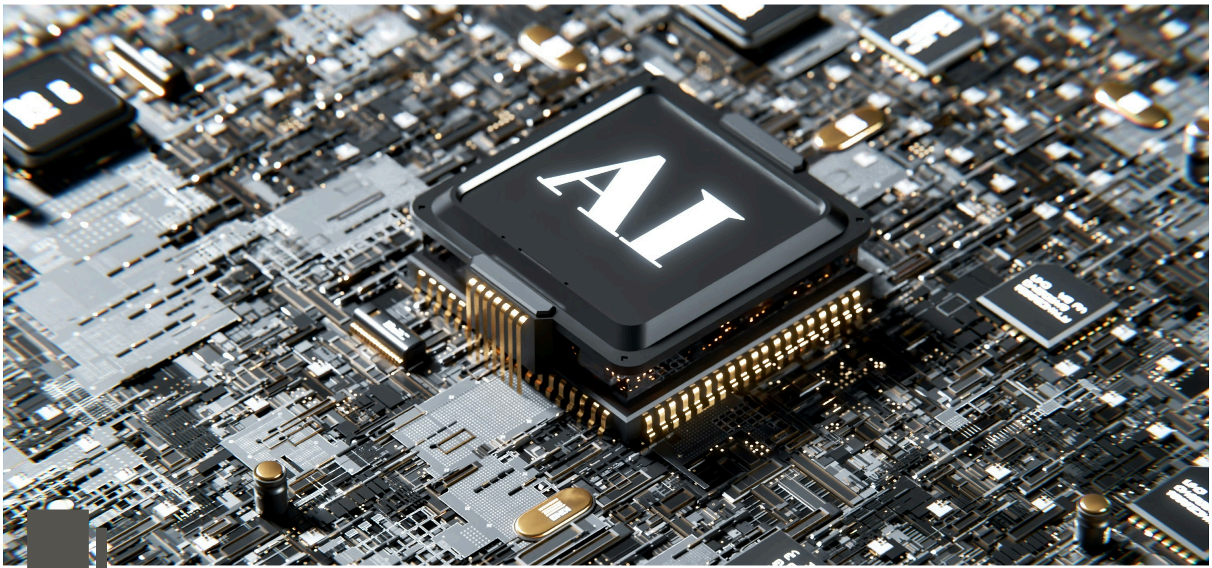

AI-HPC Hybrid Project Doc - Mid Review Deliverables

Tags

AI-HPC Hybrid Project – Mid Review (Review 1)

Course: High-Performance Computing

Phase: Mid Review (Review 1)

Deadline: 19 Feb (Tentative)

Team: Individual

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1. Project Overview

The **AI-HPC project** explores a **hybrid scientific computation workflow**:

1. Students select a **computationally expensive sequential HPC workload**, such as:
   - Solving **ODEs / PDEs**
   - Iterative solvers (Jacobi, Gauss-Seidel, Conjugate Gradient)

- Simulation-based computations (fluid dynamics, molecular dynamics, N-body systems)

2. Students implement HPC computation **up to a critical state or checkpoint**, generating **accurate intermediate states**.
3. Students then develop an **AI model** that **predicts subsequent states or accelerates computation** beyond the checkpoint.

> Key Principle: HPC complements AI — it provides critical input data for the AI model. Optimized HPC output ensures that AI predictions are accurate and meaningful.

This project combines **classical HPC computation** with **AI-driven acceleration**. Students have **full freedom in selecting the AI model**, but they must implement the HPC computation, reach the checkpoint, and integrate AI predictions in the Mid Review.

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2. Mid Review Objectives

By the end of the Mid Review, students must:

1. **Select a computationally intensive problem** from the provided list (or propose their own).
2. **Implement the HPC computation** to reach a **critical state or checkpoint**, generating intermediate data/states.
3. **Develop an AI model** that:
   - Predicts subsequent states
   - Or accelerates the computation beyond the checkpoint
4. **Demonstrate acceptable accuracy** of the AI predictions compared to full HPC computation.
5. Ensure **reproducibility**: results must be replicable on the same system with the same code and data.

> Note: Optimizations for performance (hardware utilization) are not mandatory at this stage. Accuracy and reproducibility are the priorities.

