

PASUMS in the Era of Generative AI: Toward AI-Assisted Workflows and New Approaches to Human Resource Development

Kazuyoshi Yoshimi

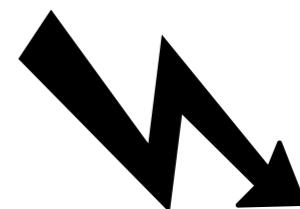
Institute for Solid State Physics, Univ. of Tokyo

2025/12/5 Fri. 17:10-17:30

State-of-the-Art in Code Generative AI
for High-Performance Computing

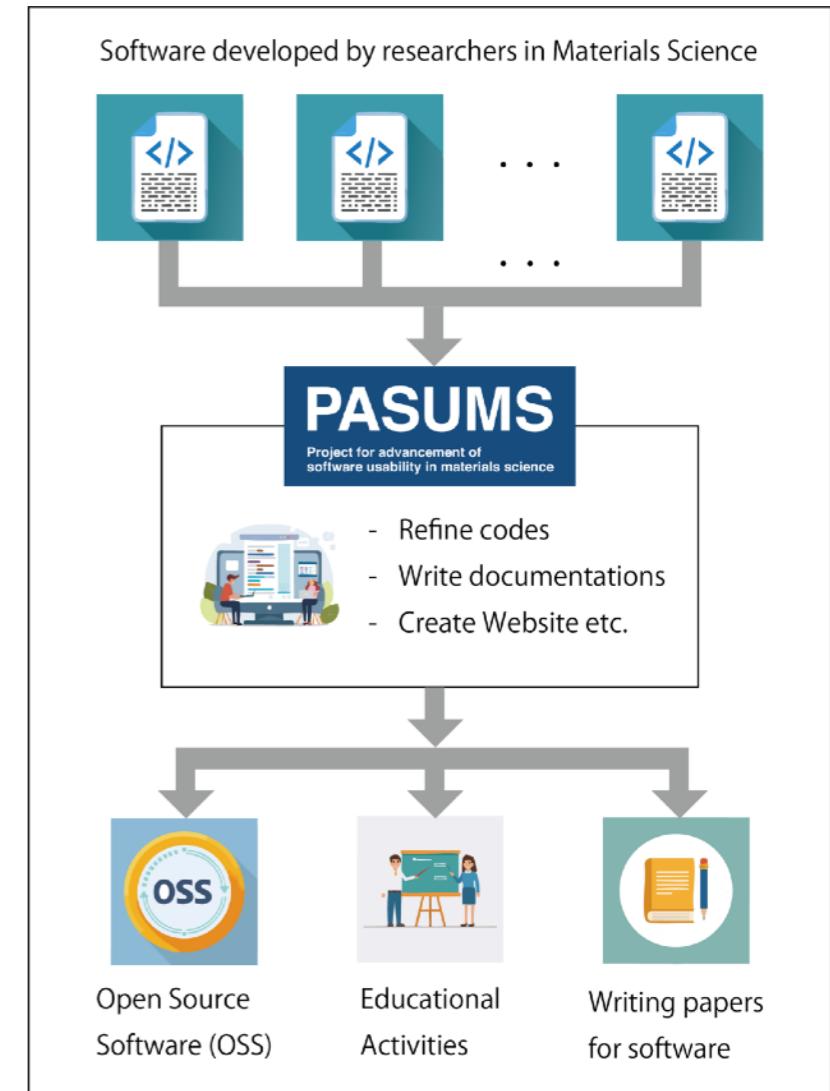
What is PASUMS ? — Background

- Research projects often produce highly sophisticated software
 - Designed for cutting-edge simulations
 - Includes advanced features and new algorithms
- But usability improvements are not prioritized
 - Documentation, tests, manuals, and websites are often delayed
 - Researchers must focus on many other tasks
- As a result
 - Excellent software does not spread widely
 - Opportunities for community improvement are lost



What is PASUMS ? — Project Overview

- **PASUMS is a long-term project launched in 2015**
 - Supports software developed in computational materials science
 - Aims to improve usability, maintainability, and accessibility of research software
- **Annual open call and development cycle**
 - 1–2 software packages selected each year
 - Continuous usability improvement, documentation, testing, and website support
- **Goal**
 - Enable community-wide use, contribution, and recognition of research software



What is PASUMS ? (4)

**Aim: Improve usability & publication of software
in the field of materials science**

Annual open call in December each year.

