



OptiMat Alloys: a FAIR living database enabled by a conversational agent

Yang Hu, Vladyslav Turlo

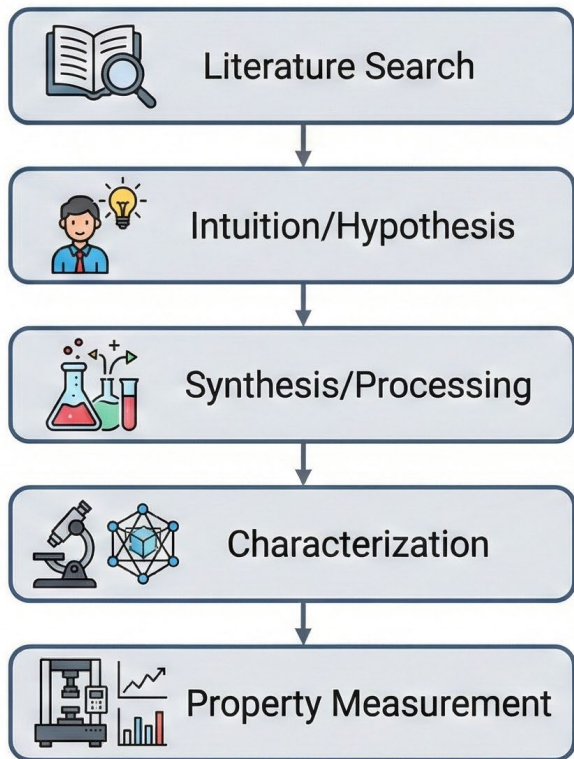
Laboratory for Advanced Materials
Processing, Empa, Thun, Switzerland