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3. Guidelines for Students

1. **Select an HPC problem** from the provided list (or propose your own).
2. **Implement HPC computation** to generate intermediate states up to a checkpoint.
3. **Develop the AI model** using any approach (LLM/NN/DL/PINN/RNN/Transformer/etc.) to predict or accelerate computation beyond the checkpoint.
4. **Validate AI predictions** against HPC computation beyond the checkpoint:
    - Maintain **acceptable accuracy** (define tolerances or error metrics)
    - Ensure predictions are reproducible
5. Document all stages:
    - HPC computation
    - Checkpoint states
    - AI model design and predictions
    - Accuracy analysis
    - Reproducibility instructions

> Students are free to choose the AI model architecture, training strategy, and prediction method.

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4. Deliverables

1. **Problem Selection**
    - Clearly state which HPC problem was chosen.
    - Justify why it is suitable for AI-HPC hybrid workflow.
2. **HPC Computation**
    - Code implementing HPC workload up to checkpoint
    - Generated checkpoint/intermediate states
3. **AI Model Implementation**
    - Code for AI model that predicts or accelerates computation beyond checkpoint
    - Training and inference methodology

4. **Validation / Accuracy Report**
   - Compare AI predictions to full HPC computation beyond checkpoint
   - Metrics (RMSE, MSE, MAE, or domain-specific error metrics)
   - Graphs or visualizations to illustrate prediction accuracy
5. **Reproducibility Documentation**
   - Instructions to reproduce HPC and AI results
   - Dependencies, dataset preparation, code execution steps

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5. Example HPC Problems (70 Options)

Students can select any problem. These generate **states/data for AI training or prediction**.

Differential Equations / Simulation

1. 1D heat equation
2. 2D heat diffusion
3. 3D Poisson equation
4. Navier-Stokes 2D fluid flow
5. 1D wave equation
6. 2D wave propagation
7. Schrödinger equation 1D/2D
8. Lorenz system chaotic simulation
9. Reaction-diffusion PDE (Turing patterns)
10. Predator-prey population dynamics (Lotka-Volterra)
11. Fokker-Planck equation
12. Burgers’ equation 1D/2D
13. Diffusion-advection equation
14. Convection-diffusion problem
15. Heat transfer in irregular geometries
16. Coupled ODE systems (mass-spring-damper)

17. Quantum harmonic oscillator evolution
18. Nonlinear pendulum
19. RLC circuit simulations
20. Fisher-KPP population PDE

Linear Algebra / Iterative Solvers

1. Sparse matrix multiplication
2. Jacobi iterative solver
3. Gauss-Seidel solver
4. Conjugate gradient solver
5. Eigenvalue solver
6. PageRank iterative solver
7. LU decomposition
8. Large-scale linear regression
9. Principal Component Analysis on large datasets
10. Sparse LU decomposition

Optimization / Scientific Computation

1. Monte Carlo integration
2. Markov Chain Monte Carlo (MCMC) sampling
3. Simulated annealing
4. Genetic algorithms
5. Particle swarm optimization
6. Molecular dynamics simulation
7. N-body gravitational simulation
8. Finite element method 1D bar
9. FEM 2D beam
10. FEM 3D structure
11. Electromagnetic field simulation (FDTD)

12. Heat conduction FEM

Signal / Image Processing

1. Large-scale FFT computation
2. Convolution on big datasets
3. Image denoising via PDE diffusion
4. Edge detection on high-resolution images
5. Tomographic reconstruction
6. MRI simulation/reconstruction
7. Seismic data modeling
8. Audio signal filtering

Stochastic / Probabilistic Models

1. Random walk simulations
2. Brownian motion
3. Epidemic spread (SIR/SEIR)
4. Stock price simulation (Geometric Brownian Motion)
5. Queueing network simulation
6. Traffic flow simulation

Other HPC Tasks

1. Cellular automata (Conway's Game of Life)
2. Lattice Boltzmann fluid simulation
3. Agent-based crowd simulation
4. Simplified climate simulation
5. Ocean circulation simplified model
6. Volcano particle simulation
7. Rocket trajectory integration
8. Protein folding simplified simulation
9. Diffusion-limited aggregation

10. Fractal generation computation
11. High-res Mandelbrot/Julia set
12. Satellite orbit simulation
13. Planetary system N-body simulation
14. Large-scale network diffusion simulation

> The AI model for prediction is entirely student-defined and will integrate after HPC data is generated.