- 1 or 2 software packages are selected
 - Released as open source software



Main members



Kazuyoshi
Yoshimi



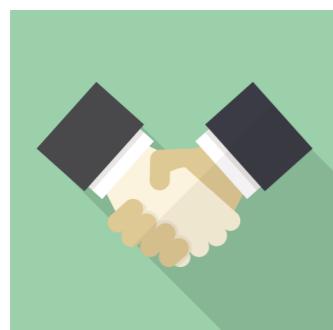
Yuichi
Motoyama



Tatsumi
Aoyama

Annual schedule

April



Kick-off meeting

May ~ Feb.



GitHub

Software development



Regular meeting/month

March ~



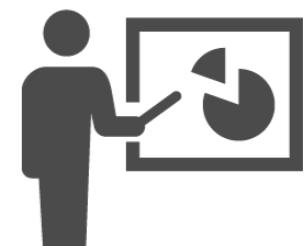
Website



Preinstall



Portal site



Lecture

PASUMS Software and Achievements

- Representative software developed under PASUMS

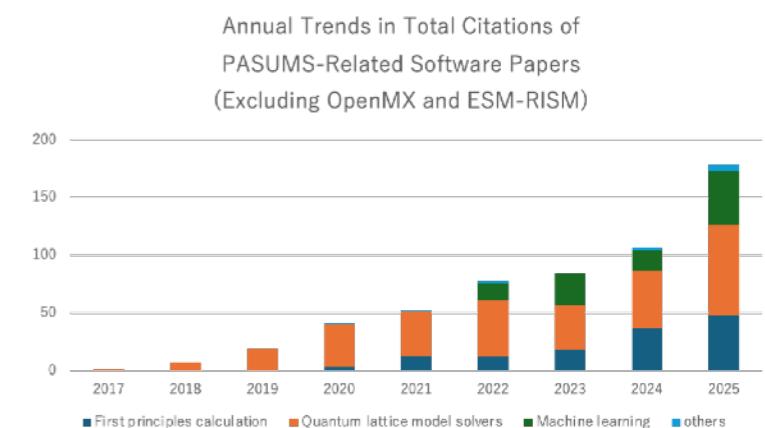
- mVMC, HΦ, RESPACK, PHYSBO, and others
- Widely used in computational materials science

- Strong impact in the community

- Increasing number of citations
- Used in many research projects and publications

- External recognition

- FY2023 HPCI Software Awards
 - mVMC: Best Performance Award
 - HΦ: Outstanding Performance Award



Google scholar 2025/12/1

Paper of PASUMS

Open Access

SCIENCE AND TECHNOLOGY OF ADVANCED MATERIALS: METHODS
2025, VOL. 5, NO. 1, 2564055
<https://doi.org/10.1080/27660400.2025.2564055>

 Taylor & Francis
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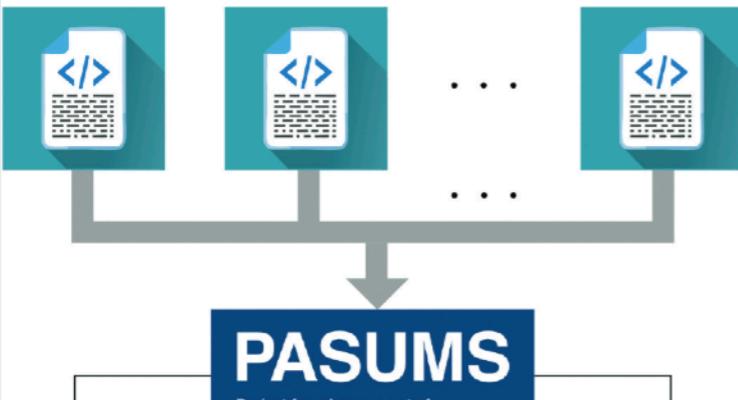
Project for advancement of software usability in materials science

Kazuyoshi Yoshimi^a, Yuichi Motoyama^a, Tatsumi Aoyama^a, Mitsuaki Kawamura^b and Naoki Kawashima^a

^aThe Institute for Solid State Physics, The University of Tokyo, Chiba, Japan; ^bFaculty of Engineering, Yokohama National University, Yokohama, Japan

ABSTRACT
The Institute for Solid State Physics (ISSP) at The University of Tokyo has been carrying out a software development project named 'the Project for Advancement of Software Usability in Materials Science (PASUMS)'. Since the launch of PASUMS, various open-source software programs have been developed/advanced, including the first-principles calculations, effective model solvers, and software for machine learning. We also focus on activities that make the software easier to use, such as developing comprehensive computing tools that enable efficient use of supercomputers and interoperability between different software programs. We hope to contribute broadly to developing the computational materials science community through these activities.

