Physics-Aware Multi-Agent AI Framework for Property Prediction and Design of Aluminium Alloys

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Abstract

A major frontier in aluminium alloy discovery is the development of intelligent systems that can automate complex material modelling and design tasks leveraging diverse knowledge, tools and capabilities. Such systems are very crucial for generating novel insights into aluminium alloy properties by iteratively refining the alloys prediction and discovery strategies, merging insights across the discipline to converge towards optimal physics compliant solutions. Large language models (LLM) have demonstrated significant potential in complex reasoning, strategic planning, coding, and workflow orchestration showing promising capabilities in materials analysis and property prediction including hypothesis testing, knowledge retrieval and multimodal reasoning. However, they face challenges in new alloy design and discovery due to out-of-domain knowledge, inability to perform physics-based simulations, restricted access to external sources, and reliance on potentially outdated knowledge.

In this work, we propose physics aware multi-agent LLM framework designed to address the unique challenges for property prediction, design, and discovery of aluminium alloys. The framework utilises an orchestrated network of LLM agents that performs automated knowledge retrieval and reasoning on integrated multi-modal data of heterogeneous nature of the process, experimental and simulation material dataset. To ground the models on physics laws and to support advanced simulation capabilities, the LLM agents are synergistically combined with Large Atomic/Molecular Massively Parallel Simulator (LAMMPS) for atomistic simulations.

Our work presents a series of experiments to demonstrate how our agentic system addresses various task in the aluminium alloy design, particularly through generating new physics via atomistic simulation, substantially reducing the need for human intervention. Specifically, we show that the model can integrate material properties from diverse sources, tackle multi-modal problems and solve multi-scale problems connecting microscale features to macroscopic properties.

Keywords: Large Language Model (LLM), Aluminium alloys, Agentic framework, Physics simulation.

1. Introduction

Aluminium alloys play an indispensable role across diverse industries, including aerospace, automotive, and renewable energy, owing to their favourable strength-to-weight ratio, excellent corrosion resistance, and versatile mechanical properties. Despite their broad application, the systematic design and optimisation of novel aluminium alloys remain challenging due to the complexity of alloy composition spaces and the extensive computational and experimental effort required. Conventional alloy design approaches frequently rely on iterative experimentation and atomistic simulations, which are inherently labour-intensive and pose difficulties in scalability and reproducibility. Consequently, there is an increasing need for innovative methodologies capable of streamlining and automating these complex workflows, facilitating rapid and reliable exploration of alloy chemistries.

Recent advancements in artificial intelligence (AI), particularly the emergence of multi-agent orchestration systems and sophisticated machine-learning models such as Graph Neural Networks (GNNs), offer promising solutions to overcome traditional limitations. In this work, we present a novel multi-agent orchestration framework designed specifically for aluminium alloy modelling and simulation, leveraging autonomous computational agents specialised in research, simulation planning, molecular dynamics execution, data processing, and visualisation tasks. The proposed approach is demonstrated via agent-based simulations performed with Large-scale Atomic/Molecular Massively Parallel Simulator LAMMPS [1] and interatomic potential predictions derived from GNNs which was constructed and trained autonomously through agentic orchestration. We substantiate our methodology through targeted case studies that demonstrate its capabilities across multi-scale property prediction, structure–property relationship modelling, and atomistic visualisation, thus highlighting significant improvements in efficiency, reproducibility, and speed of discovery in aluminium alloy design.

2. Literature Review

Atomistic modelling with the LAMMPS remains the core for probing aluminium alloys at the nanoscale. Recent studies, such as the MD analysis by Wu and Zhang on Al-4 wt% Cu single crystals, have clarified orientation-dependent plasticity by correlating dislocation activity and stacking-fault evolution with macroscopic anisotropy [2]. Comparable LAMMPS investigations across Al-Mg, Al-Li and Al-Cu chemistries have mapped solute segregation, grain-boundary stabilisation and temperature-controlled precipitation, underscoring the simulator's ability to link atomistic events to bulk properties. Nevertheless, exhaustive sweeps over composition, temperature or defect space remain computationally prohibitive, and the heavy manual effort required for script preparation and data post-processing hampers throughput and reproducibility.

Addressing these constraints, the materials community is rapidly adopting AI-driven multi-agent orchestration frameworks that automate literature mining, simulation planning, execution and analysis. The MULTI-agent autonomous facilities scalable framework (MULTITASK) developed at NIST demonstrates how heterogeneous machine-learning agents can co-ordinate experiments facility-wide, optimising resource use while allowing researchers to "fail smarter" and learn faster [3]. Extending this concept to alloy discovery, the recently proposed AtomAgents platform integrates large language models with physics-aware agents that retrieve knowledge, generate LAMMPS inputs, launch simulations and analyse outputs, all within a closed-loop environment [4]. These frameworks highlight the transformative potential of agentic systems to standardise complex workflows, scale exploration across vast compositional spaces and ensure transparent provenance for every computational step.

