CDSE DAYS

March 23-27, 2015

The Computational and Data-Enabled Science and Engineering Program invites you to join us for a **five day event**, featuring:

- **6 keynote speakers** highlighting developments in the burgeoning big-data field and big compute fields
- **8 hands-on workshops** to develop and enhance skills

To reserve your space in a workshop, please

KEYNOTE SPEAKERS:

OMAR GHATTAS

Departments of Geological Sciences and Mechanical Engineering
Institute for Computational Engineering & Sciences
The University of Texas at Austin

March 23, 2015 at 2:30-4:00 PM

Student Union Theater

"Integrating Big Data and Big Models via Bayesian Inversion, with Application to Large Scale Antarctic Ice Sheet Flow"

The flow of ice from the interior of polar ice sheets is the primary contributor to projected sea level rise. One of the main difficulties faced in modeling ice sheet flow is the uncertain spatially-varying Robin boundary condition that describes the resistance to sliding at the base of the ice. Satellite observations of the surface ice flow velocity, along with a model of ice as a creeping incompressible shear-thinning fluid, can be used to infer this uncertain basal boundary condition. We cast this ill-posed inverse problem in the framework of Bayesian inference, which allows us to infer not only the basal sliding parameters, but also the associated uncertainty. To overcome the prohibitive nature of Bayesian methods for large-scale inverse problems, we exploit the fact that, despite the large size of observational data, they typically provide only sparse information on model parameters. We show results for Bayesian inversion of the basal sliding parameter field for the full Antarctic continent, and demonstrate that the work required to solve the inverse problem, measured in number of forward (and adjoint) ice sheet model solves, is independent of the parameter and data dimensions. This work is joint with Tobin Isaac, Noemi Petra, and Georg Stadler.

Biography:

Dr. Omar Ghattas is the John A. and Katherine G. Jackson Chair in Computational Geosciences, Professor of Geological Sciences and Mechanical Engineering, and Director of the Center for Computational Geosciences in the Institute for Computational Engineering and Sciences (ICES) at The University of Texas at Austin. He is also a member of the faculty in the Computational Science, Engineering, and Mathematics (CSEM) interdisciplinary PhD program in ICES, serves as Director of the KAUST-UT Austin Academic Excellence Alliance, and holds courtesy appointments in Computer Science, Biomedical Engineering, the Institute for Geophysics, and the Texas Advanced Computing Center. He earned BS, MS, and PhD degrees from Duke University in 1984, 1986, and 1988.

Ghattas' center's current research is aimed at large-scale forward and inverse modeling of whole-earth, plate-boundary-resolving mantle convection; global seismic wave propagation; dynamics of polar ice sheets and their land, atmosphere, and ocean interactions; and subsurface flows, as well as the underlying computational, mathematical, and statistical techniques for making tractable the solution and uncertainty quantification of such complex forward and inverse problems on parallel supercomputers.

MICHEL DUPUIS

Professor, Chemical and Biological Engineering and Computational & Data-Enabled Science & Engineering
The University at Buffalo, SUNY

March 23, 2015 at 4:00-5:00 PM

Student Union Theater

"The Power of Computing for Chemistry and Materials"

Computation and simulation in Chemistry and Materials has been historically a leading consumer of high performance computing HPC resources. Recent years have witnessed transformative advances in theories, methods, and software tools whereby we can address successfully the complex fundamentals of chemistry, physics, and materials, for example relevant to new energy technologies in a renewable energy economy. Theory and modeling is now accepted as a critical and necessary partner toward revolutionary design of materials and processes in such areas as solar and electrical energy conversion and storage, catalysis, and enzymatic catalysis. In this presentation we will highlight the scope of computation and simulation in chemistry and materials, the computational requirements and necessary developments for calculating properties with 'chemical accuracy', and for addressing all relevant length and time scales, from atomistic to meso- to macro-scales. Examples will draw from modeling fuel cell membranes, molecular catalysts, and bio-catalysts. These examples underscore the power of computation and the impact of HPC in enabling fundamental understanding of complex molecular, bio-molecular, and solid state environments. Successes and challenges point to the key role of high performance and massively parallel computing and the essential need for further advances in methods and computer codes for multi-scale modeling. We will also illustrate how, as an outgrowth of successes to date, virtual high throughput screening, Big Data analytics, machine learning, and materials informatics are pushing the frontiers of innovation with in silico rational design away from the traditional Edisonian approach of trial and error discovery.

