Alex B **Buettner**

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Education

Master of Science, Chemical Engineering
University of Nevada, Reno — August 2016 – Present

Bachelor of Science, Chemical Engineering
University of Nevada, Reno — May 2016

Experience

Machine Learning
University of Nevada — May 2017 – Present

Development of Clinical Process Models from Historical Data
Utilizing semi-supervised machine learning methods for rapid extraction of process dependencies and relationships. Developing and testing of a self-consistent machine learning framework for optimization of large scale processes: including modeling of clinical processes using machine learning and advanced stochastic methods with an emphasis on highly dynamical networks. Building framework for optimization of staff and patient flow within a dynamic clinical environment with hypothetical scenario generation.

High Entropy Alloy Data Mining
Development of machine learning framework for identification of novel HEAs using commonly available material properties data. Studied mixing characteristics of HEAs using excess entropy models.

High Performance Computing
University of Nevada — May 2017 – August 2017

High Performance Computing Systems Management
Installed and setup 64-node HPC cluster in large server environment. Deployed disk-less boot and redundant distributed storage across all nodes. System was deployed with resource management software (SLURM), Ethernet MPI, and InfiniBand hardware/software capabilities.

Scientific Computing
University of Nevada — May 2014 – May 2015

Metal Hexaboride Structure and Energetics Modeling
Developed and assisted with the generation of inter-atomic pair potentials from density functional theory (DFT) and molecular dynamics (MD) simulations. Published in J. Mater. Chem. C, 2015,3, 8649-8658

Structural Modeling of Reverse-Micelle Microreactors
Performed MD study of the stability and morphology of AOT/water/iso-octane reverse micelles. Applications included the use of molecular dynamics codes for prediction and optimization of AOT/water/iso-octane reverse micelles in solution. Utilized common pair potentials for biological systems.

Computational Fluid Dynamics
Simulated dynamic fluid systems using MFiX and other open-source codes. Applied high accuracy numerical integration and differentiation schemes for analysis of multi-dimensional fluid models.

Simulation and Process Control
Designed and simulated a computational process model of a fluidized bed for validation and prediction. Implemented PID control schemes and disturbance inputs for simulated event modeling.

Publications and Presentations

2018 **Clinical Model Development From Unsupervised Machine Learning Methods**
Publication, In Progress

2018 **Real-Time Clinical Process Optimization via Machine Learning and Big Data Analysis**
Masters Thesis, In Progress

2015 **Interatomic pair potentials from DFT and molecular dynamics for Ca, Ba, and Sr hexaborides**
J. Mater. Chem. C, 2015,3, 8649-8658
DOI: 10.1039/C5TC01398D

2014 **Ionic effects on the stability and morphology of AOT/water/iso-octane reverse micelles**
XXV International Materials Research Congress
Cancun, Mexico, August 2014

Software skills

Scripting Performed advanced studies using Python languages for five years in various scientific computing settings, including machine learning, computational fluid dynamics, and molecular dynamics. Experienced in advanced numerical methods and computer algebra systems, as well as object-oriented coding with multiprocessing applications. Two years of experience using machine learning frameworks (sklearn, TensorFlow) for high-throughput data analysis. Designed and configured customized small-scale agent-based modeling framework for use in research applications. Familiar with C++ as applicable to numerical methods and CUDA-based scripting.

Linux/Bash Utilized bash language for pre and post-processing of datasets and generating input scripts. Five years of experience writing automated wrapper scripts for various optimization and simulation codes, with an emphasis in error handling and continuous processing. Utilized Awk and Sed utilities for advanced manipulation of text files and data files. Advanced experience in setup and management of numerous Linux-based operating systems, including RHEL/CentOS, Ubuntu, and Debian.

HPC Scheduling Installed and configured RHEL/CentOS HPC cluster equipped with SLURM resource manager. Handled the configuration of different resource allocations and ensured high-availability of partitions across the cluster for multiple users. Implemented high-availability distributed storage using GlusterFS in conjunction with high capacity conventional storage systems (RAID50).

MD Codes Three years of working experience with various molecular dynamics software packages including HOOMD, GROMACS, and DLPOLY. Performed stability analysis of reverse-micelle systems using GROMACS, with cross-validation and speed-up characterization using the CUDA-accelerated HOOMD codes. Handled post-processing using automated scripts.

DFT Codes Studied the energetics of rare earth hexaboride materials using the open-source Quantum Espresso DFT codes. Optimized cutoff parameters and k-point mesh sizes for various systems. Studied the effects of different pseudo-potentials on computer wall time and convergence rates. Aided in the development of automated pair-potentials extraction from DFT energetics data and temperature-dependent MSD data.

Teaching and Mentoring

Teaching Assistant Acted as primary teaching assitant to a total of six classes over four semesters of graduate study. Lead lab sections for three classes with a total enrollment of over 50 students. Administered testing materials and proctored students during exams. Offered one-on-one and group review sessions, with an emphasis on an excellent base understanding of fundamental materials.