NATIONAL SCIENCE FOUNDATION

Summer Institute on Nanomechanics and Nanomaterials and Micro/Nanomanufacturing

in collaboration with
The Argonne-Northwestern Institute

A Short Course on:

The Materials Genome: Current Practice and Future Promise

June 10 – 12, 2013
Hilton Garden Inn, 1818 Maple Avenue, Evanston, Illinois, 60201

Course Objectives: An introduction to the practice and methodology underlying this revolutionary new approach to discovering and designing materials and material systems

It has long been known that the time required to discover new materials and incorporate them into applications has been unacceptably long. For example, the ubiquitous lithium ion battery required 20 years to move from the bench top to the marketplace. This delay is largely associated with the need to design new materials through a time consuming and repetitive cycle of testing and experimentation. The recently announced Materials Genome Initiative for Global Competitiveness outlines a program to drastically reduce the time to discover and insert new materials in applications. Central to this effort is a combination of advanced computational methods, the creation and sharing of big databases of materials properties, access to fast computers, and the development of algorithms that take advantage of the architecture of these machines. For example, it is now possible using modern first-principles methods to create databases of thousands of compounds and their properties. These databases can then be mined to identify promising compounds for applications. This provides a new route to materials discovery. In addition, computational methods and accurate databases permit materials to be designed to yield certain properties. Such an approach drastically reduces the time consuming cycle of experimentation and testing needed to move new materials to the marketplace. This new approach to designing materials promises to impact the field to the same extent that bioinformatics has impacted the field of molecular biology.

Central to the modern era of mathematical materials science and engineering is the concept of building blocks and their assembly. We refer to building blocks as archetypes, and the vector of apparent properties of the assembly – the material or structural system – of these archetypes as a genome. Archetypes may be crystal lattice unit cells, nano-sized precipitates or inclusions, monomers, turbine blades, or any other substructure in a system of interest. Assemblies may be a polycrystal alloy specimen, nanowire, polymer-matrix composite, jet engine, or any other conformation of component-level archetypes. The entirety of properties of those assemblies are their genomes, such as yield strain, ultimate strength, energy dissipation capacity, fracture toughness, conductivity, permeability, or size effects. Understanding this dependence is at the core of all multiscale methods, mechanism-based or simulation-based constitutive laws, and stochastic micromechanics: pillars of the *Modern Era of Mathematical Science and Engineering*.

Due to the ubiquity of computational resources, the proliferation of experimental observations indescribable by classical mathematical and computational methods, the Materials Genome and the Integrated Computational Materials Science and Engineering research initiatives are creating unprecedented opportunities for the multiscale material models that account for structure variability at different scales that have not been addressed by traditional multiscale approaches. One focus aim of this short course is targeted at developing a novel class of multiscale and multiphysics micromorphic material models for prediction of multiscale material fracture processes: cracks and voids initiation/nucleation, growth and coalescence, local fracture, and ultimate failures, which is part of the effort to build virtual material genome database that is integrated into a predictive simulation toolbox. The ultimate goal is that the proposed archetyoe-genome exemplar will enable the certification of materials leading to predictable and desired performance at the macroscale. The proposed research in system genome can further develop and maximize the impact of science and engineering research collaborations in energy, biological and environmental systems, and national security.

The summer institute addresses the entire range of methods that impact the materials genome initiative. In addition, case studies will be given to illustrate the applications of these methods, for example for materials discovery for nanoporous materials and battery materials, and the rapid insertion of new alloys into aerospace applications. The participants from Argonne National Laboratory will provide tutorials on the unique challenges of big data and the move to exascale computing.

Course Organization

Day 1 Atomistic Methods

9AM – 12PM Chris Wolverton (http://wolverton.northwestern.edu/)

Many of the key technological problems associated with alternative energies may be traced back to the lack of suitable materials. Both the materials discovery and materials development processes may be greatly aided by the use of computational methods, particular those atomistic methods based on density functional theory (DFT). Here, we present a series of three lectures which illustrate the various roles of DFT calculations in the Materials Genome Initiative.