Software developed by researchers in Materials Science



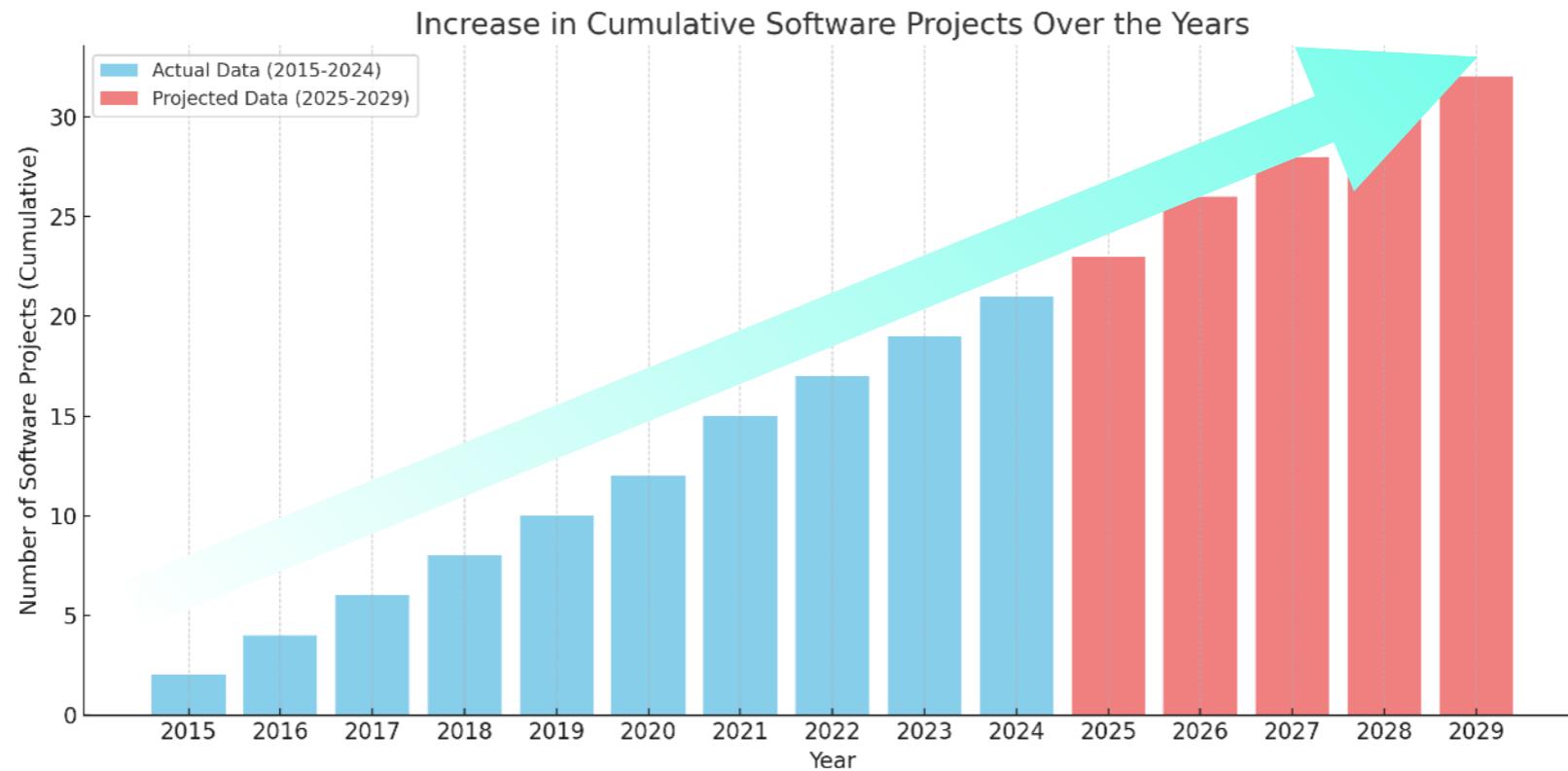
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KEYWORDS
Computational materials science; software development; open source software

