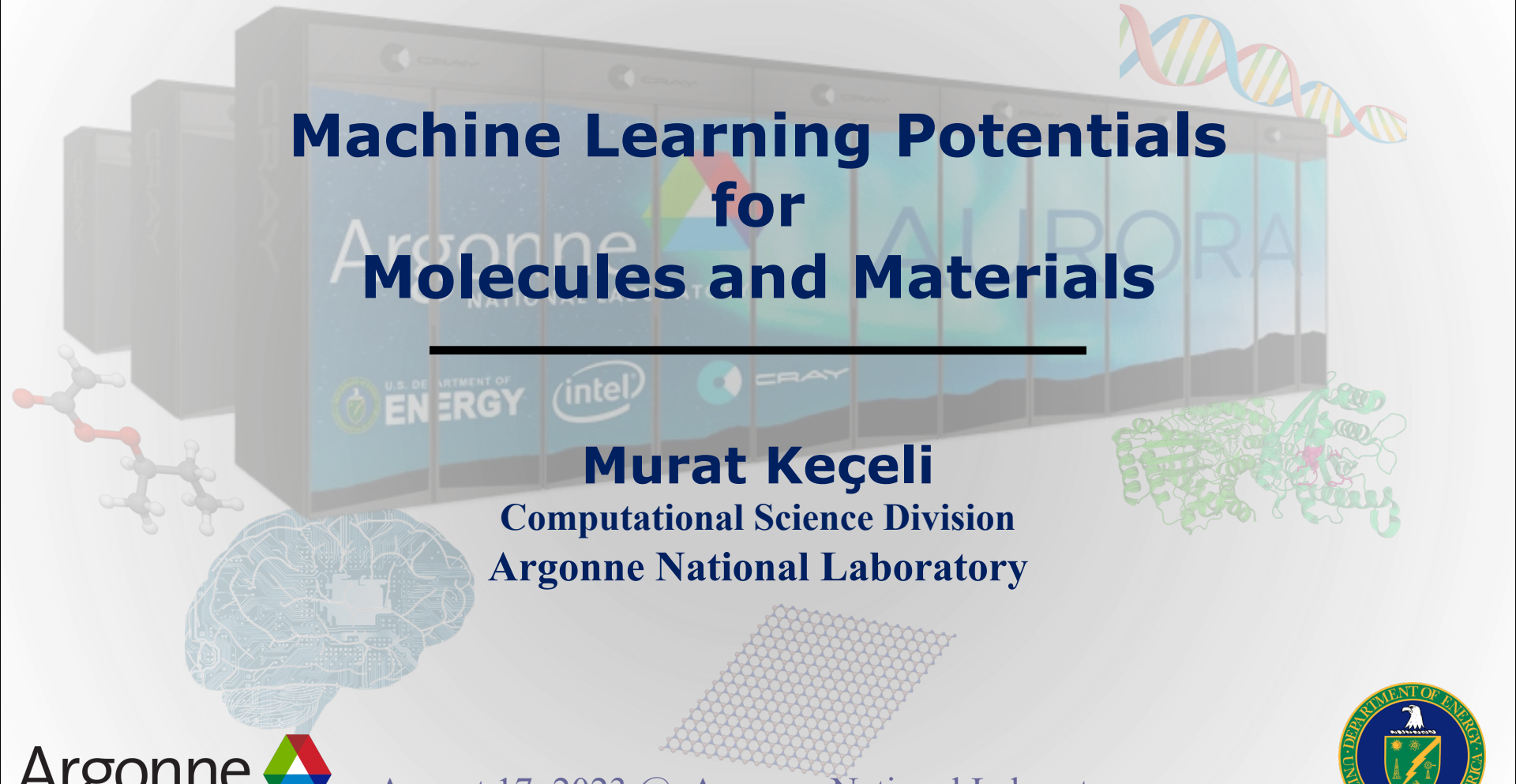

Machine Learning Potentials for Molecules and Materials

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Argonne NATIONAL LABORATORY

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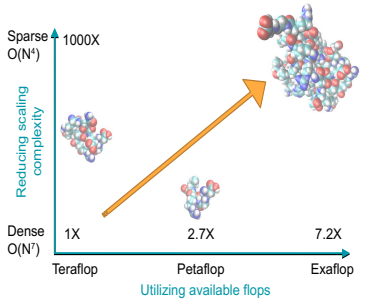
Research Overview

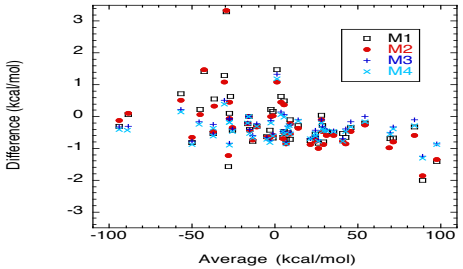
- Development of NWChemEx, VALENCE, QTC, Auto-Mech, SIESTA-SIPs, MaVi.
- Accurate electronic structure calculations and thermochemistry with composite methods
- Workflows for high-throughput quantum chemistry calculations
- Machine learning interatomic potentials
- Thermoelectric properties of 2D materials
- Molecular growth and soot formation