In the first lecture, we describe the Virtual Aluminum Castings (VAC) methodology, developed at Ford Motor Company. This VAC approach successfully resulted in optimized alloy design and processing conditions to quickly achieve Al-alloy castings with suitable mechanical properties. VAC is a suite of predictive computational tools that span length scales from atomistic to macroscopic to describe alloy microstructure, precipitation, solidification, and ultimately, mechanical properties. We describe the role of first-principles computations in the Virtual Aluminum Castings methodology.

In the second lecture, we show how DFT approaches can be used in true materials discovery applications, such as those associated with hydrogen storage technologies. Practical hydrogen storage for mobile applications requires materials that exhibit high hydrogen densities, low decomposition temperatures, and fast kinetics for absorption and desorption. Unfortunately, no reversible materials are currently known that possess all of these attributes. We present an overview of our recent efforts aimed at developing computational tools which enable accurate prediction of hydride decomposition thermodynamics, crystal structures for unknown hydrides, thermodynamically preferred decomposition pathways, and ultimately novel predicted hydrogen storage reactions and materials.

In the third lecture, we present an overview of recent work utilizing high-throughput computation and data mining approaches to accelerate materials discovery. We show how computational crystal structure solution may be addressed via a new hybrid approach, the First-Principles Assisted Structure Solution (FPASS) approach, which combines experimental diffraction data, statistical symmetry information, and first-principles-based evolutionary algorithmic optimization to automatically solve crystal structures. We also describe a newly-developed data mining approach, clustering-ranking-regression (CRR), which allows us to *automatically* identify chemical descriptors in large materials datasets.

1:30 PM – 4:30 PM Randy Snurr (http://www.iec.northwestern.edu/)

Nanoporous materials have great potential for a variety of energy and environmental applications, including energy storage (e.g. natural gas vehicles) and separating mixtures (e.g. removing CO_2 from power-plant exhaust). Metal-organic frameworks (MOFs) are a new class of nanoporous materials synthesized in a "building-block" approach from inorganic nodes and organic linkers. Given the diversity of possible building blocks, there are an almost unlimited number of possible

structures. Molecular modeling can play a key role in the high-throughput screening of MOFs for desired applications. This screening requires three key steps: 1) generating the possible structures, 2) calculating their gas-adsorption properties, and 3) analyzing the enormous amount of resulting data. We will discuss each of these topics using examples from our recent work.

We have developed a computational method for generating all possible structures (subject to certain constraints) from a given library of MOF building blocks (nodes and linkers). From a library of 102 building blocks, for example, we created over 137,000 hypothetical MOFs on the computer. The MOF structures were screened for their methane (natural gas) storage capabilities using short, atomistic Monte Carlo simulations. The basics of developing an atomistic model and performing Monte Carlo simulations will be discussed. Finally, methods for extracting insights from the large amounts of data will be illustrated with examples for natural gas storage and CO_2 capture in MOFs.

Day 2 Multiscale Methods and Data Visualization

9AM – 12PM Wing Kam Liu (http://www.tam.northwestern.edu/people/liu.html)

The construction of a genome from building blocks (archetypes) is the archetype-genome exemplar. All natural and synthetic systems critical to both mankind's infrastructure and the global ecosystem may be viewed in this physical representation. We will present the mathematical construction and computational implementation of new theories that contain new forms of traditional balance laws and physically consistent constitutive relations that, by rethinking conventional micromechanics, account for each piece of the genome assembly triplet: *archetypes, interactions, and their conformation*. Continuum theories that consider the entire triplet are rare, but an additional complication arises in the archetype-genome exemplar. Since archetypes and their interactions contain properties difficult to characterize with high fidelity, and since after mixing and processing these same archetypes conform into pseudo-random microstructures characterized by statistical descriptors, the material genome is governed by a statistical distribution that reflects these uncertainties propagating through the assembly process. The presence of uncertainty does not debar the quantitative prediction of material genomes; instead it forces predictions to be a genome's relevant statistical quantities such as its mean, correlations, and failure reliability in the same way that computational biologists provide probabilities of contracting cancer based on patient-specific health attributes.