PASUMS
Project for advancement of

[Invited Review] Yoshimi, K., Motoyama, Y., Aoyama, T., Kawamura, M., & Kawashima, N. (2025). , "Project for advancement of software usability in materials science.", *Science and Technology of Advanced Materials: Methods.* , <https://doi.org/10.1080/27660400.2025.2564055>

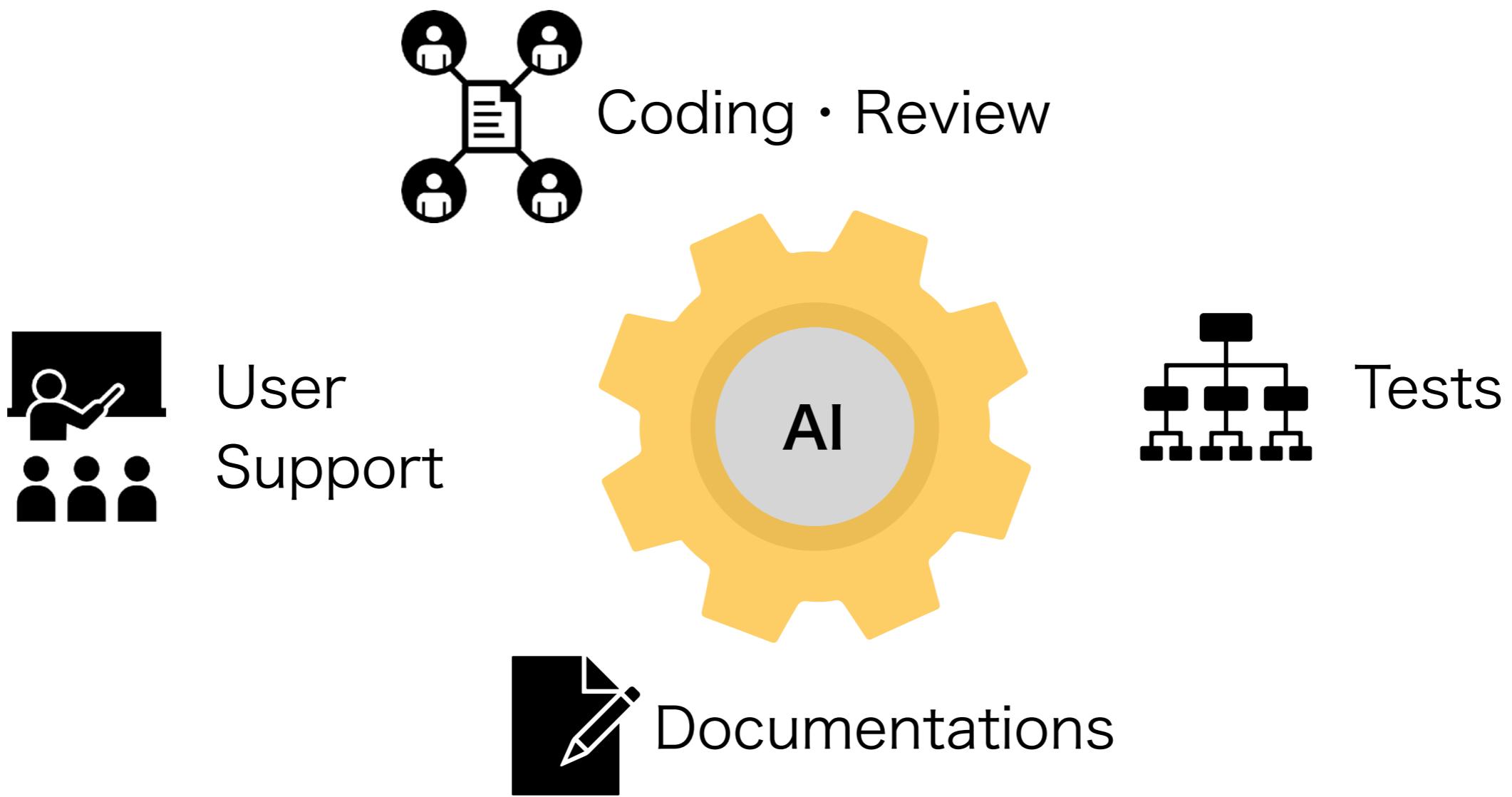
Growing Maintenance Workload and the Move Toward Generative-AI Development