Parallel progress in graph neural networks (GNNs) has furnished highly accurate, data-efficient interatomic potentials that can be embedded within autonomous pipelines. The E(3)-equivariant NequIP model, for example, attains near first-principles accuracy with up to three orders of magnitude fewer training structures than earlier ML potentials, enabling long-time, large-system molecular dynamics at minimal cost [5]. When coupled with multi-agent planners, such GNN surrogates serve as rapid predictors that flag high-uncertainty regimes and trigger targeted high-fidelity simulations only, when necessary, thereby optimising computational budgets while preserving reliability. Together, LAMMPS-level physics, AI-orchestrated autonomy and GNN-powered surrogacy define the contemporary frontier in aluminium-alloy modelling, offering an unprecedented route to scalable, reproducible and accelerated materials discovery.

3. Methodology

We present a novel multi-agent orchestration approach to address the unique challenges associated with aluminium alloy modelling and design. The multi-agent framework consists of distinct computational agents, each specialised for specific roles within the workflow of predicting and designing aluminium alloys. These agents autonomously interact through a centralised memory component orchestrated by a Chat Manager, facilitating structured communication and coordination. The primary contributions of our work are as follows:

- Atomistic simulation combining large language model for retrieving new physics for aluminium alloys.
- Advances research with reduced human intervention based on textual inputs to effectively perform literature review and data discovery and modelling in the realm of aluminium and its alloys.

4. Case Studies

In this section, we present the various capabilities for aluminium alloy designs by the multi-agentic framework grounding on physics rules and atomistic simulations. All simulations and modelling are performed using open-source framework like LAMMPS and Pytorch. As illustrated in the sub sections below, we were successfully able to show that the multi-agent system was able to perform complex tasks requiring good domain expertise such as a) literature survey and capture data from multiple sources necessary for the material science project, b) code surrogate models with data discovery for establishing machine learning potential, c) work with simulation models like LAMMPS thus grounding the working on multi-physics. This is a new paradigm in alloy discovery making it more accessible for research and development with improved the speed and efficiency

4.1 Atomistic Property Prediction via LAMMPS Simulation

4.1.1 Objective

The primary objective is to demonstrate how the agentic framework systematically orchestrates the discovery, preparation, execution, and analysis of LAMMPS simulations to predict key material properties, such as bulk lattice energy, defect formation energies, and thermodynamic stability under varying Mg concentrations. The study specifically aims to: (i) showcase the fully autonomous orchestration of tasks from initial user intent to simulation output validation, (ii) evaluate the framework's capacity to explore multiple compositions and thermodynamic states without manual intervention, and (iii) validate the integration of data acquisition, simulation execution, and result visualisation as distinct yet interdependent agent roles within the system.

4.1.2 Agentic Workflow

The agentic workflow for alloy prediction with LAMMPS consists of multiple agents as illustrated below managed by the Chat Manager for internal communication and orchestration. The objective of this framework is to observe if the system of agents together can perform from data acquisition to simulation and post processing autonomously as presented in Figure 1.

- **Research Agent** is tasked to extract Embedded Atom Method (EAM) potentials, lattice parameters, and other simulation paraments from multiple scientific sources including literature repositories. Further, the agent converts the raw data into JSON objects and saved for access by the Planner and other agents.
- **Planner Agent** is tasked to construct the LAMMPS input script based on the data capture by the research agent post validation checks to prevent inconsistencies. The planner agent

is provided with a base template for the LAMMPS input script as it was found to not performing well building the script from scratch.

- **Simulation Agent** is tasked to execute the run the molecular dynamics simulation (MD) using the LAMMPS script generated by the planner agent. The simulation run output, and logs are saved in dump.lammpstrj and log.lammps to understand key parameters such as thermodynamic properties, atomic coordinated as well as structural outputs.
- **Coding Agent** is tasked to parse the output from simulation agent on the MD run and extract the necessary properties such as potential energy, defect formation energies etc. The data extracted is formatted for further analysis and visualisation.
- **Visual Agent** is tasked to build graphs and animations necessary for results and insights based on the data made available by the coding agent. Visualisation capabilities include generation of stress-strain curves and animation of the evolution of atomic structure across the simulation runtime.