31.08.2026

Traditional materials discovery is slow



Traditional materials discovery workflow



Limitations



Process is slow



Labor-intensive



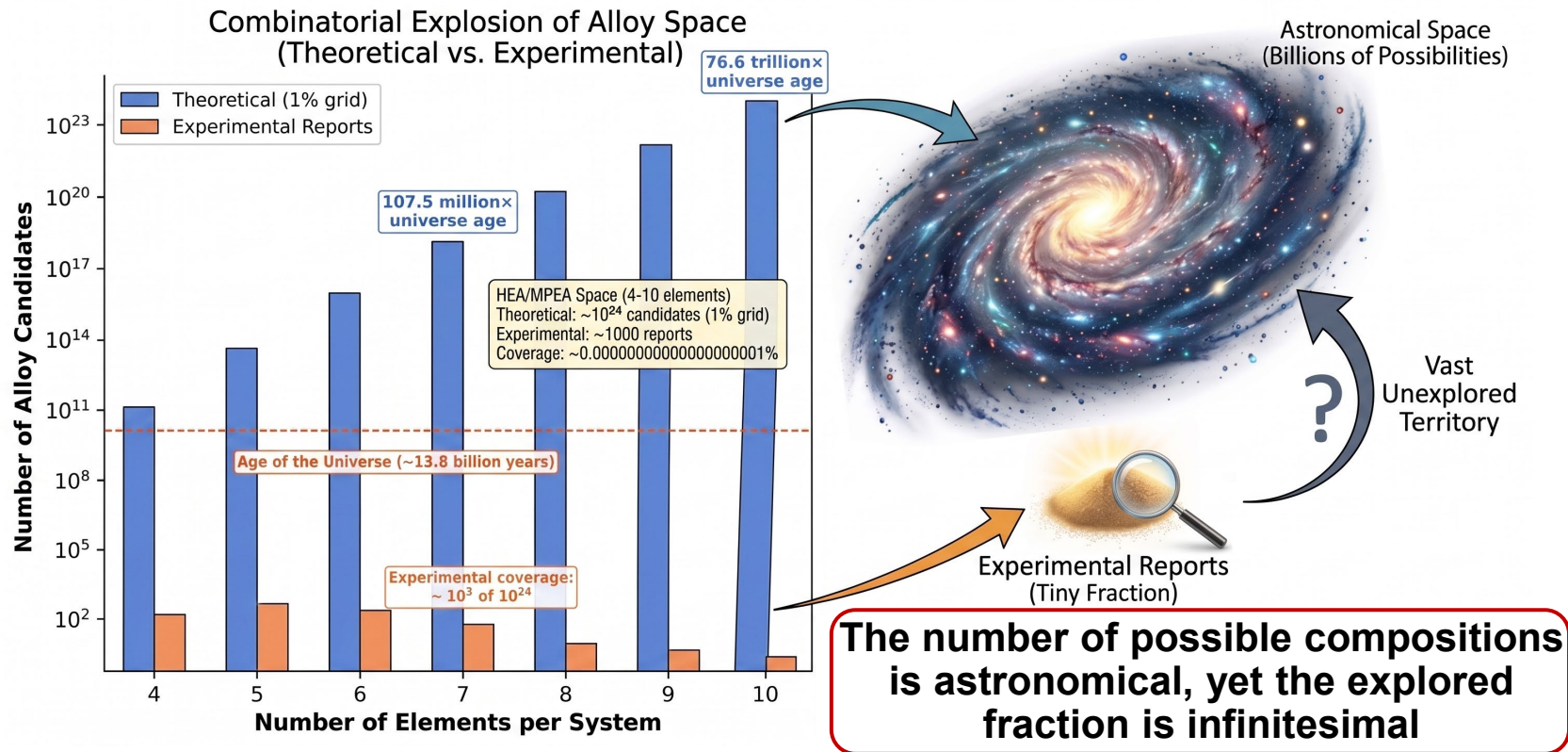
Linear & Sequential



Relies on “Edisonian” trial-and-error

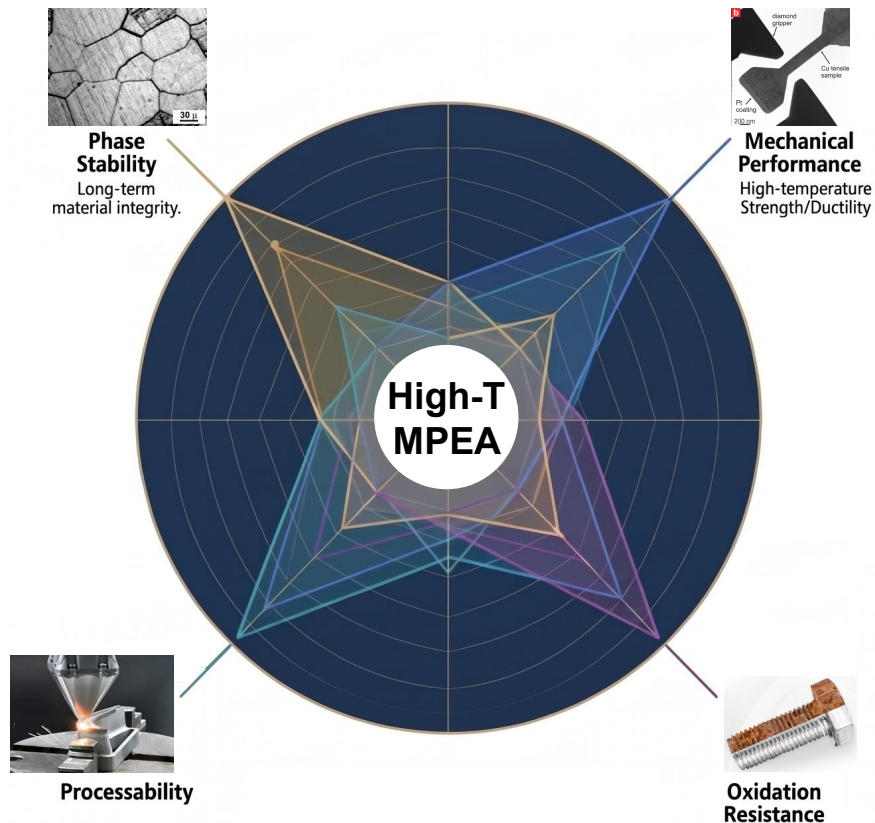
**High cost, long development cycles,
low success rate**

The design space of complex materials is vast

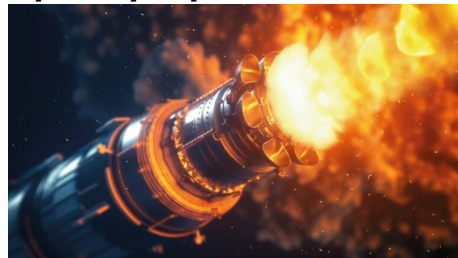


MPEA: multi-principal element alloy

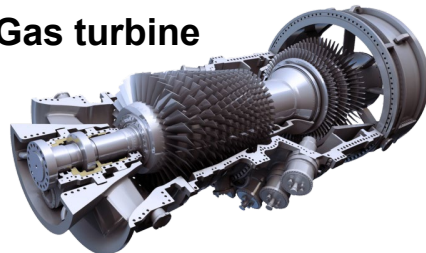
The design of complex materials is multi-objective



Space propulsion



Gas turbine



Fusion and fission applications

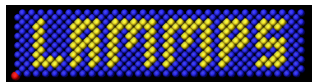


Potential applications

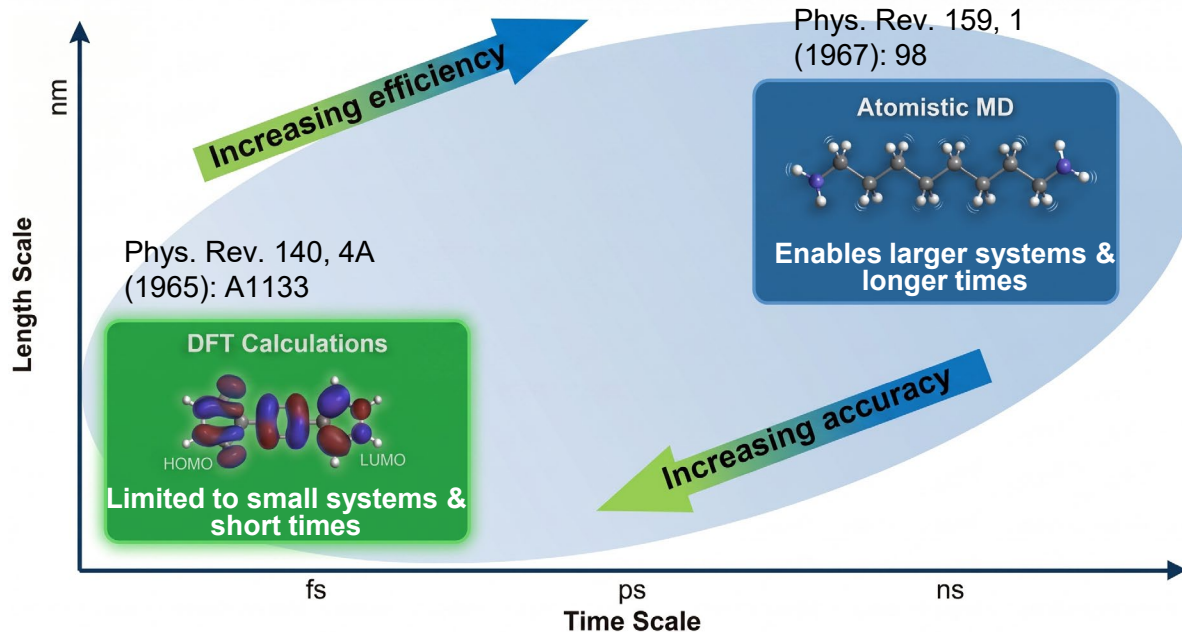
Simulations can accelerate materials discovery



Robust Atomistic Codes



Mature simulation engines provide a reliable foundation for executing complex workflows.