Wavefunction based accurate methods for large scale calculations



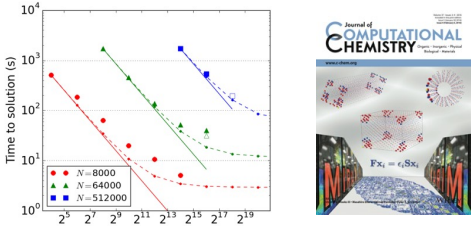
"From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape", *Chem. Rev.*, **2021.**
"PluginPlay: Enabling Exascale Scientific Software One Module at a Time", J. Chem. Phys., **2023.**

Automated workflows for accurate thermochemistry and kinetics



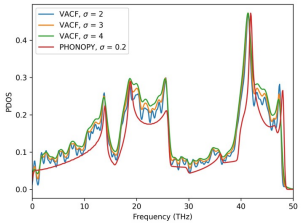
"Automated Theoretical Chemical Kinetics: Predicting the Kinetics for the Initial Stages of Pyrolysis" *Proc. Combust. Inst.* **2021**.
"Systematically derived thermodynamic properties for alkane oxidation", *Combustion and Flame*, **2023.**

Massively Parallel Sparse Eigensolvers

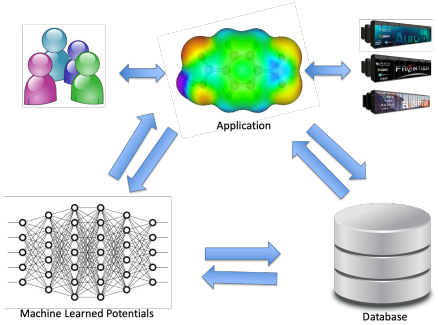
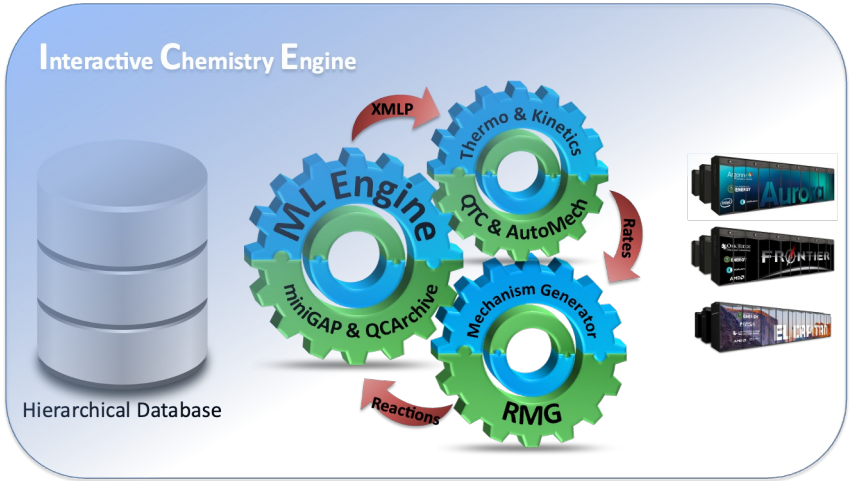
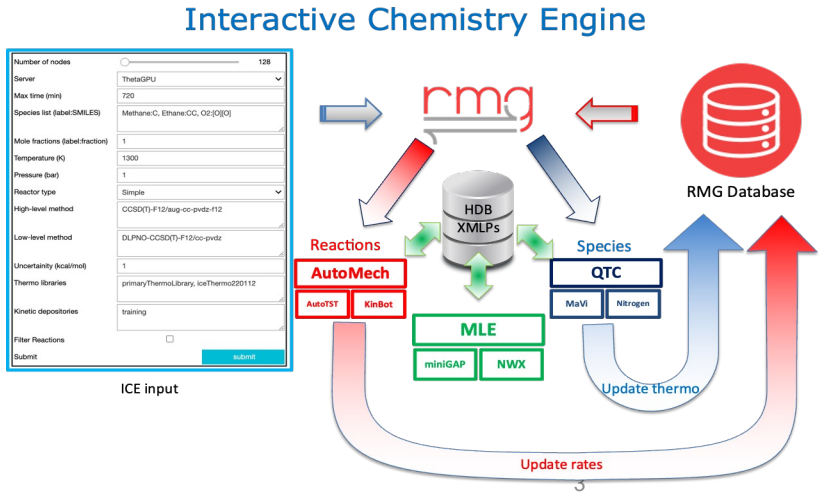


"SIESTA-SIPs: Massively parallel spectrum-slicing eigensolver for an ab initio molecular dynamics package" *J. Comput. Chem.* **2018.**
"ELSI — An Open Infrastructure for Electronic Structure Solvers" Comput. *Phys. Commun.* **2020.**

ML-based potentials for 2D materials



"Computation of the Thermal Expansion Coefficient of Graphene with Gaussian Approximation Potentials". J. Phys. Chem. C **2021**
"Gaussian approximation potentials for accurate thermal properties of two-dimensional materials" *Nanoscale* **2023**

Accelerating Quantum Chemistry

- Ever-increasing computing power, simulation data, and machine learning tools.
- Coupling machine learning and simulations and providing a user-friendly interface to these tools and HPC resources are the keys to solve challenging problems in chemistry and material science.