HPC² Project Overview
Stony Brook University

Project Director: Jason R. Trelewicz
Principal Investigator: Robert J. Harrison

HPC² Meeting, April 23, 2015
Rensselaer Polytechnic Institute
Center for Computational Innovations
• Enabling Stable Nanocrystalline Tungsten Alloys as Plasma Facing Materials for Fusion Reactors
  Project Lead: Jason Trelewicz, Department of Materials Science and Engineering
  *Industrial Partner: TheoretiK*
  o Plasma-facing components for reactor scale fusion devices require materials to operate under far-from-equilibrium conditions of extreme temperature, radiation, and stress.
  o The team is employing thermodynamic modeling and atomistic simulations to study nanograin stability, radiation tolerance, and mechanical behavior of nanostructured tungsten alloys.
  o Computations include Molecular Dynamics and Kinetic Monte Carlo simulations.

• Molecular Dynamics Study of Sulfur Crystals for Sustainable Concrete
  Project Lead: Juhyuk Moon, Department of Civil Engineering
  *Industrial Partner: Green SulfCrete, LLC*
  o Concrete is the most widely used manufacturing material, with global concrete production exceeding 20 billion tons per year, leading to 5~7% of global CO2 emissions.
  o The team is developing a new green concrete based on sulfur, “SulfCrete,” which is produced by the recycling of industrial by-product materials of sulfur, fly ash, and catalytic cracking oil.
  o Molecular dynamics simulations are being used to study the formation of sulfur polymorphs using the large-scale atomic/molecular massively parallel simulator (LAMMPS) platform.
HPC$^2$ Projects: Continuum Simulations in Project Design

**Partial Reformation of Mixed Fuels for Combustion in Heavy-duty Engines**

Project Lead: Sotirios Mamalis, Department of Mechanical Engineering

*Industrial Partner: Innoveering, LLC*

- Heavy-duty diesel engines are operated using fuels of mixed properties (thermodynamic and chemical) that have variable hydrocarbon and CO$_2$ content, resulting in inefficient combustion.
- To address these and other issues, the team is studying how to enable decomposition (a.k.a., reformation) of larger hydrocarbon molecules into smaller, more reactive species.
- Computational fluid dynamics (CFD) simulations are being employed to perform chemistry and heat transfer calculations to assess combustion efficiency and predict emission formations.

**Computational Modeling of the Thermomechanical Properties of the Regenerator in a Thermally Driven Heat Pump**

Project Lead: T. A. Venkatesh, Department of Materials Science and Engineering, and Maen Alkhader, Department of Mechanical Engineering

*Industrial Partner: ThermoLift, Inc.*

- The team is developing a disruptive and transformational thermally-driven heat pump that provides heating, cooling, and hot water all in one device. Materials selection for various components (e.g. heat exchangers, regenerators) play a crucial role in determining efficiency.
- Finite element based computational models are being employed for controlling thermal and mechanical coupling and predicting thermal history.
HPC\textsuperscript{2} Projects: Software Development for Data Analytics

- **Source-to-Source Translator for High-Performance Computing with R Language**
  
  Project Lead: Xiangmin Jiao, Department of Applied Mathematics and Statistics
  
  *Industrial Partner: ParaLab Computing, LLC*
  
  - The team is working with ParaLab Computing, LLC on the development of a new source-to-source technology to translate user-written R codes into high-performance C++ codes.
  
  - A myriad of commercial applications exist for this technology in the handling of large datasets in the insurance, advertising, and pharmaceutical industries.
Summary of SBU HPC\textsuperscript{2} Projects

Atomistic Simulations

- W alloys as plasma facing materials for fusion reactor
  - PI Trelewicz
- MD of sulfur crystals for sustainable concrete
  - PI Moon

Finite Element Modeling

- Partial reformation of fuels for heavy duty engines
  - PI Mamalis
- FE modeling of thermally driven heat pump
  - PI Venkatesh
  - PI Alkhader

Software Development

- Big data analytics in R using advanced software tech
  - PI Jiao
- Source-to-source translation technology
Nanocrystalline Tungsten Alloys for Fusion Applications

- Radiation hardening and embrittlement (<0.4 $T_M$, >0.1 dpa)
- Phase instabilities from radiation-induced precipitation (0.3-0.6 $T_M$, >10 dpa)
- Irradiation creep (<0.45 $T_M$, >10 dpa)
- Volumetric swelling from void formation (0.3-0.6 $T_M$, >10 dpa)
- High temperature He embrittlement (>0.5 $T_M$, >10 dpa)

Zinkle and Busby, Materials Today (2009)
Radiation Tolerant Nanocrystalline Metals

- Why nanocrystalline metals?
  - Han et al., JMR (2013)

- Does the sink proximity effect operate in nanocrystalline tungsten?
  - El-Atwani et al., Scientific Reports (2014)
Constructing Nanocrystalline Simulation Cells

- **Voronoi tessellation (VT)** - partitions space in a Voronoi-Poisson distribution

- **Orientation**
  Euler angles \((\alpha_i \beta_i \gamma_i)\) used to assign orientations via orientation matrix \(O_i\):

\[
\begin{bmatrix}
\cos \alpha_i \cos \beta_i \cos \gamma_i & -\sin \alpha_i \cos \gamma_i + \sin \alpha_i \cos \gamma_i & \sin \beta_i \cos \gamma_i \\
\sin \alpha_i \cos \gamma_i + \cos \alpha_i \cos \beta_i \sin \gamma_i & -\sin \alpha_i \cos \beta_i \sin \gamma_i + \cos \alpha_i \cos \gamma_i & \sin \beta_i \sin \gamma_i \\
-\cos \alpha_i \sin \beta_i & 
\end{bmatrix}
\]