Biography:

Dr. Michel Dupuis joined the Faculty of the Department of Chemical and Biological Engineering of the University of Buffalo (UB) in January 2015. Dupuis obtained a Diplome d'Ingenieur from the Ecole Polytechnique, Paris, in 1972 and a PhD in Theoretical Chemistry in 1976 in the Department of Chemistry at UB under the supervision of Professor H. F. King. He worked at the Lawrence Berkeley National Laboratory, at IBM, and more recently at the Pacific Northwest National Laboratory as a Laboratory Fellow. He is a Fellow of the APS, a Fellow of the AAAS, and a Member of the International Academy of Quantum Molecular Science IAQMS, elected for his contributions to the development of Quantum Molecular Science. Over the years he contributed to the development and application of quantum chemical methods and codes (HONDO, GAMESS, and NWChem) for electronic structure studies of molecules and materials. He is author or co-author of over 205 journal articles and has been an invited speaker at over 160 national and international workshops and conferences. His research at UB will be in the area of computation-enabled chemical and materials science and engineering, in particular for new energy technologies relevant to sun-to-fuels and fuels-to-electricity conversions.

BUFFALO INSTITUTE FOR GENOMICS AND DATA ANALYTICS

Norma Jean Nowak, Peter Winkelstein, Thomas Furlani

March 24, 2015 from 2-3PM

120 Clemens Hall

"BIG"

The Buffalo Institute for Genomics and Data Analytics (BIG) was created in 2014 with $50M from New York State to advance healthcare by providing genomic, computational science and biomedical informatics capabilities. In addition to helping advance medical research through advanced data analytics, one of the core missions of BIG is that of economic development and job creation in WNY.

This presentation will discuss the goals of BIG, its capabilities and some of the early projects it has launched in collaboration with several industrial partners in the healthcare industry.

Biographies:

Norma Jean Nowak, Ph.D., is recognized as a leader in the field of human genomics. Her research contributed directly to the Human Genome Project, as well as to genomic based approaches to understanding heritable disorders and cancer. In 2015, Dr. Nowak was named executive director for the University at Buffalo New York State Center for Excellence in Bioinformatics and Life Sciences, and holds the rank of Professor of Biochemistry. In addition, Dr. Nowak is the founder and Chief Scientific Officer of Empire Genomics LLC, a molecular diagnostics firm focused on enabling personalized medicine. Dr. Nowak was appointed to the Empire State Stem Cell Board in 2014. Dr. Nowak received the 2008 American Association of Cancer Research (AACR) Team Science award for the development of CGH (Comparative Genomic Hybridization) and array CGH technology. In addition she was awarded the 2008 Thomas B.Tomasi award for her outstanding achievements in science by the Roswell Park Cancer Institute.

Dr. Peter Winkelstein is a physician executive with extensive experience in medical management, medical informatics – including big data and data science – financial analysis and computer modeling. He serves as the executive director of the University at Buffalo (UB) Institute for Healthcare Analytics (IHI), as chief medical informatics officer (CMIO) of UBMD, a multispecialty faculty practice of over 500 UB physicians, and as CMIO of Kaleida Health, the largest health care provider in Western New York with over 1200 hospital beds. His particular interest is ethical issues in informatics. Dr. Winkelstein is a long-time member of the American Medical Informatics Association (AMIA), past chair of the AMIA Ethical, Legal and Social issues Working Group and past chair of the AMIA Ethics Committee. He also co-founded the Advanced Certificate in Medical/Health Informatics program at UB and have advised many commercial providers of medical content, including Zix Corporation, ePocrates Inc., Wolters Kluwer Health Inc. and ExitCare LLC. He is a Board-certified Pediatrician who continues to practice in inner-city Buffalo, New York.