1:30 PM – 4:30 PM Rob Ross (http://www.mcs.anl.gov/about/people_detail.php?id=395)

The term "Big Data" has received a lot of press lately. Scientists as well as the broader business market are realizing that many key computational problems really depend on solving problems on very large data sets. In the scientific community, these data sets come primarily from two places: experimental data and simulation data. The growth of both types of data is outpacing our ability to store and analyze it. Many data sets are generated or collected, only to age into obscurity on a tape archive because the tools and methods to quickly analyze the data are still young and evolving. To address this challenge, new I/O libraries, storage systems, and analysis tools have been developed. This talk will start with a short explanation of how current parallel file systems work, and then move to the I/O libraries and tools that can be used today. To wrap up the

discussion, we will describe how the I/O path is evolving and how new analysis and visualization techniques for big data can be applied to today's science problems.

Day 3 Exascale Computing and Materials Design

9AM – 12 PM Pavan Balaji (http://www.mcs.anl.gov/~balaji/index.php)

CPU clock speeds have peaked at about 3 Gigahertz and the era of "always faster" on the next CPU is over. Individual processing units in CPUs have stopped getting significantly faster across subsequent generations. Today, performance comes from parallelism and all software must adapt to this new paradigm. The parallelism within a high-end server CPU is roughly doubling every year. To move from today's petascale computers to tomorrow's exascale systems will require embracing this architectural shift as well as understanding how future machines will manage increasing levels of hardware faults, improved electrical power efficiency, heterogeneous computing elements such as GPGPUs, and new memory technology such as nonvolatile RAM. We expect that managing parallelism and fault will significantly impact the parallel programming models currently used. While MPI has been a key communications library for inter-node programming, it will not scale down to use within future CPUs with hundreds or thousands of lightweight cores. Instead, programmers will initially shift toward an MPI+X model, where X could be GPU programming, OpenMP, lightweight threads, or some other method for executing highly parallel intra-node work. This talk will provide a background on where we are, the current petascale systems, and the important changes to application codes and system software as we enter the exascale era.

1:30 PM – 4:30 PM Greg Olson (matsci.northwestern....gregory-b-olson.html)

The numerical implementation of established materials science principles in the form of purposeful engineering tools has brought a new level of integration of the science and engineering of materials. Building on a system of fundamental databases now known as the Materials Genome, parametric materials design has integrated materials science, applied mechanics and quantum physics within a systems engineering framework to create a first generation of designer "cyberalloys" that have now entered successful commercial applications, and a new enterprise of commercial materials design services has steadily grown over the past decade. The DARPA-AIM initiative broadened computational materials engineering to address acceleration of the full materials development and qualification cycle, and a new level of science-based AIM modeling accuracy has now been achieved under the ONR/DARPA "D3D" Digital Structure consortium. A surface thermodynamic genome database predicted directly from validated DFT quantum mechanical calculations has generated novel “Quantum Steels” completely eliminating intergranular stress corrosion cracking at the highest strength levels. Integration with the full suite of fundamental databases and models has recently demonstrated the historic milestone of accelerated flight qualification for aircraft landing gear through application of the fully integrated computational design + AIM methodology. Past success defines a clear path forward for major enhancement of materials genomics technology.

