Efficient Implementation of Key Graph Algorithms

Fundamental changes in the way electric power is generated, transmitted, and consumed today have resulted in an unprecedented need for computation to solve problems related to the design, planning, and operation of the power grid. This endeavor and the need to computationally design and model chemicals, materials, and biosystems at a molecular level are fundamental to accomplishing DOE's energy, environment, and national security missions. Recent advances in systems-based approaches coupled with ever-increasing data volumes require extreme-scale computing.

Combinatorial algorithms in general and graph algorithms in particular play a critical enabling role in numerous scientic applications. The irregular memory access nature of these algorithms makes them some of the most difficult algorithmic kernels to implement on parallel systems. Efficient implementation of key combinatorial (graph) algorithms chosen from four exascale application domains—smart grids, computational biology, computational chemistry, and climate science—will be captured in a unified software framework, **ExaGraph**, that targets a diverse set of current and future extreme-scale architectures.

PI: Mahantesh Halappanavar, Pacific Northwest National Laboratory

Collaborators: Pacific Northwest National Laboratory, Argonne National Laboratory, Lawrence Berkeley National Laboratory, Purdue University, Sandia National Laboratories