Dr. Thomas Furlani serves as Director of the University at Buffalo's Center for Computational Research (CCR), a leading academic supercomputing center. A National Science Foundation Pre-doctoral Fellow, Dr. Furlani has more than 25 years experience in scientific computing, including computational chemistry and high performance computing. Dr. Furlani serves as principal investigator on several externally funded projects, including the XSEDE Technology Audit Service award. In addition, Dr. Furlani serves on the NYSERNet Board of Directors and is a founding member of the Visualization in Transportation Committee of the National Transportation Research Board. Dr. Furlani also coordinates on-going K-12, undergraduate and graduate level programs, including the Eric Pitman Annual Summer Workshop in Computational Science for High School Students.

BARRY SCHNEIDER

Staff Member
NIST Applied and Computational Mathematics Division

March 24, 2015 from 3-4 PM

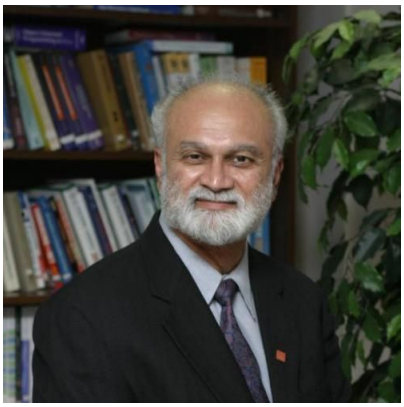
120 Clemens Hall

"The Influence of Heterogeneous Computational Resources on Computing in Physics"

As a consequence of the slowing down of Moore's Law and the need to reduce the power requirements required in modern computers, there has been an ever increasing trend to reduce processor clock speeds, increase the number of cores on a chip and to look to specialized co-processors such as the NVIDIA graphical processing units and the Intel Many Integrated Core technology to provide the needed computational power for modern high performance computing engines. These developments have come with a substantial price. To utilize these technologies effectively codes need to be re-written with a non-trivial impact on the communities that want to be at the leading computational edge in their discipline. The objective, as always, is to keep pushing the envelope to extend the computational models and produce more accurate and realistic science. The physics community has traditionally been one that has always wanted to push this envelope. As such the American Physical Society sponsored a set of symposia, organized by the Division of Computational Physics, at the March and April 2014 meetings in Denver and Savannah devoted to "The Influence of Heterogeneous Computational Resources on Computing in Physics". The speakers at those meetings also agreed to write articles for a special edition of the magazine, Computers in Science and Engineering, to be published this spring to disseminate the material to a much wider audience. As Editor of that special edition, I requested that the speakers send me their presentations so I could present a talk for the Buffalo "CDSE Days" symposium. My talk will examine the trend and illustrate what has been learned in a few of the physics communities that have taken up the baton and are using these new devices.

Biography:

Dr Barry I. Schneider (b. 1940 in Brooklyn, New York) is a staff member of the NIST Applied and Computational Mathematics Division. He is also a General Editor for the DLMF project. A graduate of the NYC Public Schools, he received his B.S. in chemistry from Brooklyn College, his M.S. in chemistry from Yale University and a Ph.D. in theoretical chemistry from the University of Chicago. Before coming to NIST in 2014, he was a postdoctoral research associate at the University of Southern California (1969-1970), and a staff member of the General Telephone and Electronics Laboratory (1970-1972). He joined the Theoretical Division of Los Alamos National Laboratory (1972-1991) and then the National Science Foundation (1991-2013). In early 2014, he came to NIST as a General Editor of the DLMF project. Schneider's current research interests span a broad number of areas of theoretical chemistry, atomic and molecular physics, numerical methods and high performance computing. His current principal focus is developing novel methods for the solution of the time dependent Schrödinger equation in ultra-short, and intense laser fields. He has authored or co-authored 130 refereed papers and books and has given numerous invited talks in the US and abroad. Schneider was awarded a Poste Rouge by the CNRS in 1980, was elected a Fellow of the American Physical Society (APS) in 1983 and received the prestigious Humboldt prize from the German government in 1987. He was a visiting scientist at NIST from 1995 to 2013 and spent a sabbatical year at NIST in 2000-2001. Schneider has served as Chair and Co-Chair of the APS Division of Computational Physics and Few Body Topical group and has been the organizer of a number of conferences and invited sessions here and abroad. He also serves as a reviewer for a variety of journals inside and outside the US.