Speaker Biographies

Dr. Pavan Balaji holds appointments as a Computer Scientist and Group Lead at the Argonne National Laboratory, as an Institute Fellow of the Northwestern-Argonne Institute of Science and Engineering at Northwestern University, and as a Research Fellow of the Computation Institute at the University of Chicago. His research interests include parallel programming models and runtime systems for communication and I/O, modern system architecture (multi-core, accelerators, complex memory subsystems, high-speed networks), and cloud computing systems. He has nearly 100 publications in these areas and has delivered nearly 120 talks and tutorials at various conferences and research institutes. He is a recipient of several awards including the U.S. Department of Energy Early Career award in 2012, Crain's Chicago 40 under 40 award in 2013, Los Alamos National Laboratory Director's Technical Achievement award in 2005, Ohio State University Outstanding Researcher award in 2005, five best paper awards and various others. He serves as the worldwide chairperson for the IEEE Technical Committee on Scalable Computing (TCSC). He has also served as a chair or editor for nearly 50 journals, conferences and workshops, and as a technical program committee member in numerous conferences and workshops. He is a senior member of the IEEE and a professional member of the ACM. balaji@mcs.anl.gov

Wing Kam Liu, Walter P. Murphy Professor of Mechanical Engineering at Northwestern University, Founding Director of the NSF Summer Institute on Nano Mechanics and Materials, Founding Chair of the ASME NanoEngineering Council, and Vice Chair of the US National Committee on Theoretical and Applied Mechanics within the National Academies, received his B.S. from the University of Illinois at Chicago; his M.S. and Ph.D. both from Caltech. He is a world leader in multiscale simulation-based engineering and science and has applied a spectrum of atomistic, quantum, and continuum strategies towards the understanding and design of nano-materials, biological processes, and recently the mathematical science and mechanics of materials, uncertainty, and the archetype-genome exemplar. In 2001, he was cited by the ISI as “one of the most highly cited, influential researchers in Engineering, and an original member highly cited researchers database”. Selected honors include the International Association of Computational Mechanics (IACM) Gauss-Newton Medal, the highest award given by IACM; the ASME Dedicated Service Award, the Robert Henry Thurston Lecture Award, the Gustus L. Larson Memorial Award, the Dedicated Service Award, the Pi Tau Sigma Gold Medal and the Melville Medal, (all from ASME); the John von Neumann Medal and the Computational Structural Mechanics Award from the US Association of Computational Mechanics (USACM), the highest honor given by USACM; and the IACM Computational Mechanics Award, and the Japanese Society of Mechanical Engineers. Liu chaired the ASME Applied Mechanics Division and is a past president of USACM. He is the editor of two International Journals and honorary editor of two journals and has been a consultant for more than 20 organizations. Liu has written three books; and he is a Fellow of ASME, ASCE, USACM, AAM, and IACM.w-liu@northwestern.edu.

Robb Ross is a computer scientist at Argonne National Laboratory and a senior fellow at the Computation Institute of the University of Chicago. He was the lead architect of the PVFS parallel file system and has been instrumental in the enhancement of the ROMIO MPI-IO library and the development of the Parallel netCDF high-level I/O library. Rob was a recipient of the 2004 Presidential Early Career Award for Scientists and Engineers for his work on parallel file systems, and he is a member of the MPICH2 development team awarded the R&D 100 award in 2005. He is the Deputy Director of the DOE SciDAC Scalable Data Management, Analysis, and Visualization Institute, helping provide data storage and analysis tools to the DOE computational science community, and he leads a team of researchers at Argonne developing solutions for storage and analysis challenges in computational science and, recently, in data-driven science domains.

Greg Olson is Walter P. Murphy Professor of Materials Science and Engineering at the McCormick School of Engineering and Applied Science at Northwestern University. He directs the Materials Technology Laboratory/Steel Research Group, and is a founder of QuesTek Innovations LLC, a materials design company that was selected for Fortune magazine's list of the 25 breakthrough companies of 2005. He is a member of the National Academy of Engineering, the American Academy of Arts and Sciences, and a fellow of ASM and TMS-AIME. He has authored more than 250 publications. He received a BS and MS in 1970 and ScD in 1974 in materials science from MIT and remained there in a series of senior research positions before joining the faculty of Northwestern in 1988. Beyond materials design, his research interests include phase transformations, structure/property relations, and applications of high resolution microanalysis. Recent awards include the ASM Campbell Memorial Lectureship, the TMS-SMD Distinguished Scientist/Engineer Award, the Cambridge University Kelly Lectureship, the ASM Gold Medal and the TMS Morris Cohen Award.

