SINAPSE: Scalable Infrastructure for AI-coupled Predictive Simulation at Exascale

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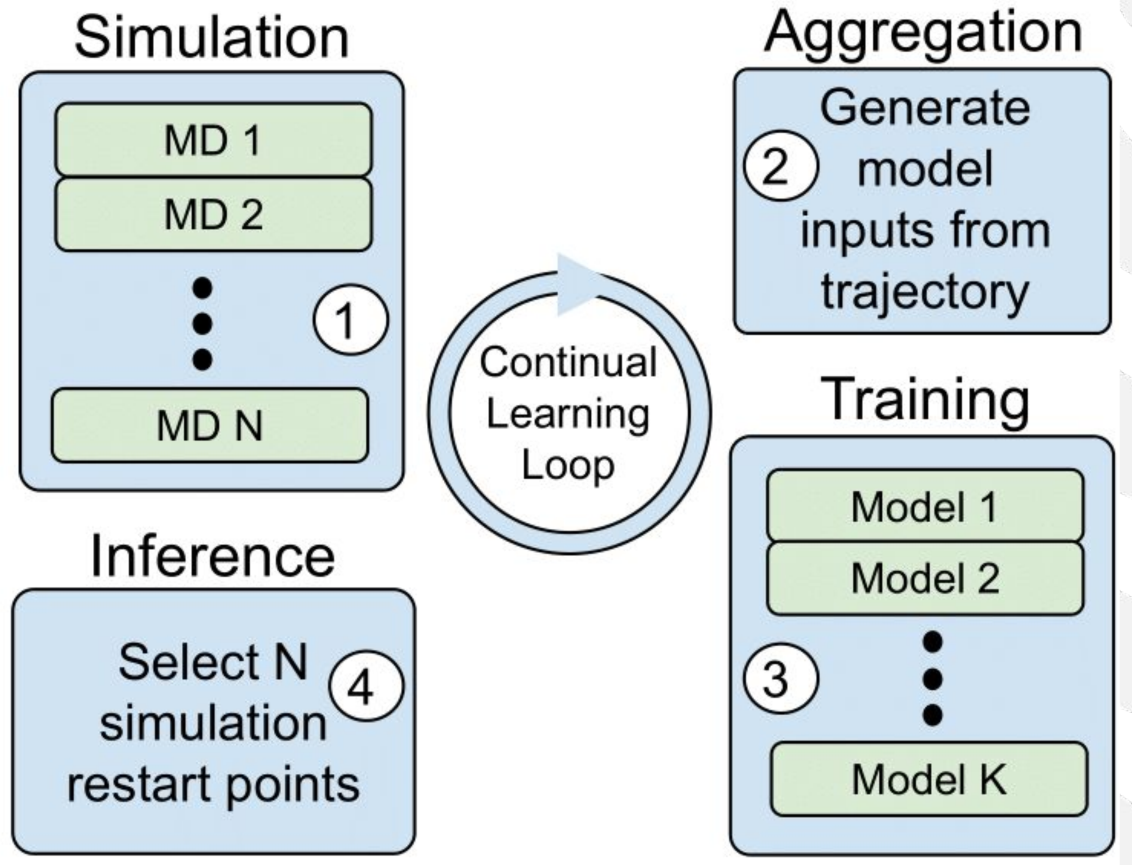
URL: `https://radical-cybertools.github.io/sinapse/`

Overview

This project will deliver the SINAPSE Software Development Kit (SDK), a robust and extensible kit that integrates artificial intelligence (AI) with high-performance computing (HPC) to enable next-generation scientific discovery. SINAPSE features a scalable runtime system that concurrently executes AI and HPC tasks and advanced tools for coordinating simulations with AI models. These capabilities bridge critical gaps in AI-HPC integration by providing reusable, optimized components for addressing complex, high-dimensional problems.