VIJAY RAGHAVAN

Computer Science at the Center for Advanced Computer Studies, University of Louisiana at Lafayette

March 26, 2015 from 3-4PM

120 Clemens Hall

"Massive data analysis: applications and challenges"

We will highlight a few trends of massive data that are available for corporations, government agencies and researchers and some examples of opportunities that exist for turning this data into knowledge. We provide a brief overview of some of the state-of-the-art technologies in the massive data analysis landscape. Then, we describe two applications from two diverse areas in detail: recommendations in e-commerce, link discovery from biomedical literature. Finally, we present some challenges and open problems in the field of massive data analysis.

Biography:

Vijay V Raghavan is the Alfred and Helen Lamson/BoRSF Endowed Professor in Computer Science at the Center for Advanced Computer Studies and the Director of the NSF-sponsored Industry/University Cooperative Research Center for Visual and Decision Informatics, at the University of Louisiana at Lafayette. His research interests are in data mining, information retrieval, machine learning and Internet computing. He received his PhD in Computing Science, in 1978, from the University of Alberta, Canada. He is an ACM Distinguished Scientist and a senior member of the IEEE Computer Society.

E. BRUCE PITMAN

Dean, College of Arts and Sciences, University at Buffalo, SUNY

March 26, 2015 from 4-5PM

120 Clemens Hall

Data, Prediction, Errors, and the Compute Budget

The easy availability of data and access to large computing resources has created opportunities for scientists to make testable predictions of physical and biological phenomena. But, although data storage and CPU cycles are orders of magnitude cheaper than they were just a decade ago, they are finite. Often more important, the analysis of a specific problem can be time bound. That is, sometimes you need an answer by tomorrow, no matter what. This presentation will discuss the trade-offs that must be made when planning the computational workflow required to make predictions based on simulations and data. In addition to digital issues, we will highlight the role of statistical errors and uncertainty propagation, and just what it means to make a prediction that is "good enough".

Biography:

E. Bruce Pitman was appointed Dean of the College of Arts and Sciences at the University at Buffalo in July, 2011. Pitman earned his Ph.D. in mathematics at Duke University in 1985 and was a post-doctoral fellow at the Courant Institute of Mathematical Sciences at New York University. After spending time at the New Jersey Institute of Technology and the Institute for Mathematics and Its Applications at the University of Minnesota, he came to UB in 1989. Pitman is the author or co-author of more than 70 scholarly papers, and has been investigator or co-investigator on some $10M of research funding. To help excite and train the next generation of scientists, since 1999 Pitman and colleagues at UB's Center for Computational Research have organized an annual workshop in computational science for high school students.

WORKSHOP LEADERS:

DENNIS PATRONE

March 24, 2015 from 10AM-1PM

113A Davis Hall

"Big Data with Apache Accumulo"

Apache Accumulo is a distributed key-value data store. Modeled after Google's BigTable, Accumulo allows high-volume storage and efficient retrieval of big data-scale tables consisting potentially of millions of columns by billions of rows. Accumulo supports server-side iterators, cell-level security, and integration with Hadoop M/R, all of which will be introduced in this workshop. Representative use cases where Accumulo can provide utility will also be presented.

In this hands-on workshop, attendees will learn the basics of working with Apache Accumulo. Experience with Apache Hadoop M/R and Java development will be helpful but are not required.

Biography:

Dr. Dennis Patrone is a member of the senior professional staff at The Johns Hopkins University Applied Physics Laboratory (JHU/APL) in Laurel, MD. During his 17 year-tenure at JHU/APL, Dr. Patrone has worked on a wide range of projects that have been used on submarines, in space applications, and everywhere in between. For the last 5 years as a member of the Asymmetric Operations Sector he has been working with big data technologies including Hadoop, Accumulo, and Storm. In 2013 he was awarded the JHU/APL Invention of the Year Award as a co-inventor of an architecture utilizing big data technologies for identifying related code variants across compiled binary software.