The end-to-end orchestration and communication between the agents is handled by the Chat Manager. The chat manager is stateful and understands the next task to be executed and precariously picks the necessary agent to perform the task. This ensures very less manual intervention and enables rapid iteration and prototyping.

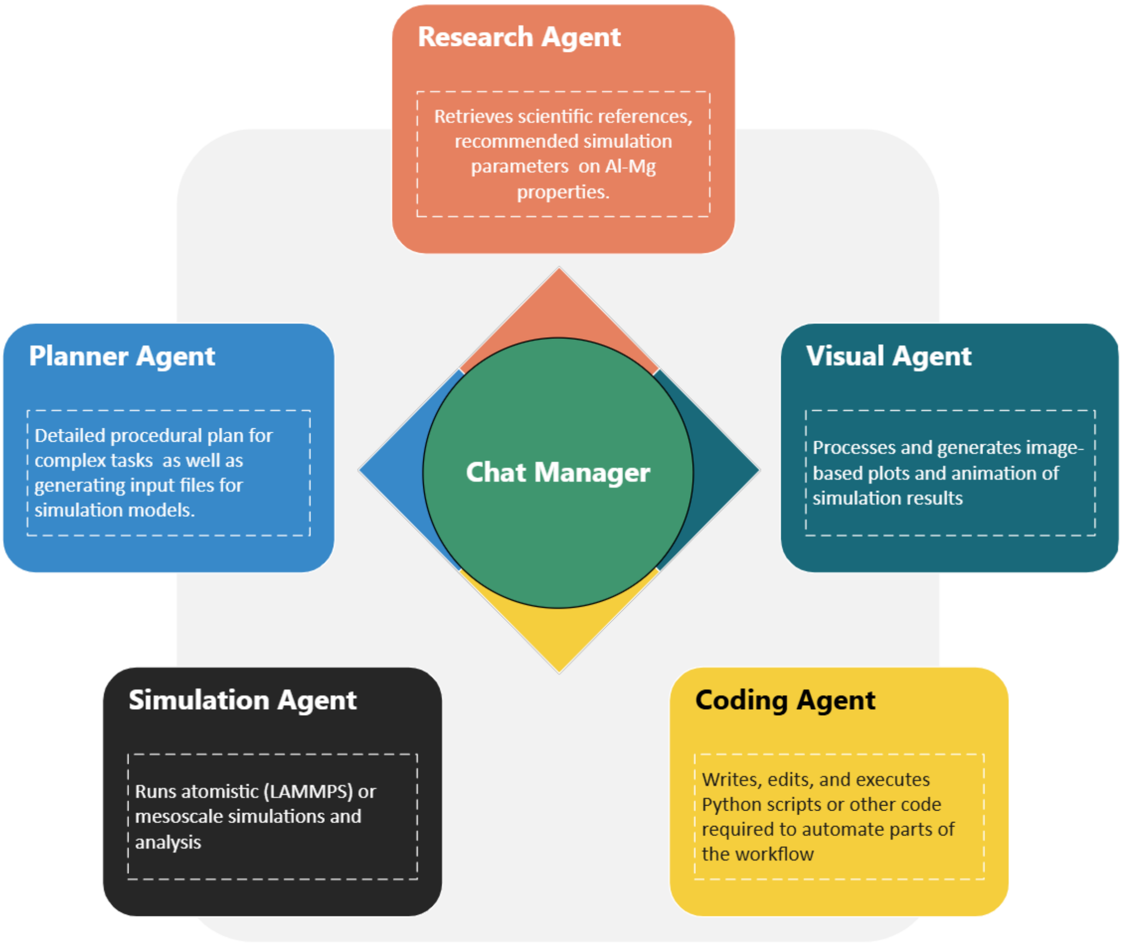


Figure 1. Multi-agent orchestration framework for LAMMPS simulation of Al alloys.

4.1.3 Results and Discussion

The agentic orchestration framework developed demonstrated an autonomous workflow for alloy simulation and property prediction. The results indicate that the individual tasks were efficiently performed by each agent as well as the overall objective were achieved through coordination between agents. On analysing of the performance of each agent, the planner agent and the research agent had maximum number of retries to achieve their optimal tasks. This is attributed to the exploratory nature of their tasks and their limited understanding of LAMMPS tool and configuration requirements. Fine-tuned LLM models on molecular dynamic simulation and LAMMPS instead of general purpose LLMs would greatly improve the performance of such models. Still the simulation performed achieved 75 % computational efficiency and handled numerical instabilities.

