

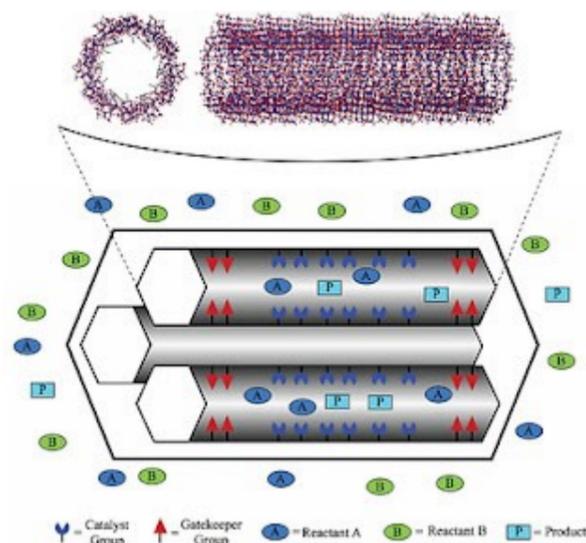
DSATS

DSATS : Research & Project

March 24, 2020



Project 1 : The GAMES Exascale Computing Project

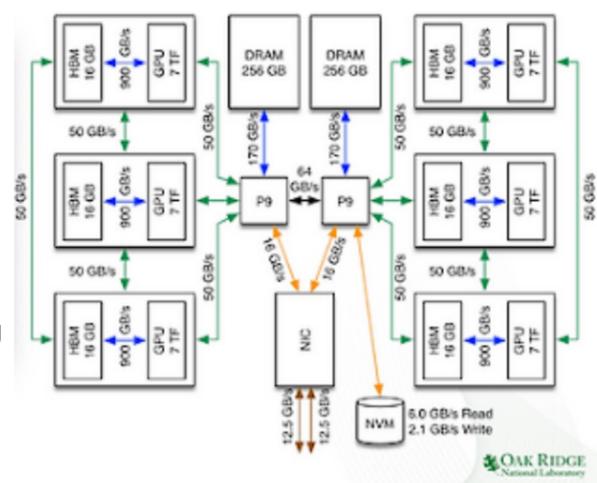


Heterogeneous catalysis and the design of new catalysts is a grand challenge problem in computational chemistry that will require the capabilities of exascale computing. The GAMES project is extending methods and algorithms based on chemical fragmentation methods and coupling these with high-fidelity quantum chemistry (QC) simulations to solve this problem.

As part of the Exascale Computing Project, GAMESS is currently being refactored to take advantage of modern computer hardware and software, and the capabilities of the C++ libcchem code that is co-developed with GAMESS are being greatly expanded.

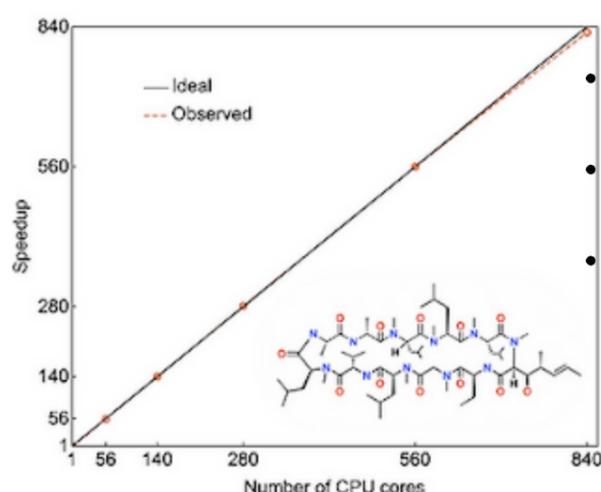
Heterogeneous catalysis and the design of new catalysts is a grand challenge problem in computational chemistry that will require the capabilities of exascale computing. The GAMESS project is extending methods and algorithms based on chemical fragmentation methods and coupling these with high-fidelity quantum chemistry (QC) simulations to solve this problem.

As part of the Exascale Computing Project, GAMESS is currently being refactored to take advantage of modern computer hardware and software, and the capabilities of the C++ libcchem code that is co-developed with GAMESS are being greatly expanded.



- Our group is at the forefront of the GAMESS ECP initiative, which is a concerted effort of the Oak Ridge and Argonne Leadership Computing Facilities, the Ames National Lab, and various other US collaborators and vendors.
- Our development in this project involves leveraging novel hardware architectures and programming model with the ultimate goal of devising software that can be executed on the exascale machines Frontier and Aurora to push the edge of what is currently achievable in chemical modelling.

Project 2 : Architecture and Structure Aware Linear Algebra



- Linear algebra (LA) operations are fundamental to a large number of computational science algorithms.
- LA algorithms is complicated by the increasing architectural heterogeneity of the high-performance computing (HPC) platforms.
- This project aims to build an Architecture and Data-Structure Aware Linear Algebra (ADSALA) software package that will use machine learning to learn the hardware/data-structure/package/algorithm relationships when compiled on a specific hardware architecture for a spectrum of LA packages.

The pursuit of optimal LA algorithms is significantly complicated by the increasing architectural heterogeneity