Dr. Patrone earned his Ph.D. in Computer Science from the University at Buffalo (2013), and his M.S. and B.S. in Computer Science from the Johns Hopkins University Whiting School of Engineering (2000) and Saint Bonaventure University (1996), respectively. He is also a Cloudera Certified Developer for Apache Hadoop (2013).

PAUL BAUMAN

Mechanical and Aerospace Engineering, Computational and Data-Enabled Science and Engineering, University at Buffalo

March 25, 2015 from 2PM-5PM

250 Math Building

“Unstructured, Parallel Finite Element Analysis with the C++ Library libMesh”

This workshop will cover application development leveraging the open-source C++ finite element library libMesh. libMesh is designed to support adaptive mesh refinement on general unstructured meshes for use on local computing environments all the way to the largest supercomputers available today. Geometric element support includes lines, quadrilaterals, triangles, hexahedra, tetrahedra, prisms, and pyramids; manifold geometries are also supported. A wide variety of finite elements are also available. Interfaces to existing solver packages, including PETSc and Trilinos, are directly supported. libMesh has active developers contributing to libMesh through GitHub. It will be assumed the audience has a basic knowledge of the finite element method. From there, the workshop will cover existing examples in the library, illustrating basic library usage to developing a program for solving systems of partial differential equations on parallel computing environments using adaptive finite element methods.

Biography:

Dr. Paul T. Bauman joined the University of Buffalo as an Assistant Professor in the Mechanical and Aerospace Engineering department in 2014. He is also a core faculty member of the Computational and Data-Enabled Science and Engineering program. He earned his in B.S., M.S., and Ph.D. at the University of Texas at Austin in 2002, 2003, and 2008, respectively. Dr. Bauman has previously studied hypervelocity impact as well as developed numerical methods for multiscale models of polymers used in semiconductor manufacturing. More recently, his research focus has been on developing modern numerical methods for studying chemically reacting flows and bringing them together with algorithms for quantifying uncertainty in engineering problems related to hypersonic flows and combustion. In addition to more than 15 years of software development experience in scientific computing environments, Dr. Bauman is a core developer of the libMesh finite element library and a lead developer of both the GRINS multiphysics framework, built on libMesh, and the Antioch thermochemistry library.

IFEOMA NWOGU

Research Scientist, UB Center for Unified Biometrics and Sensors
Research Assistant Professor, Computer Science and Engineering, University at Buffalo

March 25, 2015 from 6-9PM

113A Davis Hall

"Bayesian Data Analysis Workshop"

The Bayesian Data Analysis workshop will take a hands-on approach to data analysis using current Bayesian methods. This will be accomplished by first introducing the notion of Bayesian inference starting from first principles and go on to present some effective approaches to Bayesian modeling and computation in statistics. For this workshop, we will focus on working through examples drawn from real applications and review Bayesian inference for simple parametric models, regression models, hierarchical models and mixture models. Examples and exercises for this workshop will use R software. Previous experience with R is not required to participate in the workshop.

Biography:

Ifeoma Nwogu is a Research Scientist at the UB Center for Unified Biometrics and Sensors and is a Research Assistant Professor in the UB Computer Science and Engineering department. She finished her Ph.D. in 2009 at the University at Buffalo, SUNY. Her current research focuses on applied machine learning techniques, specifically in the area of machine perception and computer vision. Nwogu specializes in learning methods including Bayesian modeling for problems in detection, categorization and matching. The purpose of her research is to analyze image and video data to understand the nature of hidden patterns in the data, with a direct relation to the problem at hand. Then leveraging this data-driven knowledge, she develops statistical models to make jugdements based on the data, using appropriate inference mechnisms. Her research has been highlighted in Scientific Amercia, on the national public radio (NPR), on the BBC and other trade media.

KEITH DALBEY
Researcher, Sandia National Laboratories

March 26, 2015 from 8AM-11AM

150 Math Building

"Dakota: A Toolkit for Sensitivity Analysis, Uncertainty Quantification, and Calibration"

Dakota is an open-source toolkit with several types of algorithms, including sensitivity analysis (SA), uncertainty quantification (UQ), optimization, and parameter calibration. Dakota provides a flexible, extensible interface between computational simulation codes and iterative analysis methods such as UQ and SA methods. Dakota has been designed to run on high-performance computing platforms and handles a variety of parallelism. This workshop will present an overview of Dakota algorithms, specifically focusing on uncertainty quantification (including various types of sampling, reliability analysis, stochastic expansion, and epistemic methods) and sensitivity analysis (including variance-based decomposition methods and design of experiments). The tutorial will provide a summary of the methods and discuss how to use them. It will also briefly cover how to interface your simulation code to Dakota.