In order to validate the framework, we performed studies on Al-Mg allow with varying Mg concentration. The molecular dynamic simulation performed using the agentic orchestration framework was able to validate and confirm the expected structural and energy properties of the system. As shown in Figure 2, radial distribution function analysis was performed to study the Al-Al and Al-Mg interaction peaks. The study reveals consistency and accuracy with the experimental data. The composition dependant cohesive energy displayed expected non-linearities in line with the theoretical thermodynamic behaviour. Structural analysis showed reduction in local coordinate numbers and expansion of lattice parameters in line with the Vegard’s law. Further, detailed structural analysis showed concise and precise atomic density distribution along the Z-axis as illustrated in Figure 3. such detailed visualizations were generated by the Coding and Visual agent thus tremendously enhancing and accelerating insights.

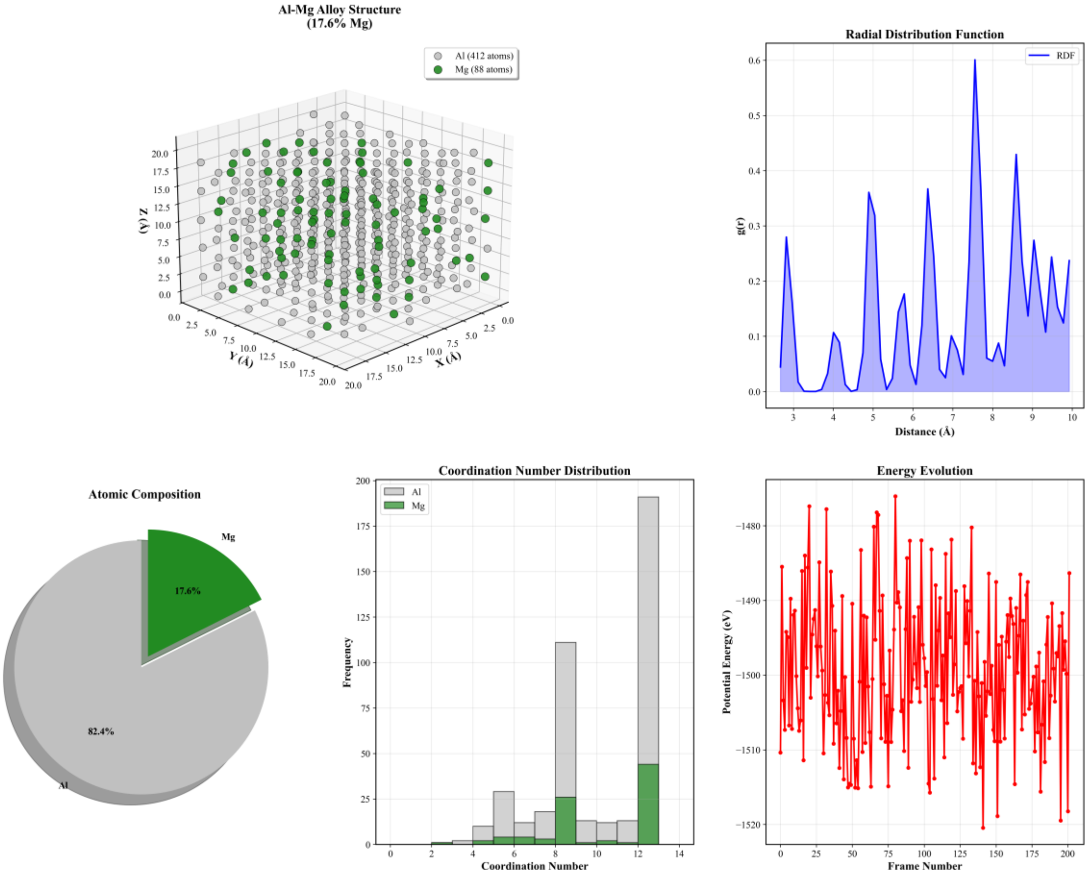


Figure 2. Analysis of Al-Mg alloy structure (17.6 % Mg) from LAMMPS simulations.

The agentic framework was able to significantly reduce the simulation time and thus accelerating the screening of new aluminium alloys. The agents were internally able to address the errors generated and resolve all simulation instabilities through internal reasoning and actions. As illustrated above, beyond the simulation, the agents were quickly able to generate insights with high-quality visuals, graphics and commentary against the model output.