- **Misorientation**
  Calculated according to the misorientation matrix \(M_{ij} = O_i O_j^{-1}\)
  where \(O_i\) and \(O_j\) are the orientation matrices of two neighboring grains

- **Monte Carlo procedure to optimize simulation structures**

- **Fill the Voronoi tessellation with atoms**
1. Designing thermally stable nanocrystalline tungsten via alloying

2. For the alloys of interest, map the W-X and deuterium potential
   • Based on stability calculations, Ti will be selected as a representative stable nanocrystalline system and Cr will be used to create duplex nanostructures

3. Perform collision cascade simulations using molecular dynamics to uncover defect accommodation mechanisms in classical and duplex nanostructures

4. Complement simulation work with experiments at the Ion Beam Laboratory at Sandia National Laboratories using an in situ irradiation HRTEM

Chookajorn and Schuh, Science (2012)
Partial Reformation of Mixed Fuels for Heavy-duty Engines

- Heavy-duty diesel or natural gas engines are used for localized power generation in oil & gas industries and landfill sites
  - Fed with fugitive gases from oil wells and landfills that have varying CH\textsubscript{4} and CO\textsubscript{2} composition
  - Combustion process is affected, resulting in poor combustion and thermal efficiencies, as well as high emissions of soot, CO and UHC
- Investigate the combustion process to improve efficiency
  - Difficult to do experimentally due to size and cost
  - In-cylinder simulations provide a robust way to understand and improve the fundamental processes
- Innoveering LLC, is exploring a partial fuel reformation technique
  - Uses a small amount of fuel in a reformer
  - Produces Syngas (H\textsubscript{2} + CO) which has multiple benefits for combustion
Computational Fluid Dynamics (CFD) modeling can be used to simulate and analyze the combustion processes. CFD includes flow, chemistry and heat transfer simulation. Detailed chemistry handled by open source chemical kinetics mechanisms. Commercial tools used that are available to academia: ConvergeCFD as the main solver and EnSight for post-processing, visualization. CFD simulations tend to be computationally expensive, but IACS cluster will be utilized for reducing runtime.
On-going Work in Converge™ CFD

- **ConvergeCFD:**
  - User imports full cylinder and port geometry as a .STL file, declares boundaries (walls), and inputs boundary conditions (fuel-air mixture, intake pressure, temperature etc.)
  - User imports chemical kinetics mechanism - can be up to thousand of species and reactions
  - Solver does automatic meshing, and solves Reynolds-Averaged Navier-Stokes equations in every computational cell

- **Investigation of reforming effects on natural gas combustion**
  - Natural gas: primarily CH$_4$, relatively simple oxidation chemistry (GRI Mechanism)
  - Working fluid will be augmented to account for syngas (H$_2$ + CO)
  - Mixed fuels or Biogas can be simulated by adding CO$_2$ (e.g. 60% CH$_4$ – 40% CO$_2$)

- **Anticipated findings based on the literature**
  - Benefit of syngas on combustion and thermal efficiency of mixed fuel engine
  - Benefit of syngas on lean combustion (excess air) or natural gas
Source-to-source Translation for R Language

• Develop software technology to speed up R language, to enable higher performance data analysis
  o Source-to-source translation
  o Performance optimization for modern computer architectures
• Data analytics has a growing market: According to IDC, market for data analysis technology grows at a 27% compound annual growth rate, to $32.4 billion through 2017
• R is widely used for data analysis in industry and academia, as it’s easy to use, open source, and has many packages available
  o Analysis of operations and market data to make business decisions
  o Analysis of financial market for investment decisions
  o Real-time recommender systems for customer retail web applications
  o Automated network intrusion detection systems
  o Analysis for optimal placement of advertisements
Areas to address with source-to-source translation

- Data analysis using R or another third-party analytics engine often encounters one or more problems with large data sets:
  1. It takes too long to get my data or to get the “right” data
  2. Cannot analyze or mine all the data – it has to be sampled
  3. *Putting R models and results into production is ad hoc and complex*
  4. *Recoding R models into C or Java takes time and is error prone*
  5. Concerns about data security, backup and recovery
  6. *Need to build 10,000s of models fast to meet business objectives*

- These issues are partially due to:
  - R is quite slow, because of its interpreter-based nature
  - Its GPL license is restrictive for commercial productions.

- This project targets intermediate-level platforms
  - Powerful workstation with many cores and potentially GPU or Intel Phi co-processor accelerations, based on either Windows or Linux

Technical Focus and Current Work

- **Algorithmic Cores of R, based on R Benchmarks**
  - **Matrix calculations**: Creation, transposition, and deformation of matrix, power of elements of matrices, sorting of large number of values, outer-product of matrices, and linear regression
  - **Matrix functions**: Eigenvalues and singular values, Cholesky decomposition, and Fast Fourier Transform (FFT)
  - **Programming controls**: Loops, recursion, and branching (if-then-else)

- **Benchmarking on GPGPUs**
  - Systematic benchmarking performance of R on GPGPUs with CUDA
  - Preliminary performance optimization

- **Development of API in R for GPGPUs and many-cores processors transparent to underlying hardware**

- **Continued development of prototype of source-to-source translator, ParaLab Coder, focusing on serial codes first, in collaboration with ParaLab Computing**