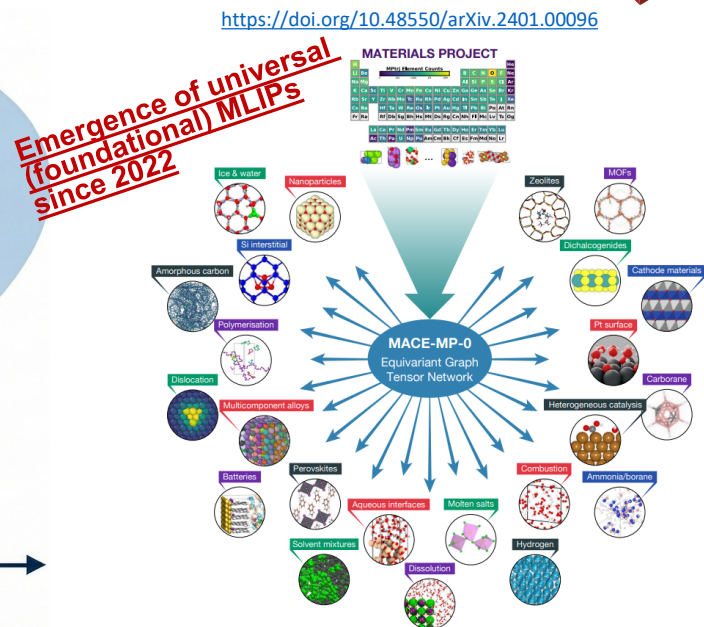
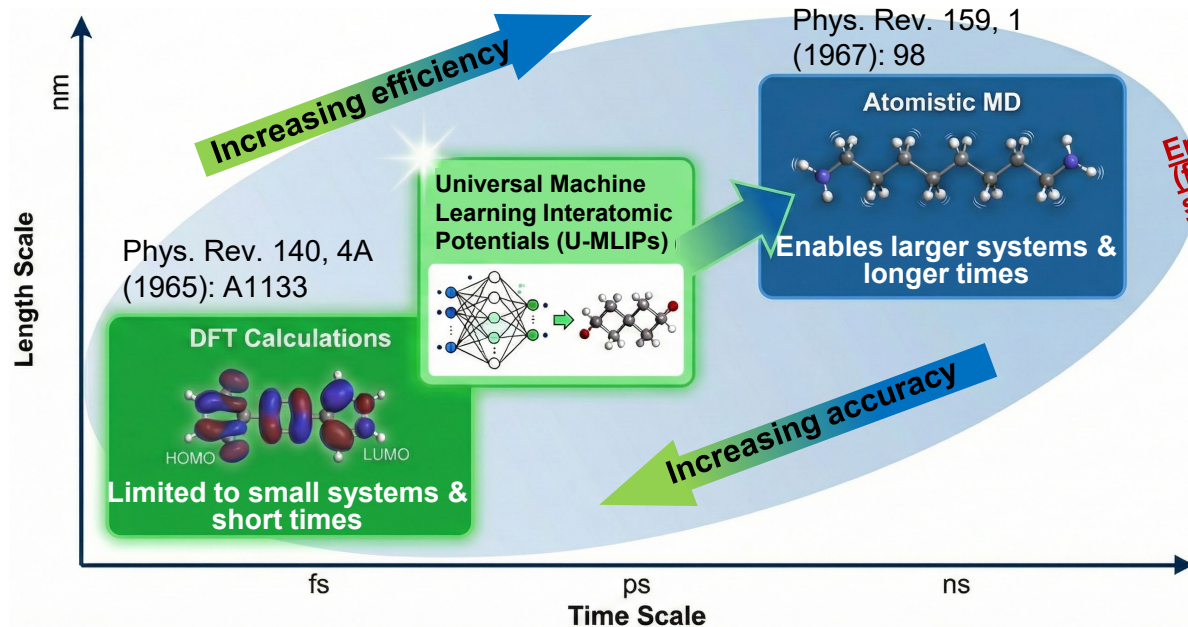


J. Comput. Phys. 117, 1 (1995): 1-19

Phys. Rev. B 54, 16 (1996): 11169

J. Phys. Condens. Matter 29, 27 (2017): 273002

U-MLIPs expand atomistic simulation capabilities



U-MLIP and VASP GPU runtime comparison on CoCrFeNi FCC supercells

Atoms	VASP GPU	U-MLIP Wall-Clock Time (ms)				Speedup
		ORB Direct	ORB Conserv.	MACE-OMAT-0	NequIP-OAM-XL	
32	11.6 min	0.10	0.09	0.09	0.10	~7,000×
108	79.5 min	0.10	0.10	0.09	0.11	~48,000×
256	3.78 days	0.10	0.10	0.10	0.11	~3.3M×

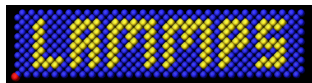
Breakthroughs enabled by U-MLIPs:

- Near-DFT accuracy
- Broad elemental coverage
- Scalable simulations

Simulations can accelerate materials discovery



Robust Atomistic Codes



Mature simulation engines provide a reliable foundation for executing complex workflows.

Universal ML Potentials



UPET
UNIVERSAL ATOMISTIC MODELS

Pre-trained foundation models offer near-DFT accuracy across broad compositions without system-specific fitting.



Simulations are powerful, but the barrier to entry is high and progress is limited by manual setup, monitoring, and analysis.

How can we make simulations more accessible?

How can we free researchers from routine, repetitive tasks?

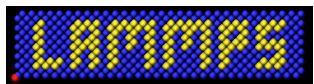
arXiv:2410.22570 (2024) Nat. Commun. 16, 1 (2025): 10653

arXiv:2607.28461 (2026) J. Chem. Phys. 163, 18 (2025)

Agentic materials discovery is now possible!



