HPC4 ENERGYINNOVATION

HPC4EI Projects Featuring Materials Design

Balasubramaniam Radhakrishnan
Oak Ridge National Laboratory

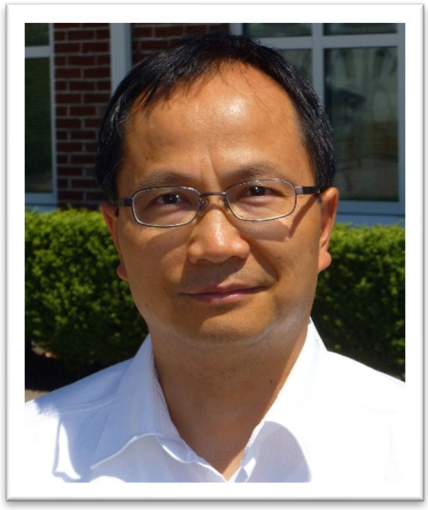
Applications of High Performance Computing to Phase-field Simulations of Microstructure Evolution during Industrial Processing of Structural Alloys

Dr. Radhakrishnan is a Distinguished Research Staff with the Multiscale Materials group in the Computational Sciences and Engineering Division at ORNL. He has worked extensively in a wide range of topics related to materials science and engineering, with particular reference to structure-processing-property relationships in structural alloys, advanced computer simulation of microstructure and texture evolution during thermo-mechanical processing, solidification processing and solid-state phase transformations using multi-scale modeling approaches. His recent research has focused on metal additive manufacturing, with specific interest on the effect of processing conditions and alloy chemistry on the microstructure evolution. As part of this effort, he is engaged in active collaborations on the development of reduced order models that can be used for the control of additive manufacturing process parameters to develop site-specific microstructures in components with complex geometries. He has been active in the development of high-performance codes related to microstructure evolution in metallic alloys that run efficiently on the Oak Ridge leadership class computing facilities.

Timofey Frolov
Lawrence Livermore National Laboratory

Modeling the Antiphase Boundary Energy in Ni_3Al-based Alloys using Density Functional Theory and Machine Learning

Dr. Timofey Frolov is a staff scientist, Lawrence Livermore National Laboratory. He joined the lab in 2015. He received his PhD from George Mason university in 2012. Prior joining the Lab, he received a Miller fellowship at UC Berkeley (2012-2015). His primary area of expertise is thermodynamics and computational modeling of materials with emphasis on materials interfaces. During his PhD, I developed a thermodynamic theory of solid-solid and solid-liquid interfaces that included effects of non-hydrostatic stresses and composition. More recently his work focused on structural transitions at grain boundaries. He has authored and co-authored 39 peer-reviewed journal publications and given 30 invited talks**.**



Michael Gao
National Energy Technology Laboratory

Accelerated Design of High-Performance High-Entropy Alloys for High Temperature Applications

Dr. Michael Gao is a Physical Scientist at National Energy Technology Laboratory (NETL). He obtained his PhD in 2002 and then did his postdoctoral research at University of Virginia (2002-2004) and Carnegie Mellon University (2004-2007). He started his career at NETL in 2008. Dr. Gao has 25 years of research experience in materials design including high entropy alloys, metallic glasses, refractory metals, and Ni-, Fe-, Al-based alloys. His recent research focus is on accelerating high-performance materials development for extreme environments by integrating multi-scale computational modeling and machine learning with critical experiments. He has published over 80 peer-reviewed journal papers, 5 book chapters, and 1 patent.

Sylvie Aubry
Lawrence Livermore National Laboratory

***Ab-initio* Guided Design and Materials Informatics for Accelerated Product Development of Next Generation Advanced High Strength Steels**

Dr. Sylvie Aubry earned her Ph.D. in Applied Mathematics from University Pierre et Marie Curie in Paris, France in 1999. After completing a Postdoctoral Fellowship at Caltech, she worked as a research staff scientist at Sandia National Laboratories in Livermore, CA and at Stanford University in Palo Alto. She joined LLNL in 2010 and established herself as a technical expert in modeling dynamic phenomena in materials. She has led several teams and delivered exquisite results that push the boundaries of our scientific understanding of materials, published over 60 peer reviewed publication, and advanced our national defense capabilities. In particular, Sylvie extended the laboratory's meso-scale capabilities such as the dislocation dynamics method, ParaDiS, to improve our prediction of the strength of metals and alloys, supporting this effort for 11 years as a both a contributor and the team leader. Her recent work investigating how the presence of helium bubbles effect the strength of metals using molecular dynamics simulations improves our understanding of aged metals. Finally, she has developed novel strategies, using LLNL's hydrocodes and machine learning models, to reduce Richtmyer–Meshkov instabilities occurring when two materials are impulsively accelerated.

Mark Messner
Argonne National Laboratory

Why does material qualification take so long and how can microstructural modeling help?

Dr. Mark C. Messner is a Principal Mechanical Engineer in the Applied Materials Division at Argonne National Laboratory. He is part of the Thermal and Structural Materials group at Argonne where he works on modeling, simulating, and designing high temperature materials and structures. His research areas include mesostuctural modeling, structural and material design and optimization, machine learning for design problems, development of simulation methods, and engineering design method development. His primary research focus is on metallic materials.