Performance Optimization of the RAMPAGE Metal Alloy Potential Generation Software

**Achievement:** Demonstrated substantial performance and scalability improvements to the RAMPAGE metal alloy potential generation software.

**Significance and Impact:** RAMPAGE is used heavily in the Center for Performance and Design of Nuclear Waste Forms and Containers (WastePD) DOE Energy Frontier Research Center project. Our performance and scalability improvements allow WastePD researchers to generate higher quality potential functions than previously possible with given time and compute resources.

**Research Details:**
- Evaluated initial RAMPAGE implementation’s scalability and performance.
- Modified RAMPAGE to use the Message Passing Interface (MPI), to run on more than one system node, and to use more than one MPI process when evaluating candidate potential functions.

**Sponsor/Facility:** DOE ASCR and NSF. Work was performed at ORNL, LBNL, and Ohio State University on OLCF, NERSC, and OSU systems.

**PI and affiliation:** P.C. Roth (ORNL) as thrust lead within larger SciDAC project led by L. Oliker.

**Team:** P.C. Roth, H. Shan, D. Riegner, N. Antolin, S. Sreepathi, L. Oliker, S. Williams, S. Moore, W. Windl


**Overview:**

The Rapid Alloy Method for Producing Accurate, General Empirical potential generation toolkit (RAMPAGE) is a program for fitting multicomponent interatomic potential functions for metal alloys. In a collaborative effort between domain scientists and performance engineers, we improved the parallelism, scalability, and maintainability of the code. We modified RAMPAGE to use the Message Passing Interface (MPI) for communication and synchronization, to use more than one MPI process when evaluating candidate potential functions, and to have its MPI processes execute functionality that was previously executed by external non-MPI processes. We ported RAMPAGE to run on the Eos and Titan Cray systems of the United States Department of Energy (DOE)’s Oak Ridge Leadership Computing Facility (OLCF), and the Cori and Edison systems at the DOE’s National Energy Research Scientific Computing Center (NERSC). Our modifications resulted in a 7× speedup on 8 Eos system nodes, and scalability up to 2048 processes on the Cori system with Intel Knights Landing processors. To improve maintainability of the RAMPAGE source code, we introduced several software engineering best practices to the RAMPAGE developers’ workflow.