, but Globus transfer, HPSS and ESGF on Titan, CADES, and other DOE computer resources.

22. **Dali Wang** (ESD, Climate Change Science Institute)
The Modular Ecosystem Software Design and Virtual Observation System presents efforts for the ACME land model simulation, as well as ongoing work for virtual observation system development, based on an in-situ data communication framework and interactive data analysis.

23. **Joseph Kennedy** (CSMD, Computational Earth Sciences)
LIVV—To address a pressing need to better understand the behavior and complex interaction of ice sheets within the global earth system, significant development of continental-scale, dynamic ice-sheet models is underway. The associated verification and validation process of these models is being coordinated through a new, robust, python-based extensible software package, the Land Ice Verification and Validation toolkit. The release of this software provides robust and automated verification and a performance evaluation on LCF platforms. The performance V&V involves a comprehensive comparison of model performance relative to expected behavior on a given computing platform. LIVV operates on a set of benchmark and test data, and provides comparisons for a suite of community-prioritized tests, including configuration and parameter variations, bit-4-bit evaluation, and plots of tests where differences occur.

24. **John Eblen** (BD, Center for Molecular Biophysics)
Eclipse PTP—Eclipse Parallel Tools Platform is an integrated development environment (IDE) that supports the development of remote parallel and high-performance computing (HPC) applications from a local Eclipse installation on a personal laptop or desktop. C, C++, and Fortran applications are supported. PTP synchronizes files between local and remote machines and can launch remote compiles and job submissions.

25. **Alex McCaskey** (CSMD, Computer Science Research)
MOOSE-Based Application Development, Input Generation, Execution, and Analysis
ICE provides a unified interface for interacting with the entire MOOSE workflow: from actual application C++ development and version control, to input generation, simulation execution, and post-simulation data analysis.

26. **Jordan Deyton** (CSMD, Computer Science Research)
Embedded Visualizations—ICE includes a “Visualization Perspective” that can connect to local or remote VisIt installations and display simulation meshes and data, but this perspective is static in nature and does not support multiple visualization engines. To address this problem, a new pluggable visualization service interface was designed to visualize scientific data. Existing infrastructure for VisIt was ported to the visualization service, while new code was developed to support integrating the ParaView toolkit into ICE. These changes will allow developers to embed advanced visualization tools within any ICE plug-in, as well as customize existing visualization plug-ins.

27. **Erica Grant & Elizabeth Piersall** (CSMD, Computer Science Research)
Analysis Tools in Eclipse ICE for Adiabatic Quantum Computing
ICE has a set of analysis tools that takes the data from an adiabatic quantum computer and generates plots, histograms, and other statistical tools relevant to the execution energy spectrum.

28. **Robert Smith** (CSMD, Computer Science Research)
3D Modeling—ICE utilizes JavaFX for geometry editors. The geometry editor provides primitive shapes such as cubes, and easy tools for moving, changing, and duplicating these shapes. Combining shapes is possible via Constructive Solid Geometry (CSG) trees.