Randy Snurr is a Professor of Chemical and Biological Engineering at Northwestern University. He holds BSE and PhD degrees in chemical engineering from the University of Pennsylvania and the University of California, Berkeley, respectively. From 1994-95, he performed post-doctoral research at the University of Leipzig in Germany supported by a fellowship from the Alexander von Humboldt Foundation. Other honors include the 2011 Institute Award for Excellence in Industrial Gases Technology from the American Institute of Chemical Engineers, the Leibniz professorship at the University of Leipzig in 2009, and a CAREER award from the National Science Foundation. He is a Senior Editor of the *Journal of Physical Chemistry* and has served on the editorial boards of *Chemistry of Materials, Journal of Molecular Catalysis A*, and *Catalysis Communications*. His research interests include development of new nanoporous materials for energy and environmental applications, molecular simulation, adsorption separations, diffusion in nanoporous materials, and catalysis.

Chris Wolverton is a professor in the Materials Science Department at Northwestern University. Before joining the faculty, he worked at the Research and Innovation Center at Ford Motor Company, where he was group leader for the Hydrogen Storage and Nanoscale Modeling Group. He received his BS degree in Physics from the University of Texas at Austin and his PhD degree in Physics from the University of California at Berkeley. After completing his PhD degree, Wolverton performed postdoctoral work at the National Renewable Energy Laboratory (NREL). His research interests include computational studies of a variety of energy-efficient and environmentally friendly materials via first-principles atomistic calculations and "multiscale" methodologies for linking atomistic and microstructural scales. Currently funded research projects include the discovery of novel hydrogen storage materials, Li battery materials, thermoelectric materials, phase transformations in light-weight Mg alloys, and discovery of new oxide materials for solar thermochemical production of fuels. Wolverton has authored or co-authored more than 140 peer-reviewed publications, holds seven patents (several others pending), and has given more than 130 invited talks. He is a Fellow of the American Physical Society. Before joining the faculty of Northwestern, he also gave the John Dorn Memorial Lecture in 2003.

Fees
The registration fee for the short course is: $2,200. An additional $220 fee will be added to late registrations received after **April 15, 2013**. Register by **March 15, 2013** and receive a 20% discount that the reduced registration fee is $1,760. The fee includes coffee breaks, and lunches each day as well as all presentation materials, lecture notes and appropriate review papers.

NSF fellowships are available to faculty members, high-school science teachers, post-docs and Ph.D. candidates from the US. The fellowship consists of full registration fee plus an accommodation allowance. A limited number of fellowships are also available for faculty and postdoctoral fellows outside the US. Download the application form from http://tam.northwestern.edu/summerinstitute/Home.htm. The deadline for fellowship application is **March 1, 2013**.

Location
The course will be held at Hilton Garden Inn, 1818 Maple Avenue, Evanston, Illinois, 60201.

Accommodations
A block of rooms has been reserved at special rates for short course attendees at the **Hilton Garden Inn**. Attendees should contact the hotel directly to make reservations by calling 847-475-6400 or through 1-877-STAY HGI or 1-800-HILTONS, to qualify for special rates guests **must** mention "**Materials Genome Short Course**". The rooms at the **special rate of $135 single and $145 double will only be held until April 15, 2013.**

Registration
Registration form can be downloaded from http://tam.northwestern.edu/summerinstitute/Home.htm.

Mail in the completed registration form with check or money order by **March 15, 2013**.
Make check or money order payable to:
Northwestern University
Send to: Northwestern University, Dept. of Materials Science and Engineering, 2220 N. Campus Drive, Evanston, Illinois, 60208
Attn: Yip Wah Chung

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