- Maintenance and quality control of individual software are important
 - We aim to manage software as community codes
 - But each code still requires continuous work
- The amount of software and functionality continues to increase
 - More updates, bug fixes, and user requests
 - Efficiency of the development process is required

→ Software development initiatives using generative AI

Background to software development initiatives using generative AI

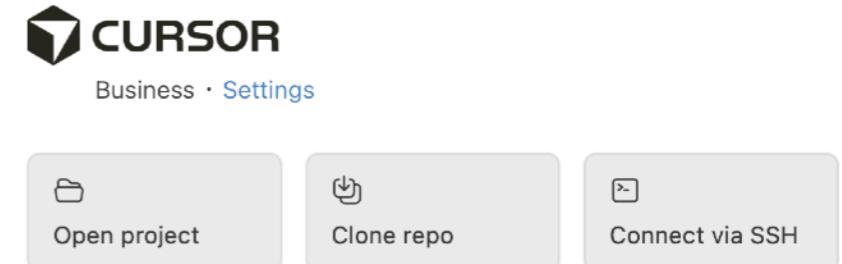


- Time savings through automation of development work
- Improvement of software quality: Coding, review, testing etc.
- Support for dissemination activities: Documentation, tutorials, user communication etc.

Development Environment with Agent Tools

- **Cursor as the main development IDE**

- Inline agent support
 - Code refactoring and debugging assistance



- **CodeX/Claude Code as agent tools**

- Code generation, analysis, and explanation
 - Multi-file reasoning and large context handling



Agent tools support coding, debugging, refactoring etc.

Documentation & Quality Control with AI

- **Predefined rules to maintain consistency**
 - Naming conventions, Folder structure and Documentation style (e.g., numpydoc)
- **Automated setup and CI support by AI**
 - AI generates initial GitHub Actions configurations
 - AI creates simple unit tests and style-check scripts
 - Quick setup of CI workflows without manual effort
- **Integrating automated tests with GitHub Actions**
 - Unit tests, style checks, CI workflow
 - Preventing regressions and ensuring code quality
- **Using multiple related project documents to support manual creation**
 - Templates, README files, examples, and API descriptions

→ These help AI generate consistent manuals and documentation



GitHub Actions

Potential of AI Tutors

- **Challenges: Legacy code becoming a black box**
 - Low readability makes old code difficult to understand
 - Hard to recall and reuse past implementations
- **Potential of AI-based Code Analysis**
 - AI can analyze legacy code and infer its meaning.
 - Tools like Copilot can automate refactoring and propose improvements
- **New Utilization Models: AI Tutors**
 - Suggest relevant APIs and functions.
 - Explain code operations and specifications.

User support

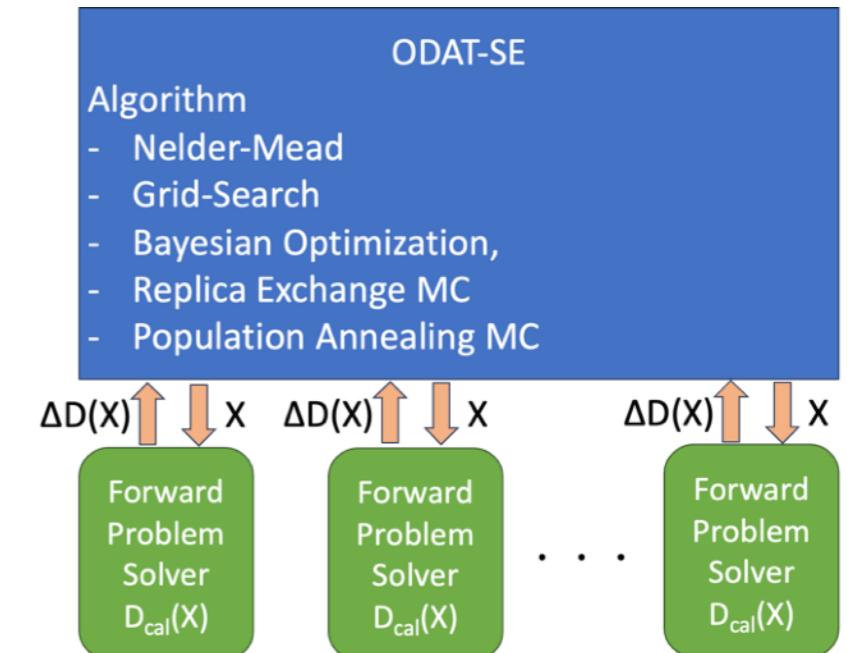
ODAT-SE-Template Expert (1)



ChatGPT

Open Data Analysis Tool for Science and Engineering (ODAT-SE)

A general-purpose data analysis platform that combines forward problem solvers and inverse problem analysis algorithms to solve optimization problems.