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Reasoning-Capable LLMs



ChatGPT



MIMO



Modern LLMs orchestrate the pipeline through scientific reasoning, tool use, and long-context processing.

arXiv:2303.08774 (2023)

arXiv:2406.12793 (2024)

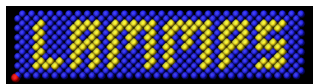
arXiv:2505.07608

(2025)

Agentic materials discovery is now possible!



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ChatGPT



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An **agent** is a software system that can **plan and take actions** toward a goal. In practice, it is an orchestrator that connects tools, data, and decision-making logic.

arXiv:2303.08774 (2023)

arXiv:2406.12793 (2024)

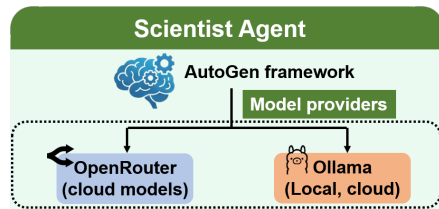
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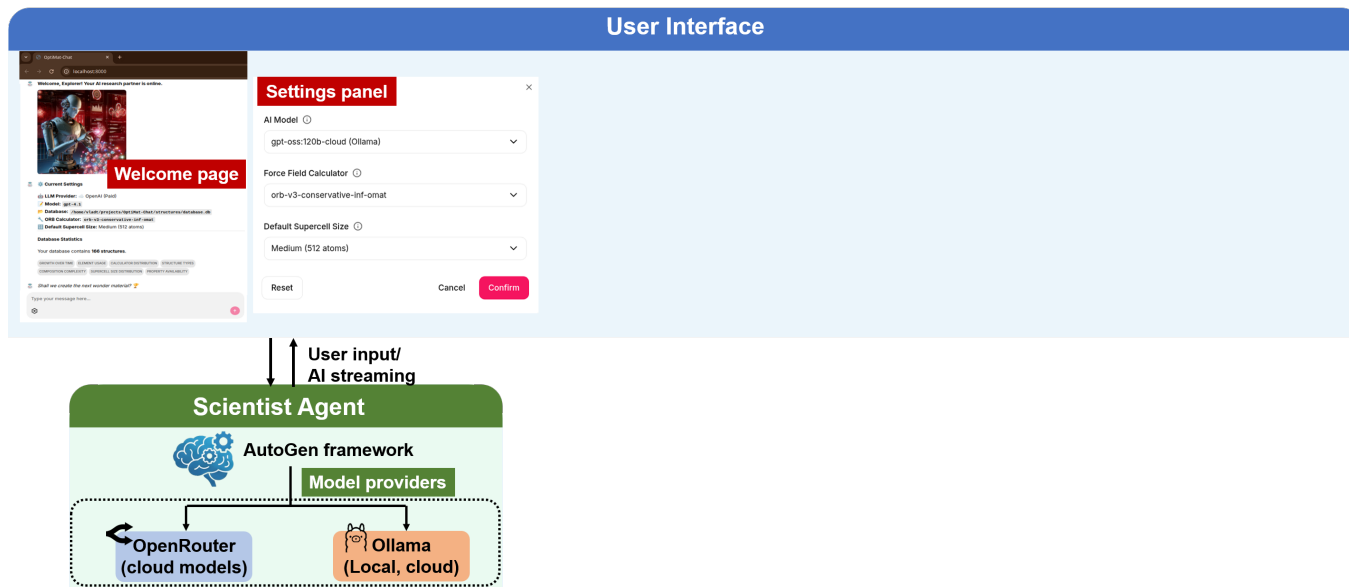
OptiMat Alloys architecture



- OptiMat Alloys is built on the Python-based **AutoGen** framework.
- AutoGen is an open-source framework developed by Microsoft for building multi-agent AI applications.
- The agent connects to cloud-hosted LLMs via APIs.



OptiMat Alloys architecture



- The agent provides a web-based GUI built with Chainlit.
- Users interact with it entirely in natural language.

