Eco-Comp: Towards Responsible Computing in Materials Science

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Abstract:

Computational methods such as Density functional theory and Molecular dynamics (MD) simulations have become a key focus in material science, especially with the rise of machine learning interatomic potentials that enables the simulation of multi-million atomic systems. The computational intensity of these simulations necessitates their deployment in high-performance computers (HPCs) and the usage of multi node runs. However large number of submitted calculation by users are targeting speed regardless of efficiency. To foster sustainable and ethical computing practices. We built Eco-Comp, a user-friendly automated Python tool that allows material scientists to optimize their simulations' computing power with one command. In this study, we employed the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) to find the optimal allocation of computing resources based on the simulation input. Through the analysis of bulk metallic systems and surface reactions, we identified various factors that affected parallel efficiency. Through this, we propose rules for responsible computing in HPC architecture that Eco-Comp uses. This Poster gives a broad overview of the Eco-Comp software and its potential use for the material science community through an interactive guide.

Background:

Thousands of High-Performance Computers allocate more than 50% to atomistic research, yet few perform benchmarking before running their simulation.

How to ensure HPCs are used sustainably?

9 INDUSTRY, INNOVATION AND INFRASTRUCTURE

Methodology:

Why are atomistic simulation not benchmarked?

- New users have limited knowledge about the system architecture.
- False assumptions: more computational power = more speed
- Scheduling files reused to save time, impacting performance
- Difficult to distinguish between efficiency and CPU time taken
- Lack of awareness surrounding Responsible Computing

The goal is to build a tool that can:

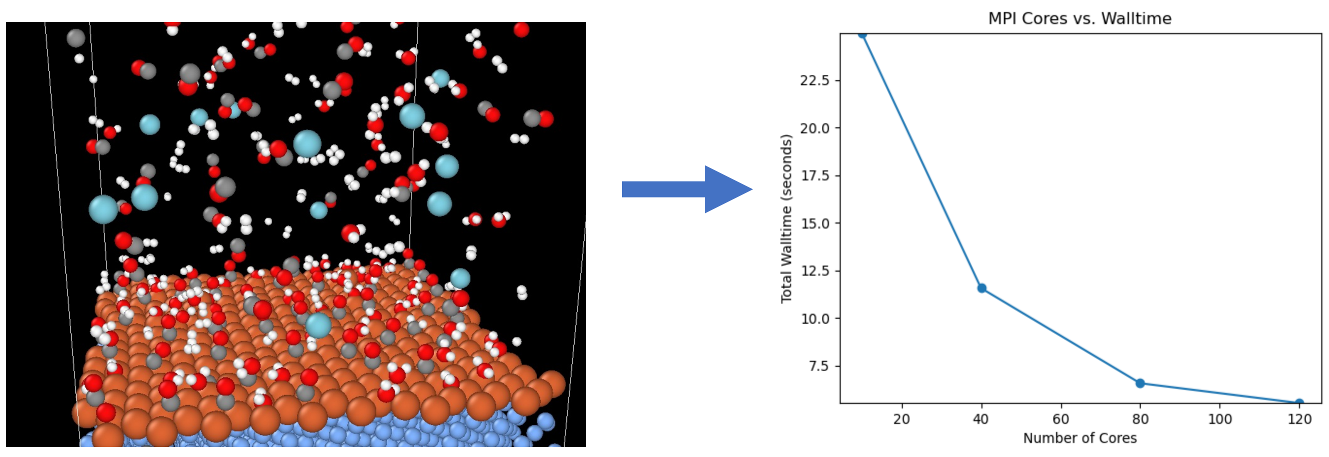
1. Read the simulation data and extract required information
2. Predict benchmark category based on system complexity
3. Run benchmarking on HPC
4. Extract & plot information to select the optimal configuration
5. Build a report and a ready-to-use job submission file

Requirements for building the tool are to understand the:

I. Impact of vacuum space in different atomic systems
II. Potentials used such as ReaxFF, ML-SNAP, etc.
III. Packages used such as Kokkos, MPI, Open-MPI
IV. Parallel efficiency of runs using various MPI cores
V. Possible bottlenecks and impact on parallel efficiency

$$Strong-scaling\ speedup\ on\ N\ nodes = \frac{Time\ on\ 1\ Node}{Time\ on\ N\ nodes}$$

$$Parallel\ Efficiency\ with\ N\ nodes\ (\%) = \frac{Strong\ scaling\ speedup\ on\ N\ nodes}{Number\ of\ nodes} \times 100$$



Acknowledgement:

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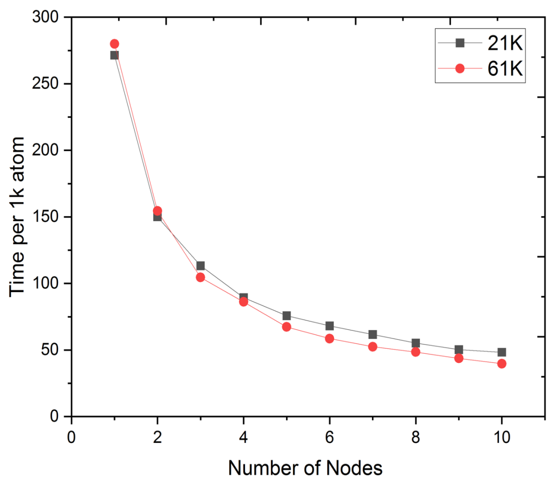
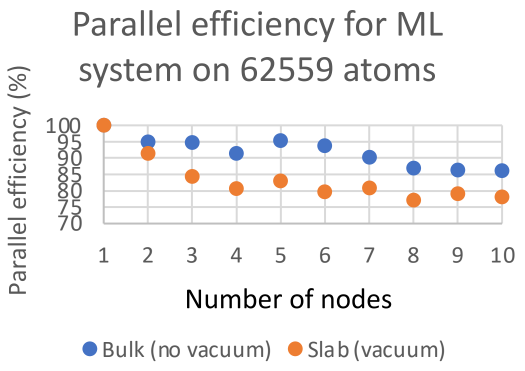
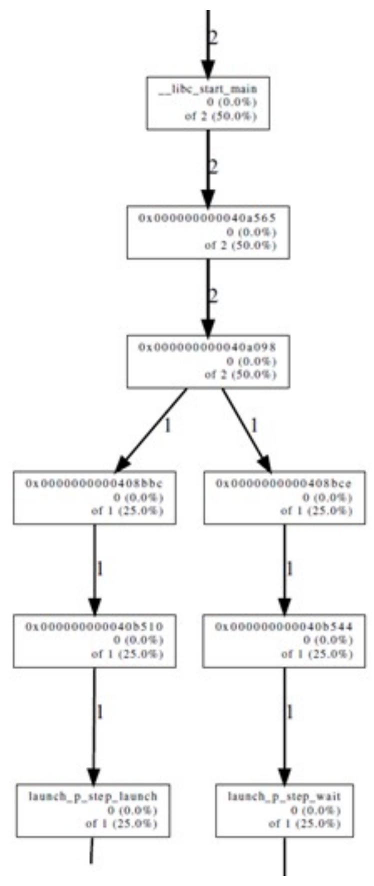
Result and Discussions:

Key takeaways:

- Performance degradation insignificant on small systems
- Kokkos package improves efficiency and speed by ~2× for large atomic systems.
- Slab system with vacuum vs. bulk system without vacuum:
  - 1.3× scale factor using ReaxFF
  - 1.45× scale factor using ML-SNAP
- 66% efficiency threshold set after profiling analysis