URL: <https://github.com/issp-center-dev/ODAT-SE>

Main Developers: Y. Motoyama, K. Yoshimi, T. Aoyama, T. Hoshi

License: Mozilla Public License v2.0

FY 2024 PASUMS project (proposer T. Hoshi@NIFS)

User support

ODAT-SE-Template Expert (2)



ChatGPT

- myGPT given the odat-se-template manual as prior knowledge.

[https://chatgpt.com/g/
g-6744675c4ee8819185d4eb6678
2c2016-odat-se-template-tutorial-
expert](https://chatgpt.com/g/g-6744675c4ee8819185d4eb66782c2016-odat-se-template-tutorial-expert)

ODAT-SE-Template Tutorial Expert ▾



ODAT-SE-Template Tutorial Expert

By KAZUYOSHI YOSHIMI ✉

ODAT-SEへの順問題ソルバー導入に関する日本語チュートリアル専門家。

ODAT-SEのインストール方法を教えてください。

ODAT-SEでモデルを設定する手順を教えてください。

ODAT-SEのデータ解析で使用する主要なコマンドは？

ODAT-SEのエラーを解決する方法を教えてください。

- It is possible to make some examples and try them out.
(Note: As mistakes are often made, this is only a reference base to build on.)

Message ODAT-SE-Template Tutorial Expert



?

ChatGPT can make mistakes. Check important info.

User support

ODAT-SE-Template Expert (3)



ChatGPT

ODAT-SE-Template Tutorial Expert

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If an error occurs when following the tutorial, paste the error into a message and it will suggest a solution.

In fact, in the current case, in `input.toml`, `[solver]` type = 'FourierSolver' was not added to the `input.toml`, so an error occurred, but once this was added, it could be executed.

CCMS hands-on training course, held on 2024/12/2 for test operation.

<https://ccms.issp.u-tokyo.ac.jp/event/7002>

User support

ODAT-SE-Template Expert (4)



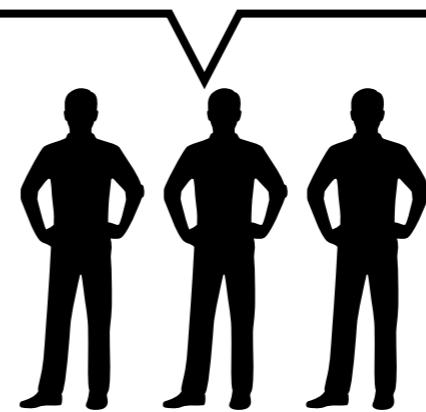
ChatGPT

Generally well received by the participants, although there were still some areas of underperformance

‘This is fantastic!’

‘I’m glad I had limited avenues to ask about things I didn’t understand’

‘I will try it. I hope it will be available for other software in the future’



Importance of Sharing AI Technologies with the Community

- **Extending AI-assisted development beyond individual projects**
 - Share tools, workflows, and best practices
 - Enable wider adoption in materials science research
- **Lowering the learning barrier for newcomers**
 - AI supports coding, analysis, debugging, and documentation
 - Helps students and young researchers begin contributing earlier
- **Building a community through education and collaboration**
 - Training events and hackathons
 - Encourage participation in scientific software development

MateriAI Hackathon — Overview

- **Hands-on event focusing on AI-assisted materials research**
 - Data-driven discovery using generative AI
 - Automation of analysis and workflow construction
- **Organization**
 - Division of Data-Integrated Materials Science, Social Cooperation Research Departments, ISSP
 - Advanced Material Engineering Div., Toyota Motor Corporation
- **Target participants**
 - Students and early-career researchers in materials science, physics, and related fields
- **Past and upcoming events**
 - MateriAI 2023: <https://ccms.issp.u-tokyo.ac.jp/event/6320>
 - MateriAI 2024: <https://ccms.issp.u-tokyo.ac.jp/event/7033>
 - **MateriAI 2025 (Feb. 2–4, 2026) — Currently recruiting participants:**
<https://ccms.issp.u-tokyo.ac.jp/event/7584>



