SINAPSE: Scalable Infrastructure for AI-coupled Predictive Simulation at Exascale (NSF 2514139)

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URL: http://project-sinapse.org

Overview

This project will deliver the SINAPSE Software Development Kit (SDK), a robust and extensible kit that enable hybrid workflows that coupled artificial intelligence (AI) with high-performance computing (HPC). The SINAPSE SDK will provide a range of extensible, reusable, and optimized components for coordinating simulations with AI models. SINAPSE will change the state of the art of hybrid AI-HPC workflows.

Motivation

Hybrid AI-HPC workflows are characterized by the online concurrent and coupled execution of AI and HPC tasks, instead of the offline or decoupled execution of AI and HPC tasks. Hybrid AI-HPC workflows are a scalable and sustainable way to obtain significant "effective performance" gains, as they can deliver effective performance gains of 10^6-10^9 relative to "vanilla" HPC applications.

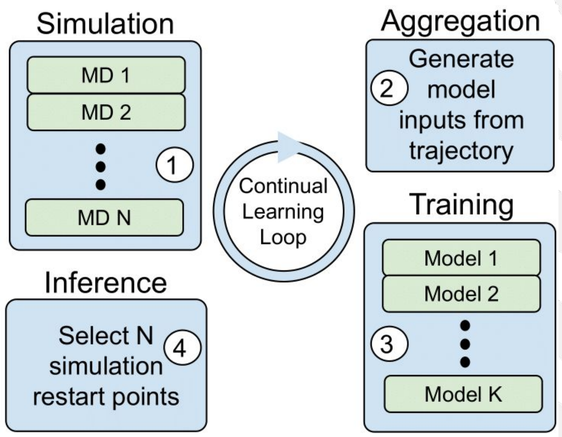
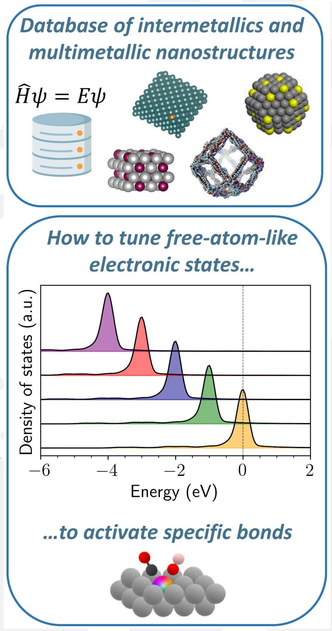


Fig. 1 represents a common mode of coupling AI and HPC tasks.

Target Applications

Key science drivers are drawn from biophysics & materials chemistry:

- **Design of Electronically Programmable Catalysts:** The density of states (DOS). The DOS is a critical tool for rationalizing surface reactivity trends and designing new catalysts. SINAPSE will deploy a deep learning-based active learning framework to discover materials that match a user-defined DOS.



- **Multiscale Protein Dynamics:** Although MD simulations can sample dynamics on the microsecond timescale, its computational cost limits its use for large system. SINAPSE SDK will overcome these challenges using advanced tools to support hybrid workflows.

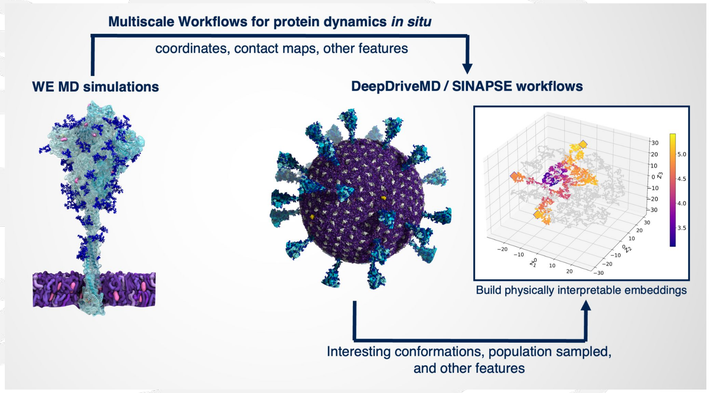


Fig 1. Hybrid AI-HPC workflow that exemplifies the use of SINAPSE SDK to unveil new features and properties of SARS-CoV-2 Spike (delta). The feedback between learning and simulation accelerated sampling by ≳60X

SDK Components

The SINAPSE SDK will develop and curate tools to advance hybrid AI-HPC workflow. The SDK core components are:

- **AIVionics** provides an event system on which developers can deploy AI logic that tunes application performance.
- **Graft** deploys AI models nto an application, reducing the cost of exchanging AI components.
- **Colmena** implements steering logic as Python programs.
- **RHAPSODY** ensures the diverse tasks for AI-enhanced workflows are deployed effectively.
- **MUSE, MUSIC and MELODY:** Application Frameworks for advanced coordination of AI-HPC tasks.

SINAPSE will also support collections of external components. It will coordinate and integrate via a community that shares **packaging, testing, and outreach** to users.

Community

The SINAPSE SDK will engage the Workflows Community Initiative and be formed around three goals:

- **Community**: Establishing places for discussing common challenges
- **Collaboration**: Shared development of common components, engineering processes, and testing infrastructure
- **Coordination**: Joint tutorials and listening sessions with users