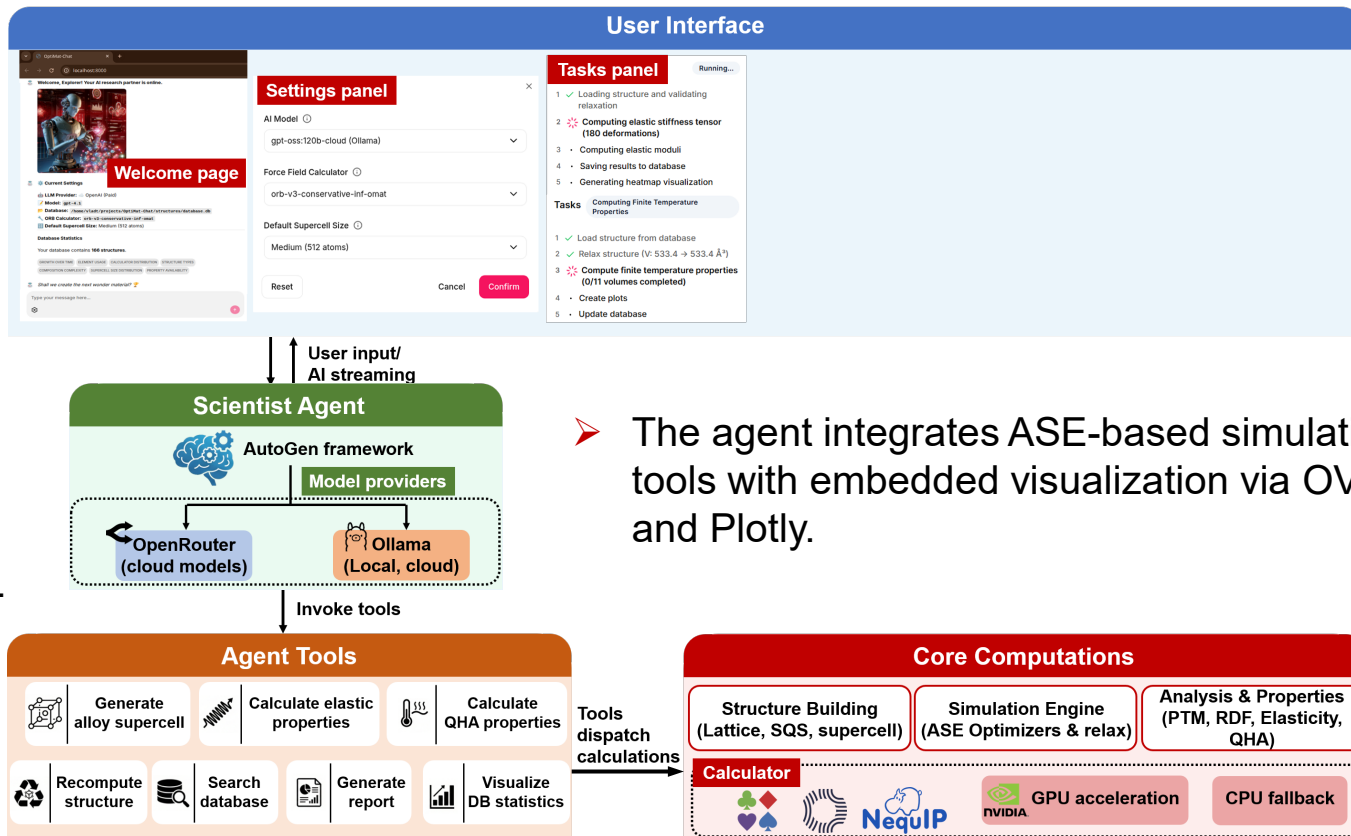
OptiMat Alloys architecture



ASE:

a Python toolkit for setting up, running, and analyzing atomistic simulations.

U-MLIPs are installed as Python packages and used as calculators within ASE.



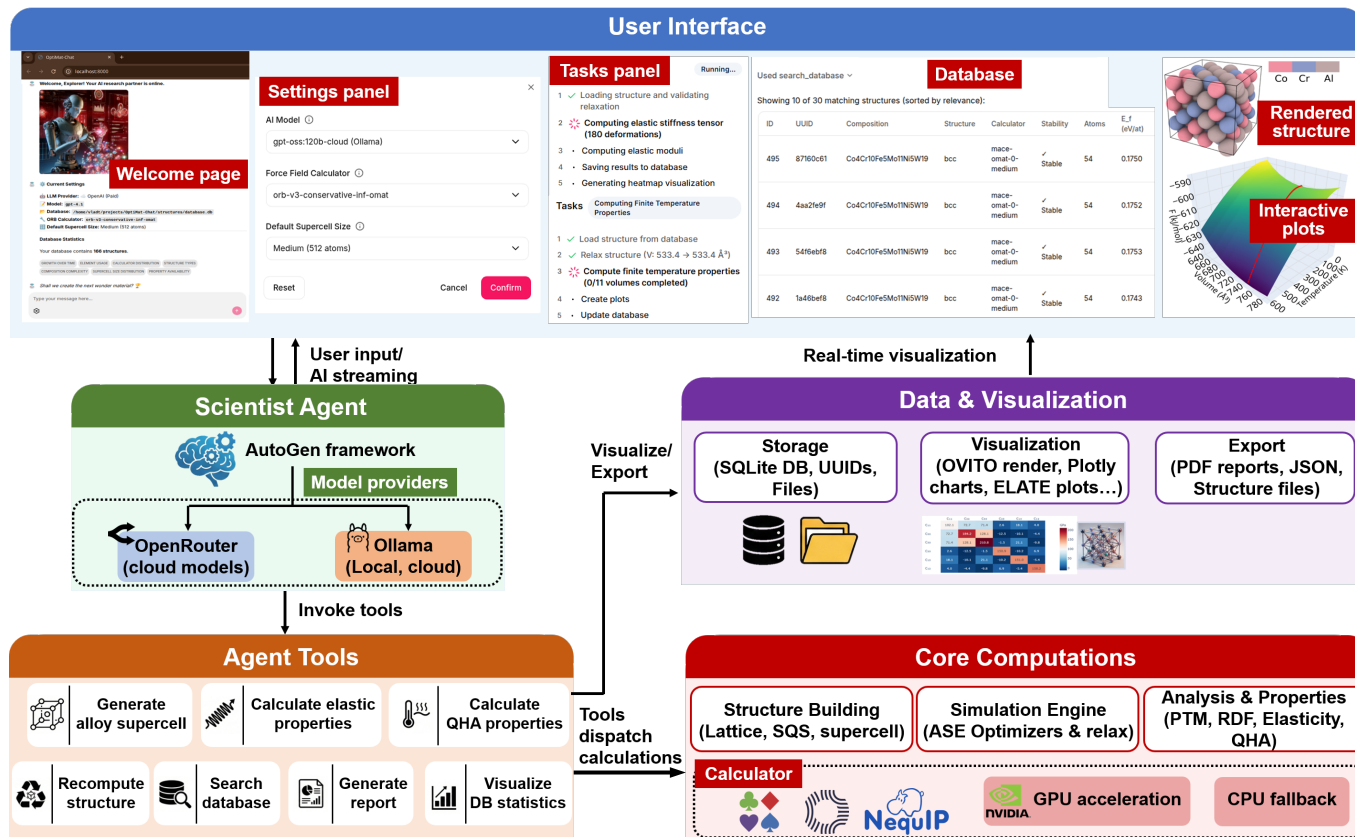
➤ The agent integrates ASE-based simulation tools with embedded visualization via OVITO and Plotly.