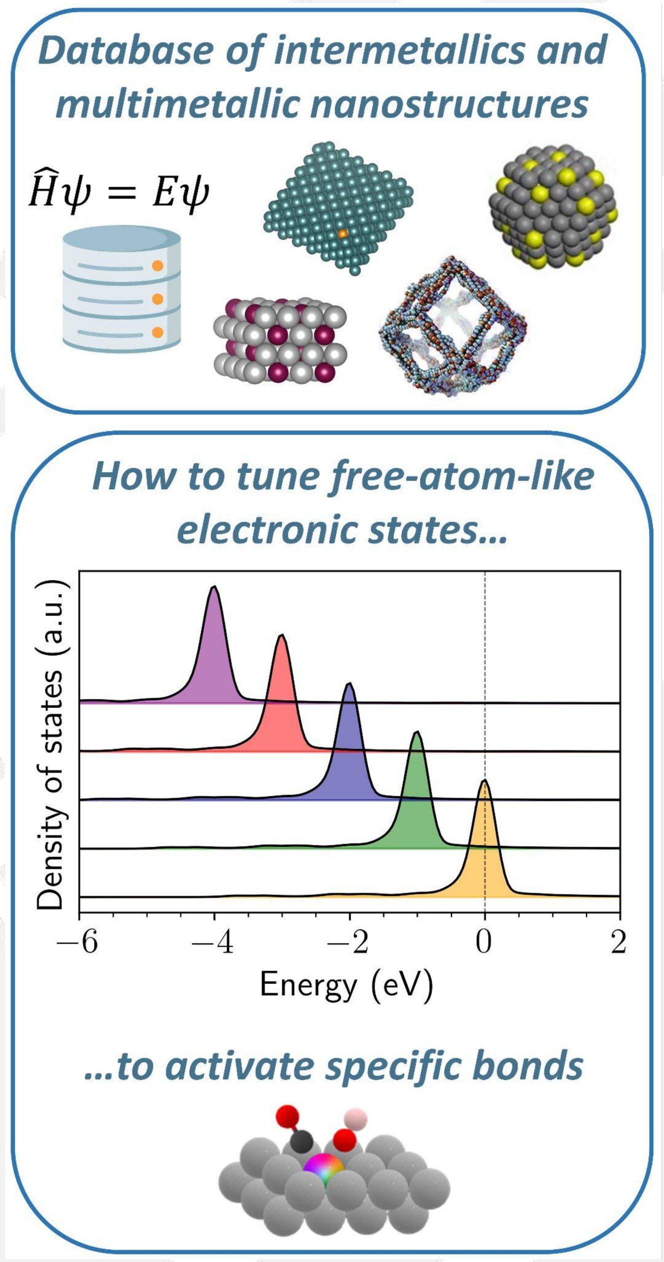
Motivation

Introducing AI models into traditional HPC workflows has been an enabler of highly accurate modeling and has demonstrated a promising approach for significant scientific discovery. AI-coupled-HPC workflows are characterized by the online concurrent and coupled execution of AI and HPC instead of the offline or decoupled AI and HPC. Integrating AI into an HPC workflow is also a scalable and sustainable way to obtain significant performance gains. AI-enhanced high-performance applications could see effective performance gains of 10^6-10^9 within the decade. **Fig. 1** is representative of applications in which AI has advanced simulations and experiments by coupling AI to HPC workflows through different mechanisms.



Target Applications

SINAPSE is exemplified through two key science drivers: in biophysics to accelerate simulations of viral glycoprotein dynamics; and in materials science to facilitate the design of electronically programmable catalysts.



- **Design of Electronically Programmable Catalysts:** In the area of heterogeneous catalysis, one of the most fundamental properties of a material is its density of states (DOS). The DOS is a critical tool for rationalizing surface reactivity trends and designing new catalysts. We propose to use SINAPSE to deploy a deep learning-based active learning framework to discover materials that match a user-defined DOS.
- **Multiscale Protein Dynamics:** Molecular dynamics (MD) simulations provide critical insights into the dynamic behavior of biological molecules at atomic resolution. While MD can sample dynamics on the microsecond timescale, its computational cost limits its use for large system. To address these challenges, AI and HPC integration via the SINAPSE SDK will enhance these workflows.