Biography:

Dr. Keith Dalbey is a senior member of technical staff at Sandia National Laboratories in Albuquerque, NM. His research involves Uncertainty Quantification and algorithm development related to simulation of the United States Nuclear-Detonation Detection System (USNDS). From 2009 to 2012, he worked on Sandia's "DAKOTA" software package for optimization and uncertainty quantification. Dr. Dalbey received his PhD in Mechanical Engineering from the University at Buffalo in 2009, where he also taught MAE376: "Applied Mathematics for Mechanical and Aerospace Engineers" from 2008 to 2009.

DANIEL GAILE, RACHAEL HAGEMAN BLAIR, JEFFERY MIECZNIKOWSKI

Department of Biostatistics, University at Buffalo

March 26, 2015 from 12PM-3PM, 120 Clemens Hall

"An Introduction to R Programming"

R (http://www.r-project.org) is described in a recent New York Times article as becoming the trade language within companies as diverse as Google, Pfizer, Merck, Bank of America, the InterContinental Hotels Group, and Shell. In addition to having the built in capabilities, both computational and graphical, to perform common statistical analyses, the versatility and extensibility of the R language make it the choice for implementation of cutting-edge statistical methods in areas such as bioinformatics (via the Bioconductor project), spatial statistics (via the R geo project), and financial analysis (via the R metric project).

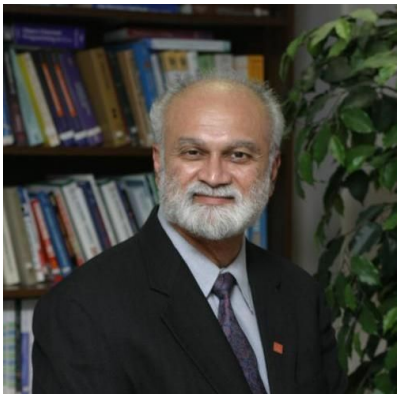
This workshop will introduce participants to R language and environment, giving both a general overview of R and specific skills that are fundamental for R users. Topics will include: 1) RStudio, 2) importing, exporting and manipulating data in R, 3) basic statistical analyses in R, and 4) graphics in R.

Biographies:

Dr. Daniel P. Gaile joined the UB Department of Biostatistics in 2003. He graduated from Texas A&M University with a PhD in Statistics. The focus of his research is on biomarker identification, expression analysis via arrays, next generation sequencing and bead-based technologies, proteomics, sparse matrix approaches, finite mixture models, and statistical computing. He has been an R user for over 16 years.

Dr. Rachael Hageman Blair joined the department of Biostatistics in the Fall of 2011. She graduated from Case Western Reserve University in 2007 with a PhD in Mathematics. The focus of her research is in systems biology, networks, and bioinformatics. She teaches the course series Statistical Data Mining I-II (STA 545/ STA 546), which emphasizes scientific computing in R.

Dr. Jeffrey C. Miecznikowski: joined the Department of Biostatistics in 2005. He graduated in 2006 from Carnegie Mellon University with a PhD in Statistics. Dr. Miecznikowski's primary research interests include spot detection in 2D images, high throughput technologies for biomarker discovery, nonparametric statistics, and software development. Dr. Miecznikowski teaches Statistical Computing (STA 511) which introduces R and statistical algorithms.