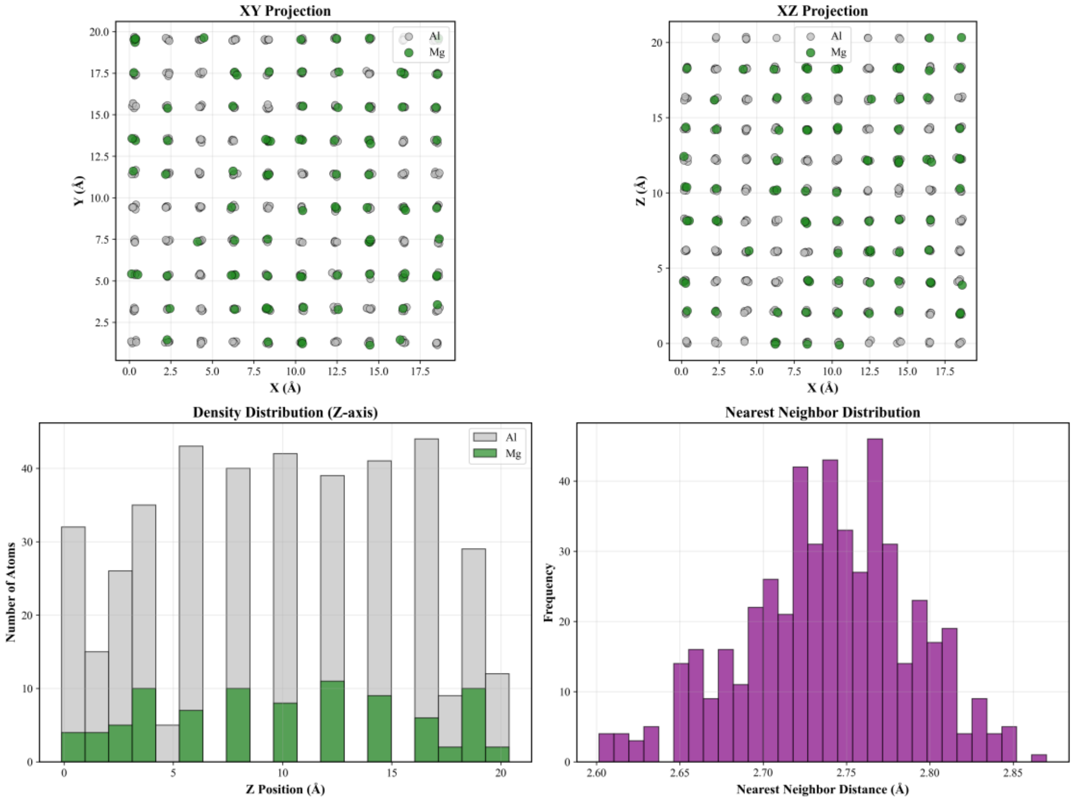


Figure 3. Structural and spatial analysis for Al-Mg alloy (17.6 % Mg).

4.2 Machine Learning Potential Estimation with Graph Neural Network

4.2.1 Objective

The primary objective of this study is to demonstrate the capabilities of the ai agentic framework in autonomously developing graph neural networks for predicting interatomic potential in aluminium alloys. Specifically, the study aims to (i) show how the agents can autonomously perform scientific survey and capture and validate data necessary for modelling GNN (Graph Neural Network) for interatomic potential (ii)capability of the agentic frameworks for graph representation of the captured data and to design and implement optimal GNN model for accurate prediction on interatomic potential (iii) validate the GNN modelling results and provide insights into the interatomic interactions and energy landscape

4.2.2 Agentic Workflow

In this illustration, the agentic orchestration framework works towards establishing a graph representation learning using deep neural networks for prediction of interatomic potentials in aluminium alloys.

- **Research Agent** is tasked to explore and save relevant data necessary for training and testing graph convolutional networks for predicting interatomic potential for aluminium alloys. The agent further checks data quality and standardizes the atomic and bonding information for the downstream pipeline