OptiMat Alloys architecture

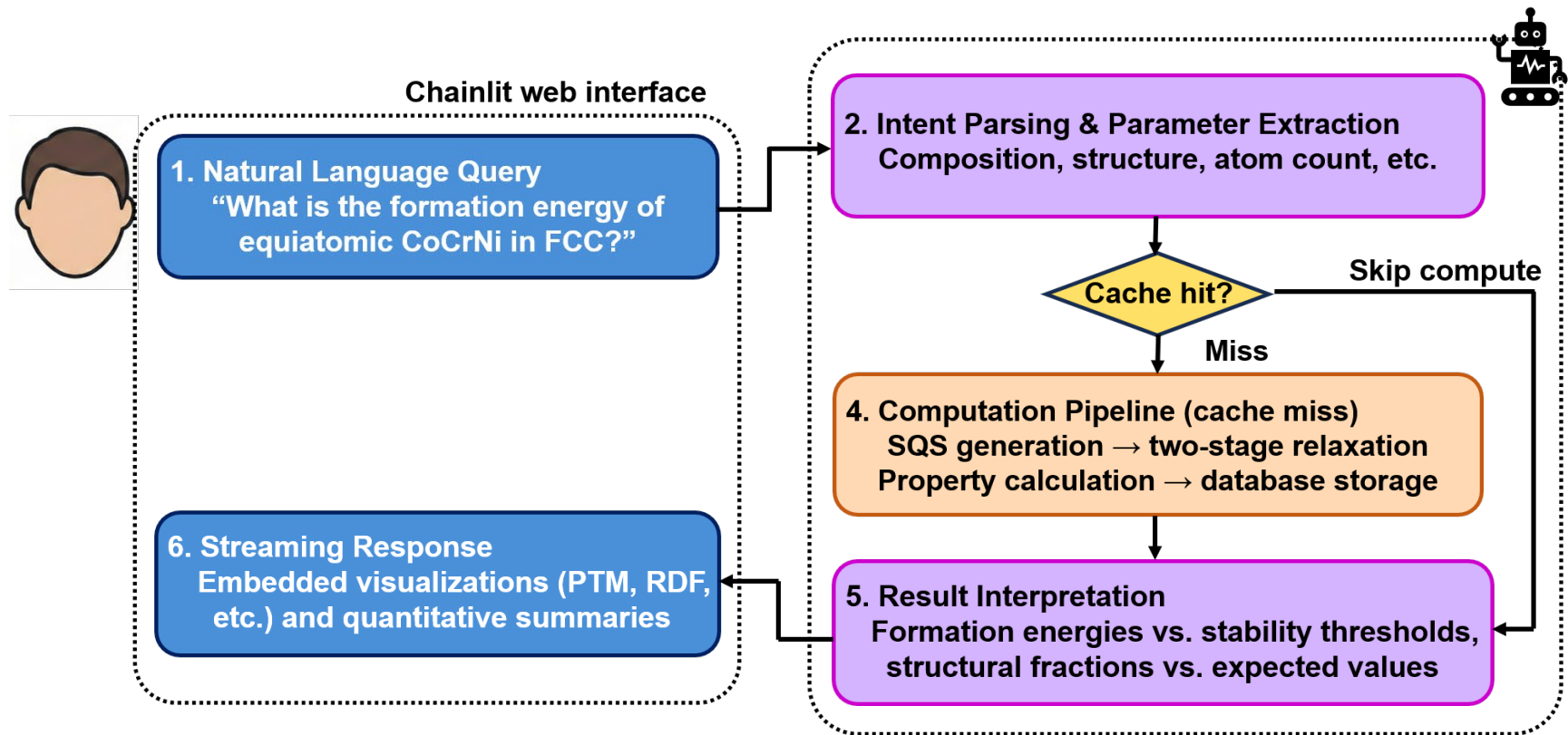


➤ The agent writes computed data into a local SQLite database.

➤ Simulation inputs and results can be summarized and exported as a report.



Agent decision and execution flow

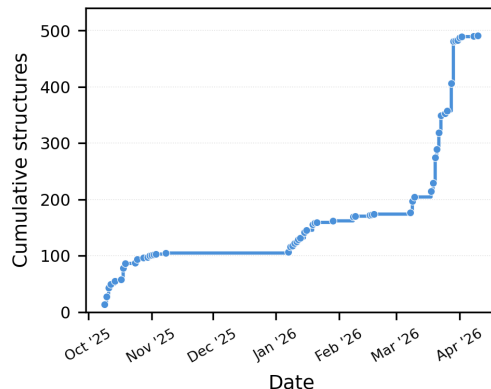


A living database that grows through usage

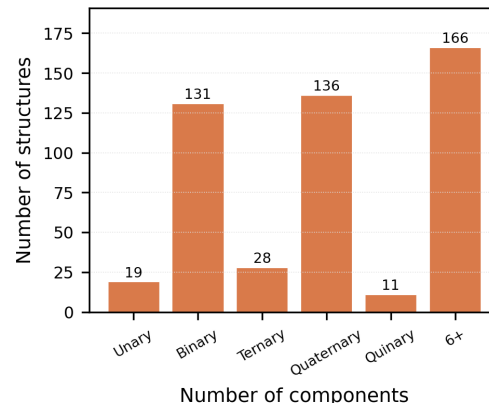


- The local SQLite database grows with every user-agent interaction.