VIJAY RAGHAVAN

Computer Science at the Center for Advanced Computer Studies, University of Louisiana at Lafayette

March 27 from 8-11AM

102 Alfiero Hall

Visual Analytics of Time-evolving Large-scale Graphs

Data streams arriving from multiple data sources such as sensors, logs, and social media exhibit structural pattern, and can be modeled as time evolving graphs. With the rapid growth in Internet of Things (IoT's) as well as the availability of large-scale data from social media, sensors, smart phones, there is great interest in structuring real world observations from these sources as dynamic graphs. The size and complexity of these graphs are however growing to span millions of nodes and billions of edges, and hence present several challenges in terms of processing, analyzing, and visualizing this data. Time evolving graphs of large scale graphs are being studied in various applications such as disaster management, cyber security, fraud detection, social community network analysis. This workshop will introduce you to time evolving graphs, their properties, various graph mining algorithms, tools for storing, processing, analyzing, and visualizing these graph data sets and some applications.

Biography:

Vijay V Raghavan is the Alfred and Helen Lamson/BoRSF Endowed Professor in Computer Science at the Center for Advanced Computer Studies and the Director of the NSF-sponsored Industry/University Cooperative Research Center for Visual and Decision Informatics, at the University of Louisiana at Lafayette. His research interests are in data mining, information retrieval, machine learning and Internet computing. He received his PhD in Computing Science, in 1978, from the University of Alberta, Canada. He is an ACM Distinguished Scientist and a senior member of the IEEE Computer Society.

ANDREW BAUER

Research and Design Engineering, Kitware

March 27, 2015 from 11:30AM-2:30PM

102 Alfiero Hall

“ParaView Tutorial”

Dr. Andrew C. Bauer from Kitware will be giving a hands-on tutorial for ParaView. ParaView is an open-source visualization and analysis package that runs on a variety of platforms and at a variety of scales. He will be presenting a hands-on introduction to ParaView that is appropriate for beginners. Additionally, he will be presenting on how to use ParaView for batch processing through Python scripts as well as ParaView Catalyst and ParaView Cinema, tools specific for in situ processing.

Biography:

Andy Bauer joined Kitware in January 2008 as an R&D Engineer. Dr. Bauer's general research area is on enabling technologies for large-scale, PDE-based numerical simulations. His two current focus areas are assisting climate scientists with analyzing simulation outputs and performing coprocessing/in-situ visualization with simulation codes on supercomputers. Previous work at Kitware focused on generically specifying simulation code inputs for large scale simulations. Prior to joining Kitware, his work was primarily focused on mesh based numerical simulations of partial differential equations. Specific tasks include being part of the TSTT/ITAPS project for enabling high performance computing on large scale computing systems, working with physicists on numerical simulations of extended MHD using adaptive methods, and working on mesh search methods.

MARCUS HANWELL

Technical Leader

Kitware

March 27, 2015 from 3PM-6PM

102 Alfiero Hall

"Computational Chemistry: Scaling to Large Systems, Improving Code Integration and Chemical Data Informatics/Analytics"

Avogadro 2 is a complete rewrite of the Avogadro project, with a suite of targeted software libraries, and an end-user application all permissively licensed under the open source BSD license. Everything from core data structures, file input/output, and rendering have been rewritten with an emphasis on extensibility and scalability while maintaining usability. Avogadro 2 has been demonstrated interactively rendering large systems with in excess of 2.8 million atoms, and small quantum results using volume rendering for electronic structure among other techniques. MoleQueue will be described, an application for running external codes, submitting jobs to high performance computing resources and monitoring execution. MonogChem offers chemical data storage, indexing, search and informatics, with both companion applications using a simple local communication protocol for seamless integration. MongoChemWeb also enables wider sharing of chemical data, sharing many of the same resources. Finally an overview of the software process, and collaborative R&D model will be described.

Biography:

Marcus D. Hanwell is a Technical Leader in the Scientific Computing group at Kitware, Inc. He leads the Open Chemistry project, which focuses on developing open-source tools to for chemistry, bioinformatics, and materials science research. He completed an experimental PhD in Physics at the University of Sheffield, a Google Summer of Code developing Avogadro and Kalzium, and a postdoctoral fellowship combining experimental and computational chemistry at the University of Pittsburgh before moving to Kitware, Inc. in late 2009. He is a member of the Blue Obelisk, blogs, is @mhanwell on Twitter, and is active on Google+ . He has also written several guest posts for opensource.com and the Kitware Source. He is passionate about open science, open source and making sense of increasingly large scientific data to understand the world around us.