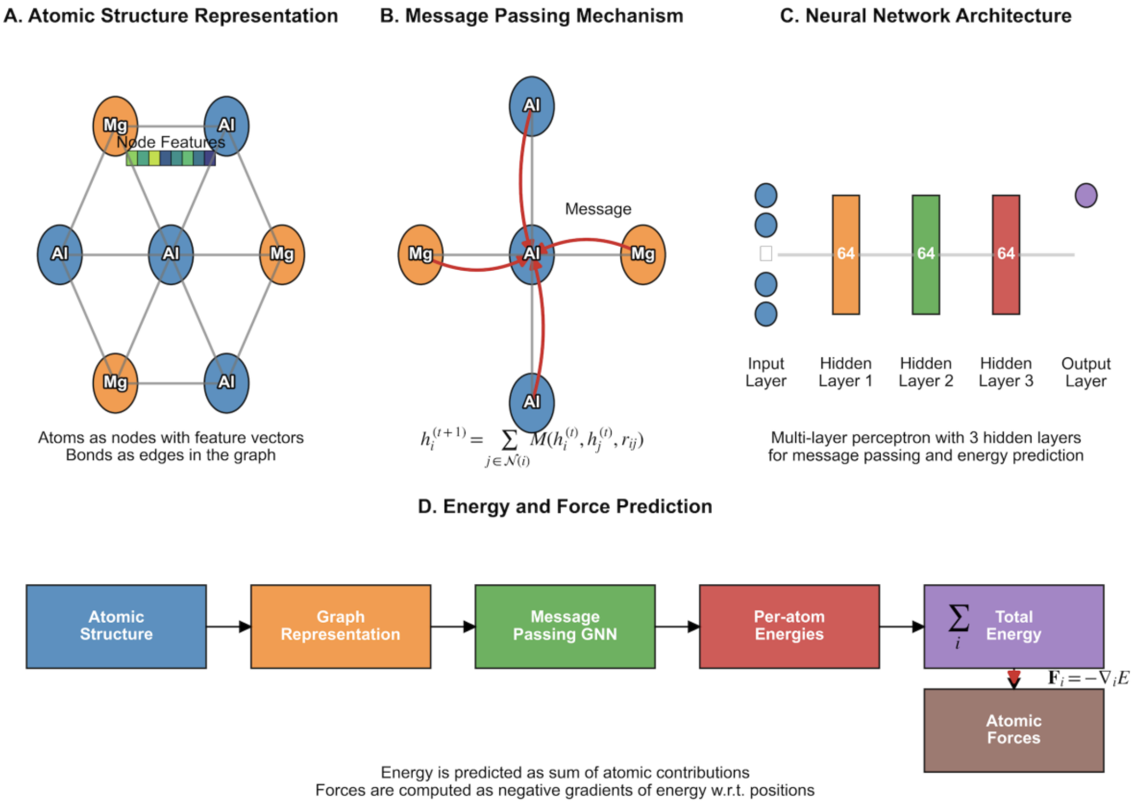
- **Data Agent** is tasked to transforms the raw data from the research agent into graph equivalent format. This includes assigning node features such as atomic number, electronegativity and edge features such as bond length, bond type etc. The data agent ensures that the graph generated is compatible for training using GNN model.
- **Planner Agent** is tasked to design the key features for the GNN model such as number of layers, hidden layers, activation functions, learning rate, batch size, training epochs and message passing architecture. The agent defined the learning function as the summation of mean squared error (MSE) for energy and force prediction weighted to balance the contribution of each.
- **Coding Agent** is tasked to code the defined GNN model by the planner agent for training and inference. The model was advised to use pytorch framework for the model development. Further, the agent was tasked to log the entire training routine across all the epochs using tensor board and save the best model as checkpoints. The model results are also formatted by the Coding agent for future visualisation.
- **Visual Agent** is tasked to build interactive graphs and plots of the prediction results of interatomic potentials and energy bands to provide insights on atomic interactions, bond energy and electronic states. The visual agent further generated comparison plots to identify model accuracy against different aluminium alloy compositions.

The agentic architecture performs sequential resolution of data dependencies enabling individual agents to function autonomously while collaborating for the overall objective. Hence the framework established a divide and conquer strategy for rapid iteration and scalability in the development of GNN model to predict interatomic potential.

Figure 4. Agentic orchestration for GNN modelling and inference for interatomic potential.

4.2.3 Model Architecture and Automated Workflow

Figure 5 illustrates the GNN model designed and developed by the planner and coding agent. This includes atomic representation of raw data (A), message passing algorithms (B), neural network architecture (C), and inference framework for energy and force prediction (D).



A. Atomic Structure Representation

B. Message Passing Mechanism

C. Neural Network Architecture

Atoms as nodes with feature vectors
Bonds as edges in the graph

$$h_i^{(t+1)} = \sum_{j \in \mathcal{N}(i)} M(h_i^{(t)}, h_j^{(t)}, r_{ij})$$

Multi-layer perceptron with 3 hidden layers
for message passing and energy prediction

D. Energy and Force Prediction

Energy is predicted as sum of atomic contributions
Forces are computed as negative gradients of energy w.r.t. positions

Figure 5. GNN model schematics for interatomic potential of aluminium and its alloys.