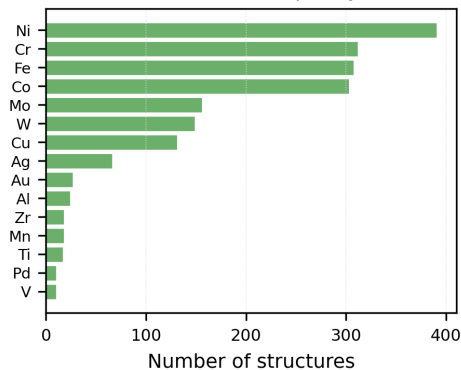
(a) Database growth



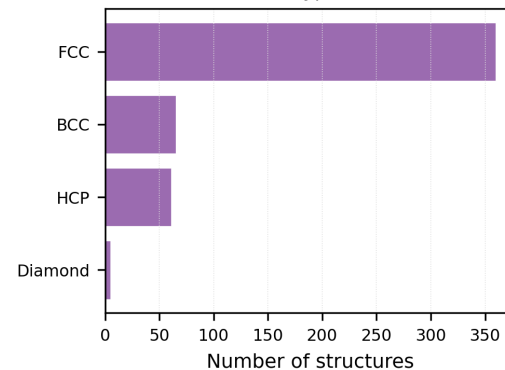
(b) Composition complexity



(c) Element frequency



(d) Structure type distribution

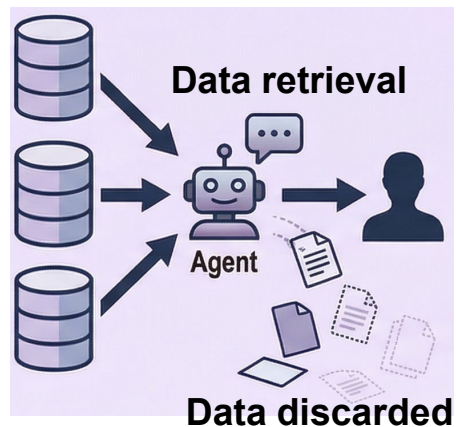


A living database that grows through usage

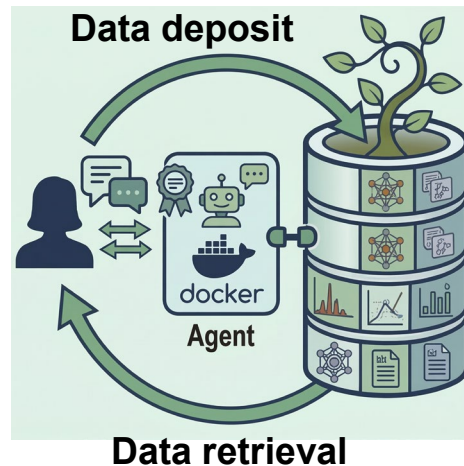


- The local SQLite database grows with every user-agent interaction.
- Data generation is no longer separated from data deposition

Other agents:
Ephemeral data



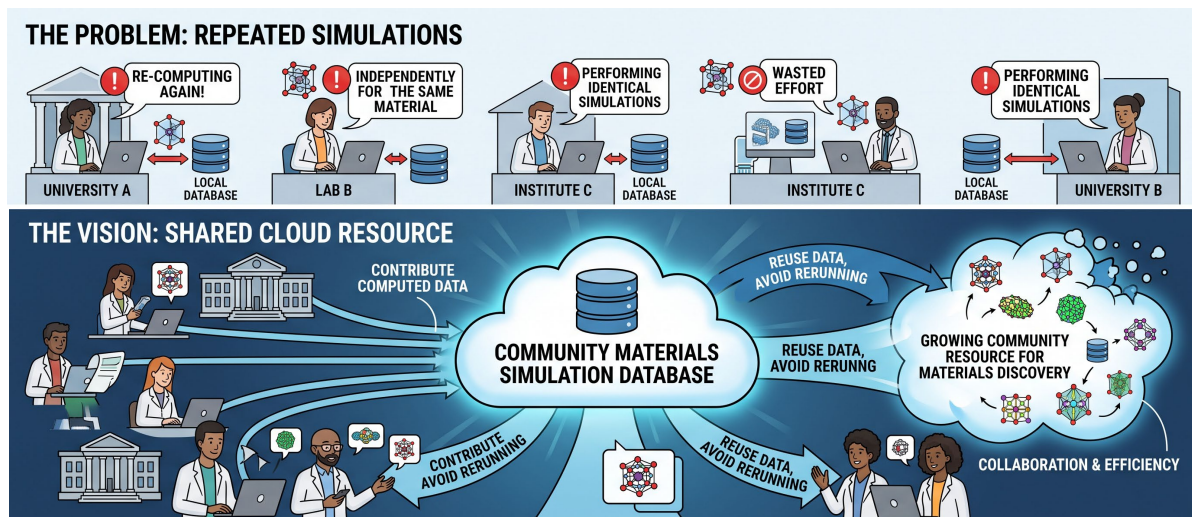
Our agent:
Living data



A living database that grows through usage



- The local SQLite database grows with every user-agent interaction.
- Data generation is no longer separated from data deposition
- Stored results avoid repeated computation



Beyond results: capturing simulation provenance



- Simulation methods, input parameters, and software versions are summarized in an exportable report.
- Generated structures can also be exported for external use.

Single Crystal Elastic Properties

Directional Properties: Single crystal elastic properties vary with crystallographic direction due to anisotropy. All directional properties are computed from the compliance tensor $S = C^{-1}$:

Young's modulus: $1/E(n) = S_{ijkl} n_i n_j n_k n_l$. **Linear compressibility:** $\beta(n) = S_{ijkl} \delta_{ki} n_j n_l$. **Shear modulus:** $1/G(n,m) = 4 S_{ijkl} n_i m_j n_k m_l$. **Poisson's ratio:** $\nu(n,m) = -S_{ijkl} n_i n_j m_k m_l / S_{ijkl} n_i n_j n_k n_l$, where S_{ijkl} is the compliance tensor, δ_{ki} is the Kronecker delta, n is the loading direction, and m is the perpendicular direction for lateral response.

Auxetic Behavior: Negative Poisson's ratio in certain directions indicates the material expands laterally when stretched (unusual mechanical behavior).

Wave velocities: $v_s(n) = \sqrt{G(n)/\rho}$ for shear waves, $v_l(n) = \sqrt{((K(n) + 4G(n)/3)/\rho)}$ for longitudinal/compression waves, where v_s is the shear wave velocity, v_l is the longitudinal wave velocity, $G(n)$ is the directional shear modulus, $K(n)$ is the directional bulk modulus, n is the propagation direction, and ρ is the material density.