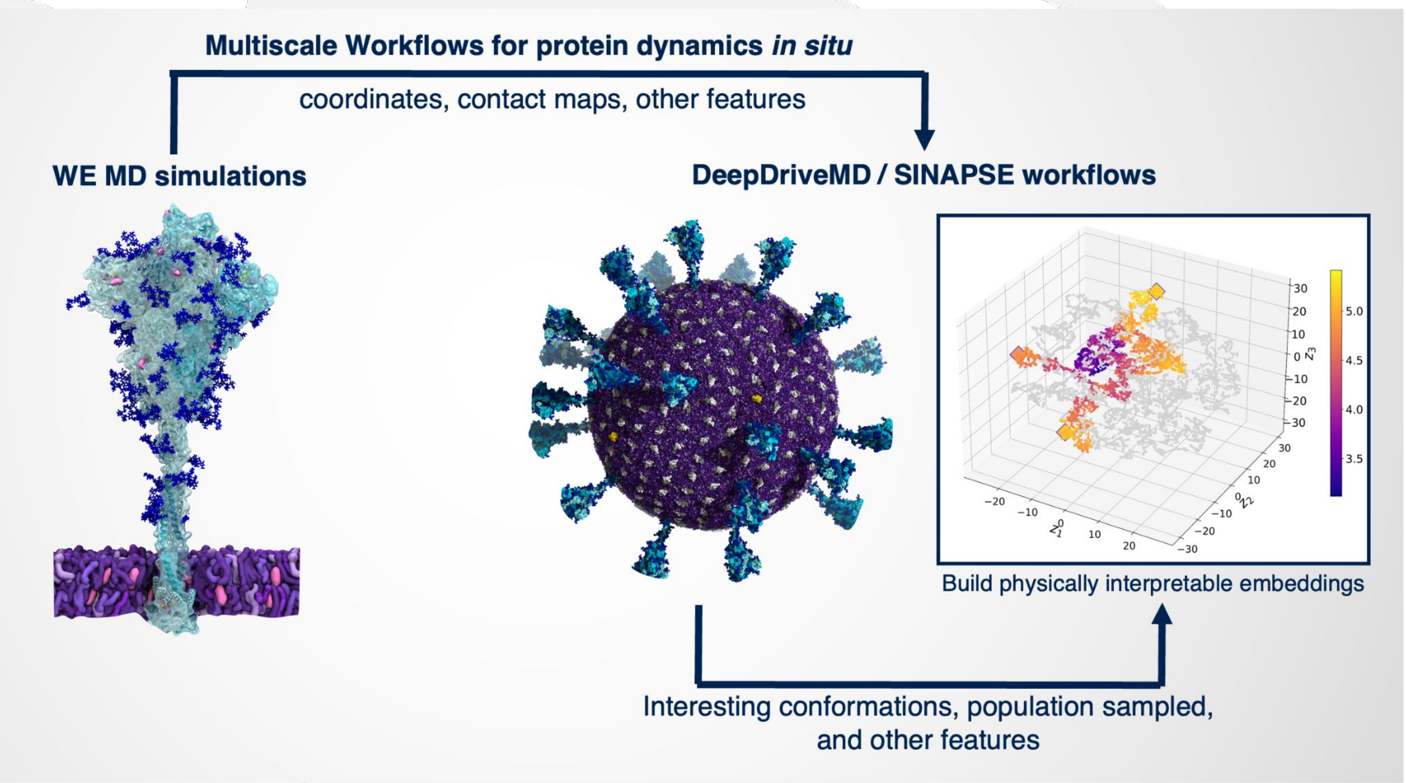
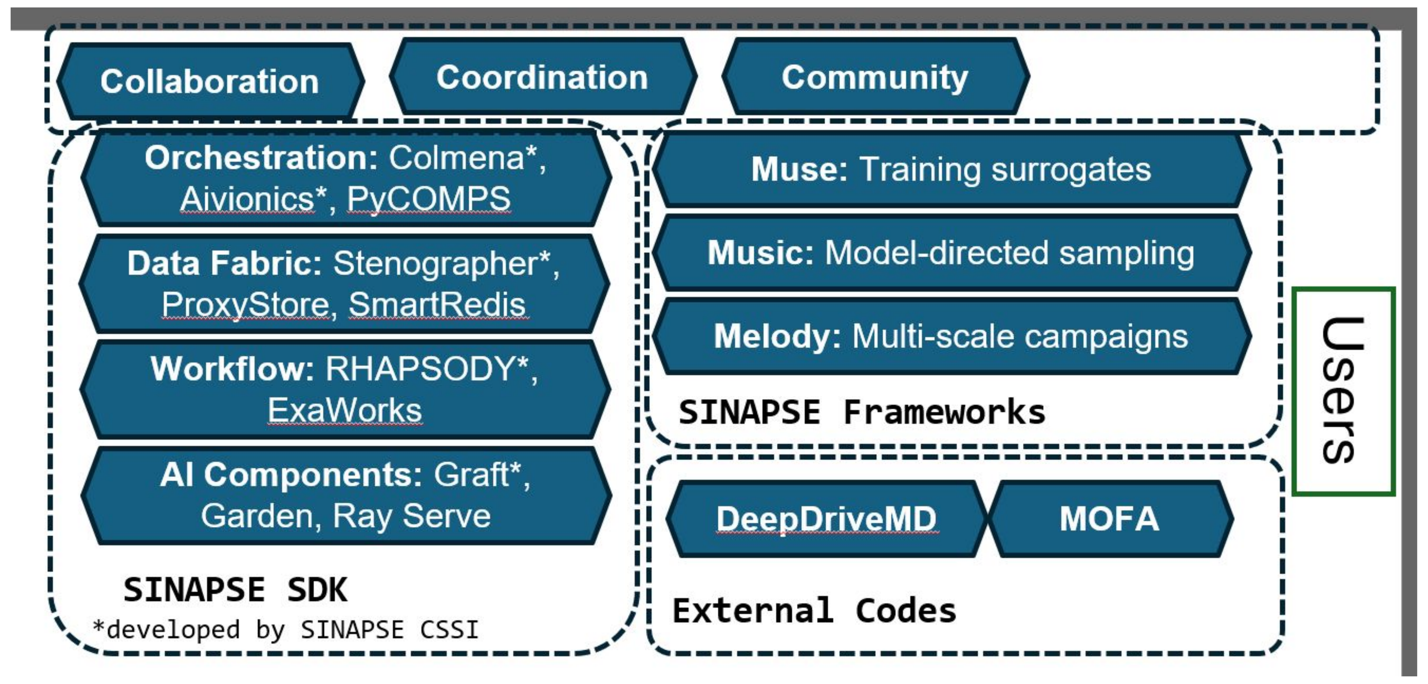


Fig 1. AI-coupled HPC workflow that exemplifies the use of SINAPSE SDK to combine weighted ensemble molecular dynamics (WE MD) simulations and AI to unveil new features and properties of SARS-CoV-2 Spike (delta) on leadership class supercomputers, The feedback between learning and simulation accelerated sampling by ≳60X

SDK Components

The SINAPSE SDK must contain tools that meet the diverse needs of AI-coupled HPC workflow applications. We will develop five core components as part of SINAPSE.

- **AIVionics** provides an event system on which developers can deploy AI logic that tunes application performance.
- **Graft** deploys AI models directly from the Garden project into an application, reducing the cost of exchanging AI components.
- **RHAPSODY** ensures the diverse tasks for AI-enhanced workflows are deployed effectively.
- **MUSE, MUSIC and MELODY: Applic**
- **Colmena** implements steering logic as multi-threaded Python programs.



SINAPSE will support collections of Components that can be composed into Frameworks which implement common application patterns. All coordinate and integrate via a Community that shares **packaging, testing, and outreach** to users. Users of SINAPSE SDK can engage from the **education materials**, using **Frameworks** for specific problems, or employing **components** in their software.

Community

The SINAPSE SDK will 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