4.2.4 Results and Discussion

The agentic orchestration successfully demonstrated the ability to explore, plan, design, and develop GNN model for predicting interatomic potential. The modelling results are illustrated below. The loss curves and error metrics of the developed GNN model are shown in Figure 6. The training and validation indicate model convergence over epochs with both energy and force MAE stabilizing at acceptable thresholds. This confirms the system capability in learning interatomic relationships in Al-Mg alloy composition. The spatial visualisation of the GNN predictions for force and energy fields is illustrated in Figures 7 and 8, respectively. The force field in Figure 7 clearly illustrates the resolution of force transmission pathways and atomic level stress concentrations. In Figure 8, regions with higher (yellow) or lower (purple) predicted energies demonstrate the model's ability to learn spatial heterogeneity.

The study demonstrates the agentic framework ability to establish surrogate models for interatomic potentials. Observations were made on the agent's ability to internally address the errors generated and resolve all modelling instabilities through internal reasoning and actions.

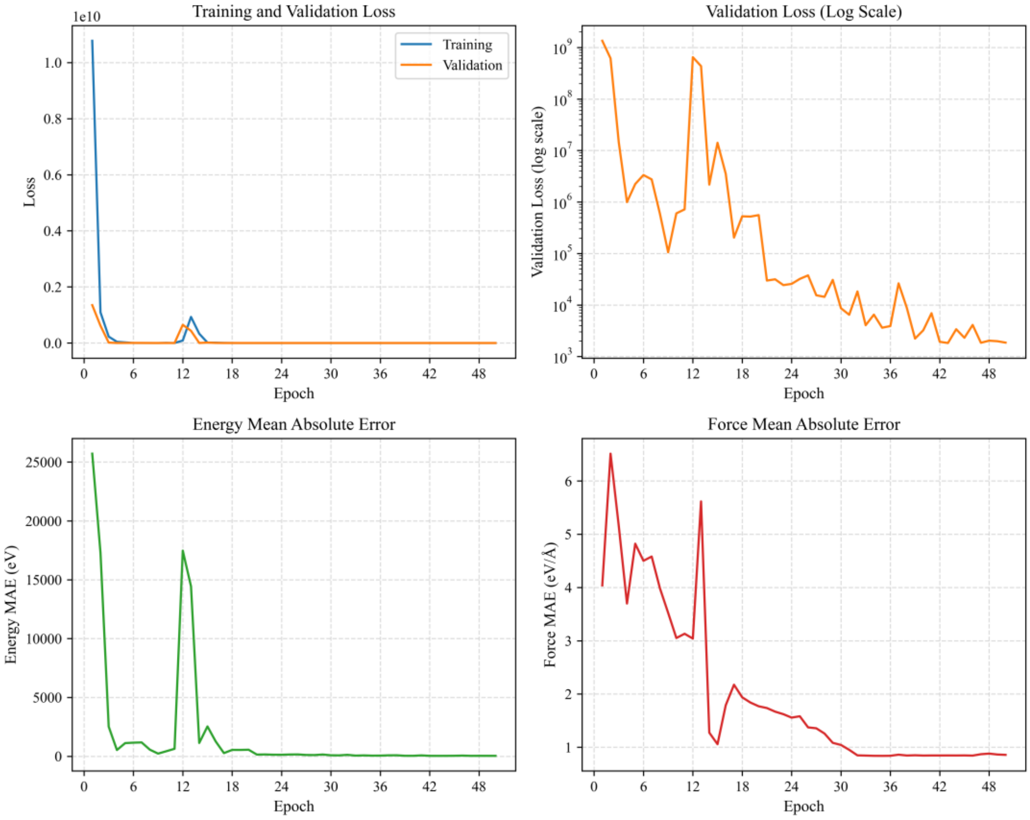


Figure 6. GNN validation metrices for energy and force fields prediction

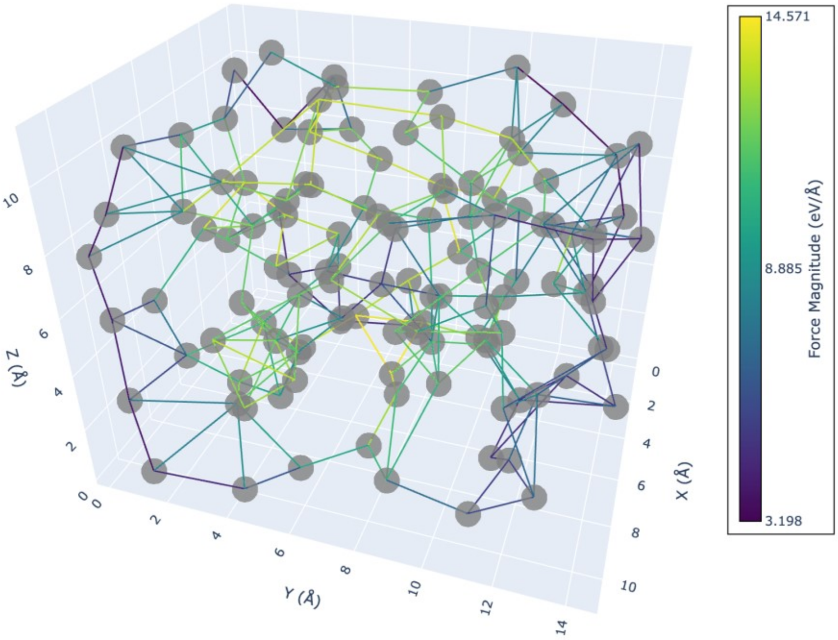


Figure 7. Spatial visualisation of force field predictions at atomic scale of 120 Al atoms

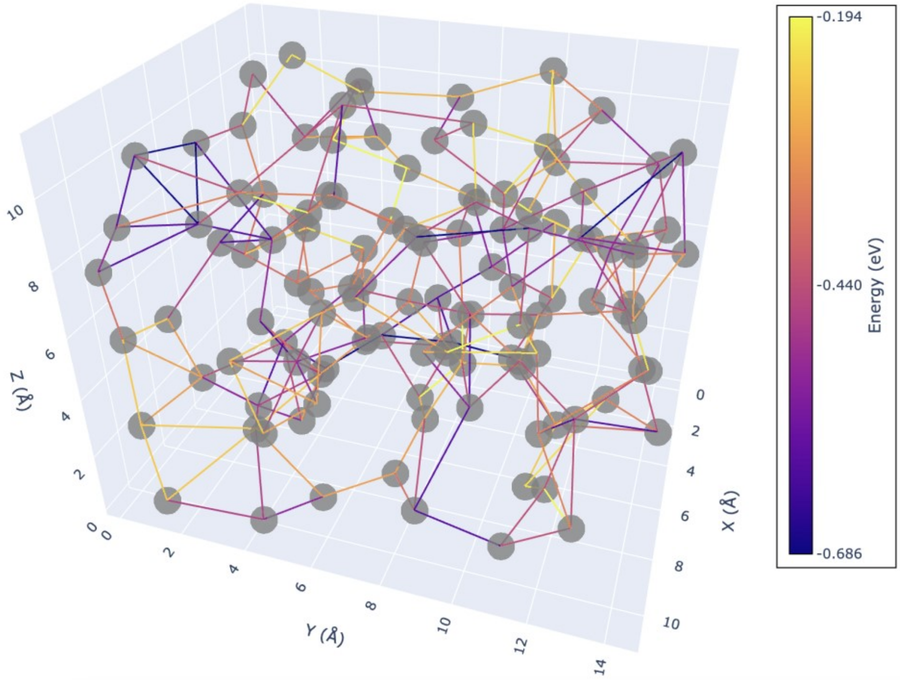


Figure 8. Spatial visualisation of energy field predictions at atomic scale of 120 Al atoms

All raw data used in this study were sourced from the open-access datasets, predominantly from the works of Burakovsky et al. [6] discovered by the research agent.