Property	Min	Max	Unit
Young's Modulus (E)	128.74	331.65	GPa
Shear Modulus (G)	46.26	139.97	GPa
Poisson's Ratio (ν)	-0.1395	0.6964	
Linear Compressibility (β)	1.822	2.053	1/TPa

Software Versions

ASE: 3.26.0, Phonopy: 2.43.6, OVITO: 3.11.1, PyTorch: 1.8.0+cu128, NumPy: 2.3.4, ORB Models: v0.5.5, MACE: 0.3.14, NequIP: 0.16.1, phono3py: 3.19.4, sqsgenerator: (0, 5, 3), MechElastic: 1.2.29

4. Computational Methods

NequIP Equivariant Neural Network Potential

E(3)-equivariant neural network potential with state-of-the-art accuracy. ORB-AMP models trained on OMat24, MPtrj, and sAlex datasets (112.8M structures). MP models trained on MPtrj only (1.58M structures). [7, 8]

Parameter	Value
Model used	nequip-oam-d
Model Oam L	nequip-oam-l (~15M params, F1=0.893)
Model Oam XI	nequip-oam-xl (~15M params, F1=0.906, highest accuracy)
Model Mp L	nequip-mp-l (9.6M params, MPtrj only)
Precision	float32

Special Quasirandom Structure (SQS)

Generates special quasirandom structures that best approximate the pair correlation functions of a random alloy. Minimizes short-range order to represent disordered solid solutions. [9, 10]

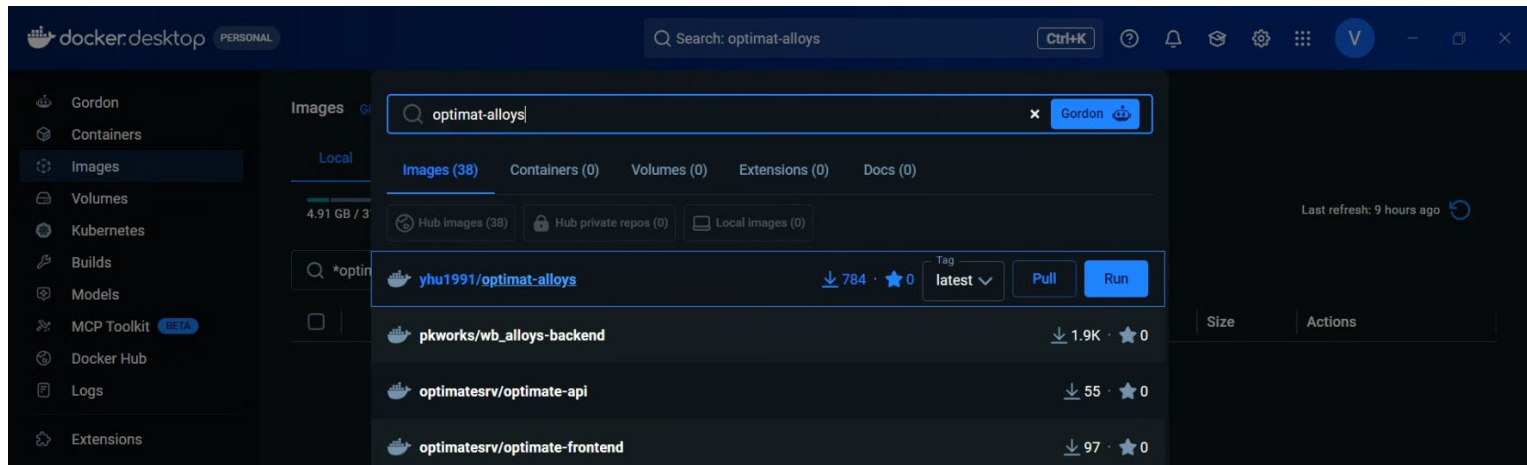
Parameter	Value
Method	sqsgenerator (gen)
Target	Minimize pair correlation deviation
Iterations	1,000,000 Monte Carlo simulation (vol default; library default is 10,000,000)
Shell Weights	(1: 1.0, 2: 0.5) — No shell weight, 2nd NN half-weighted

POSCAR	File
structure.cif	CIF File
structure.lammps	LAMMPS File
structure.xyz	XYZ File

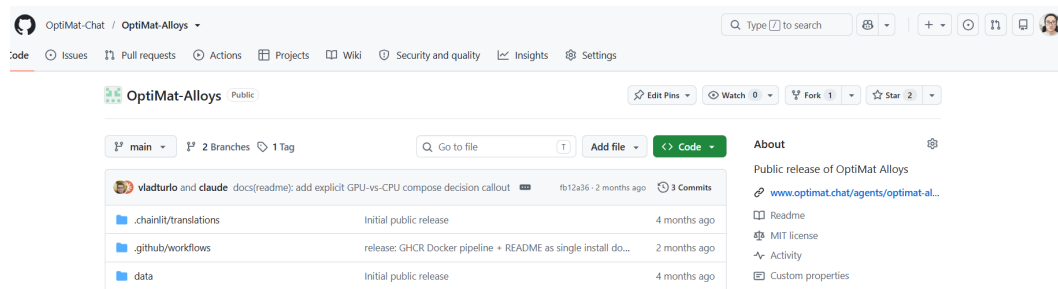
Deployment of the agent is straightforward



Docker image: yhu1991/optimat-alloys



<https://github.com/OptiMat-Chat/OptiMat-Alloys>



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Thank you!

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// CONVERSATIONAL MATERIALS DISCOVERY

Welcome to OptiMat Chat

A collaborative platform connecting AI agents, databases, and researchers to accelerate materials discovery through conversations.

Try it now Get Updates Join Discord Watch Demo

5+ RESEARCH AGENTS 117 ELEMENTS COVERED 5x LOWER COST

Contact the Team

Dr. Vladyslav Turlo
Lead Developer
✉ vladyslav.turlo@empa.ch

Dr. Yang Hu
Research Lead
✉ yang.hu@empa.ch