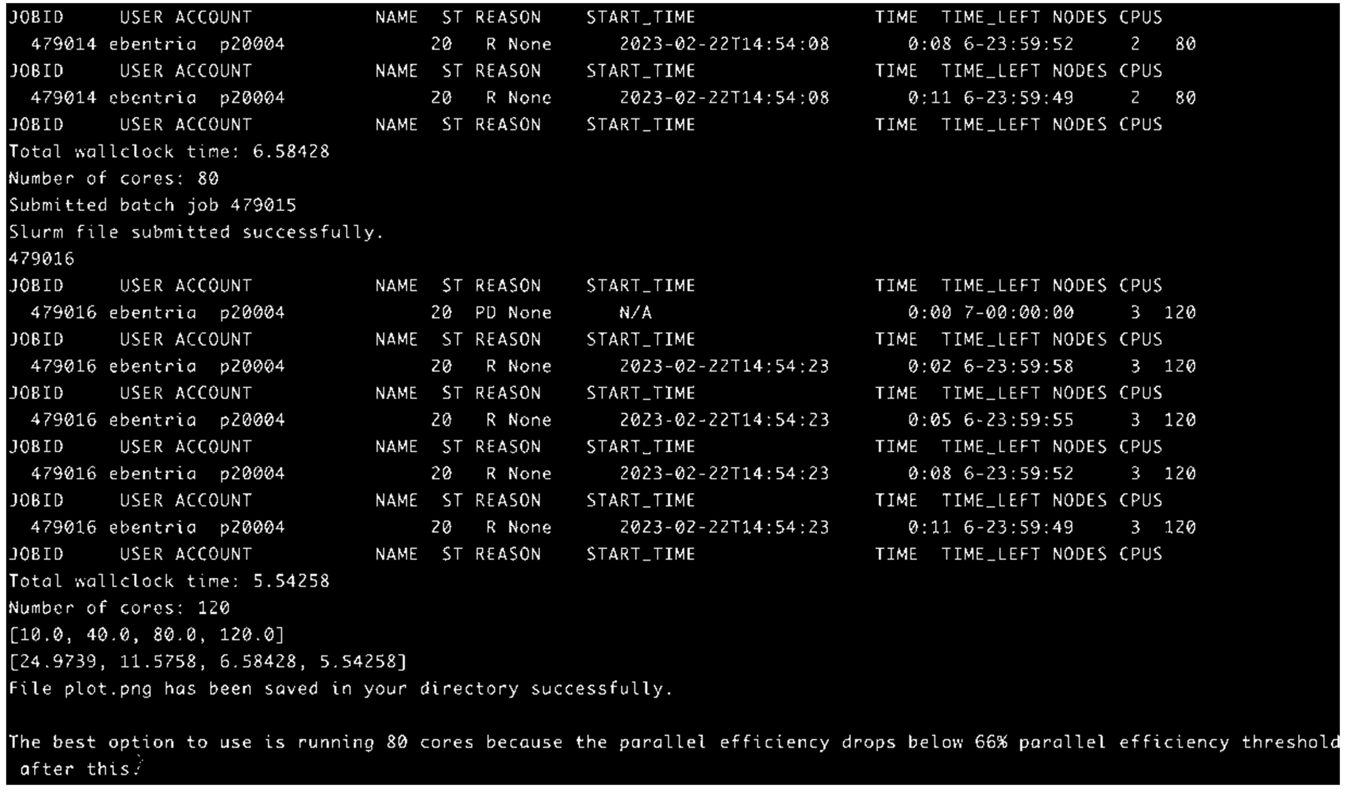
Conclusion and Future Work:

- Eco-Comp is a user-friendly Python tool that optimises simulations' computing power for materials scientists.
- User just needs to run Eco-Comp, and the tool will automatically submit jobs via schedulers and report benchmarking results for sustainable computing settings.
- If this tool gains popularity within the materials science community, the HPC footprint will be reduced considerably.
- Further efforts can be focused on incorporation into the tool, parallel programming such as OpenMP, methods such as EAM, Lennard-Jones, etc., packages such as VASP, and architectures such as GPUs.
- Raise awareness about Responsible Computing!

Outcomes:

- Eco-Comp has been elected for software copyright protection under Qatar Foundation.
- Presented at International Conference on Innovation and Technological Advances for Sustainable Development (ITAS 2023) – World Top 15 Finalist in the Arab Youth Competition.

Implementation of Eco-Comp:



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Number of cores: 80
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The best option to use is running 80 cores because the parallel efficiency drops below 66% parallel efficiency threshold
 after this.
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References:

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