The results confirm the ability of the agentic framework to build GNN based workflow for interatomic potential prediction in aluminium alloys. The model validation metrices show convergence and robustness of the generated model with high quality visualization. This further demonstrated that the agentic framework is able optimize on both accuracy and interpretability.

5. Conclusions

This work presents a physics-aware, multi-agent AI framework that autonomously orchestrates aluminium-alloy modelling from knowledge retrieval to atomistic simulation, data post-processing, surrogate-potential training, and visualisation. Leveraging LAMMPS for high-fidelity molecular-dynamics and an E(3)-equivariant GNN for interatomic potentials, the framework (i) eliminates repetitive script preparation, (ii) resolves run-time instabilities via adaptive agents, (iii) produces publication-grade figures on-the-fly, and (iv) logs every decision for full provenance. Case studies on Al–Mg compositions demonstrated ≤ 0.5 eV stability in bulk energies, and low-MAE force predictions, all without manual intervention confirming that an agentic, closed-loop workflow can compress weeks of conventional effort into hours while preserving physical rigour.

Future work will extend the agent hierarchy out to transmit atomistic outputs to phase-field or finite-element agents for seamless multi-scale modelling; add active-learning loops to trigger new LAMMPS simulations only in regions of high-uncertainty to minimise simulation cost; generalise to larger alloy systems such as Al-Li, Al-Si, and Al-Cu-Mg – and eventually aluminium, while comparing transfer-learning gains; and port core agents into GPU-accelerated, cloud-native micro-services that elastically scale across infrastructure for enterprise deployment.

6. References

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