Event

2026-MON 2026-WED
02/02 ~ 02/04 13:00 ~ 15:00

MateriAI 2025 ~ 計算物質科学分野におけるAI技術の活用 [Utilization of AI technology in the field of computational materials science]

御殿場高原 時之栖/Gotemba Kogen Tokinosumi ka
静岡県御殿場市神山1271-12 Kamiyama, Gotemba, Shizuoka

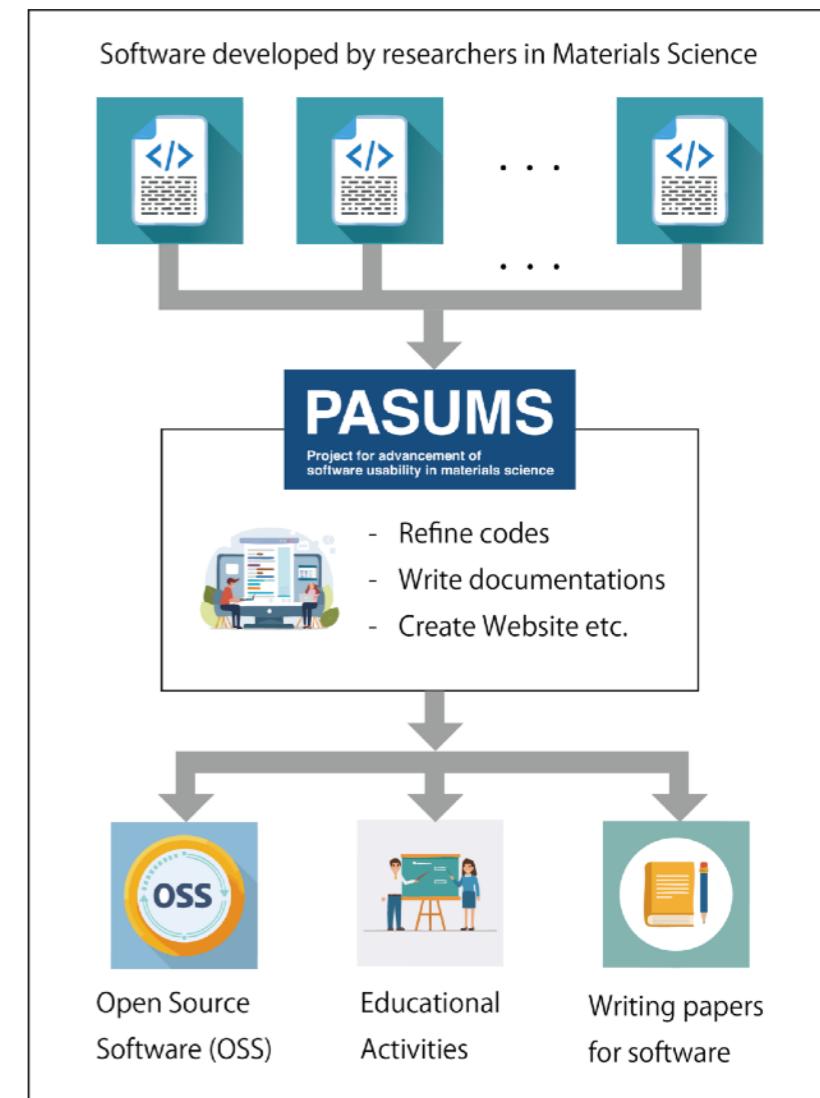
参加申込み

開催概要 | 申込要項 | 申込み | 受験者 | プログラム | 主催 | 共催/協賛 | その他 | お問い合わせ

Summary

Toward a sustainable research software ecosystem

- PASUMS improves usability and accessibility of research software
- Generative AI accelerates development workflows
 - Agent tools and AI tutors for coding and documentation
 - Sharing AI technologies strengthens the community
 - Training and hackathons lower learning barriers



Looking forward to future collaboration with the topics introduced in this symposium

Acknowledgement

- ◆ PASUMS project member

- ◆ N. Kawashima, Y. Motoyama, T. Aoyama



- ◆ MateriAI

- ◆ T. Misawa, K. Inui and K. Ido



- ◆ Advanced Material Engineering Div., Toyota Motor Corporation