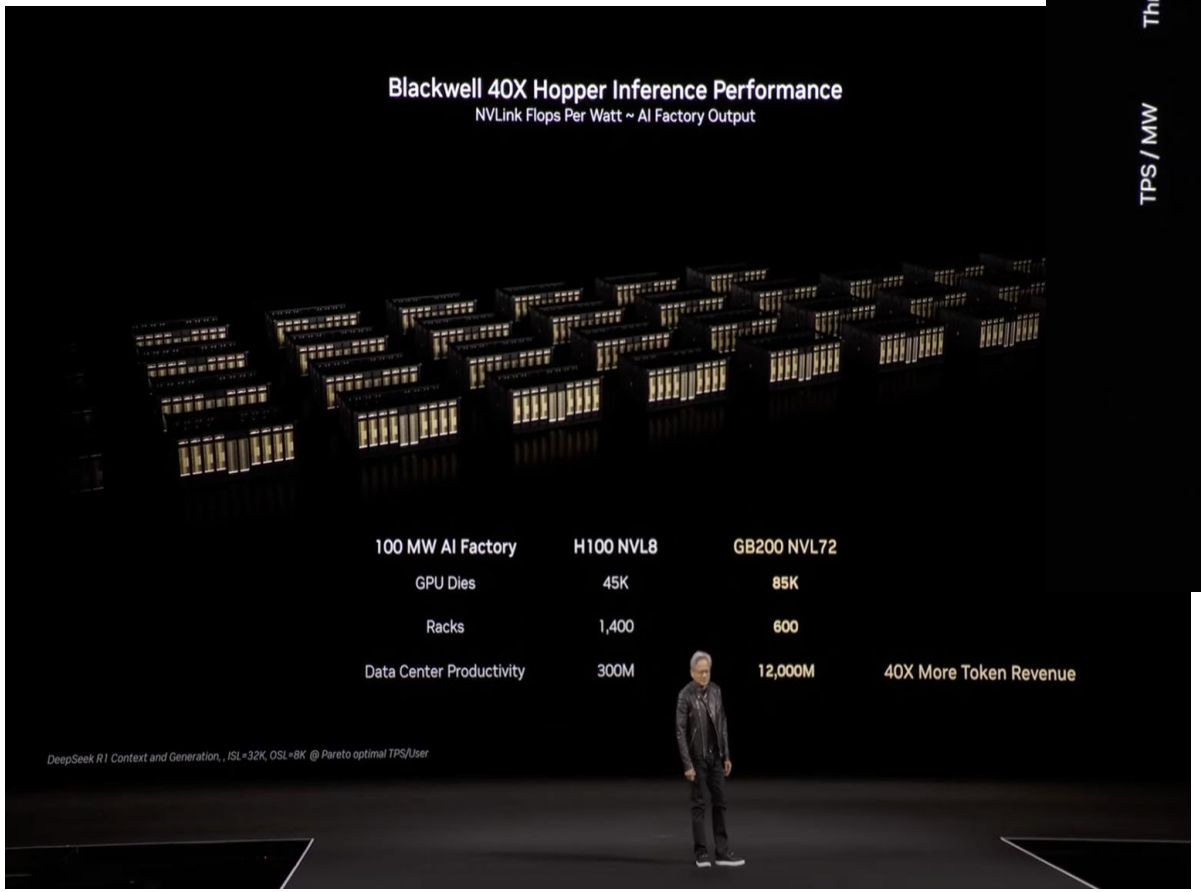
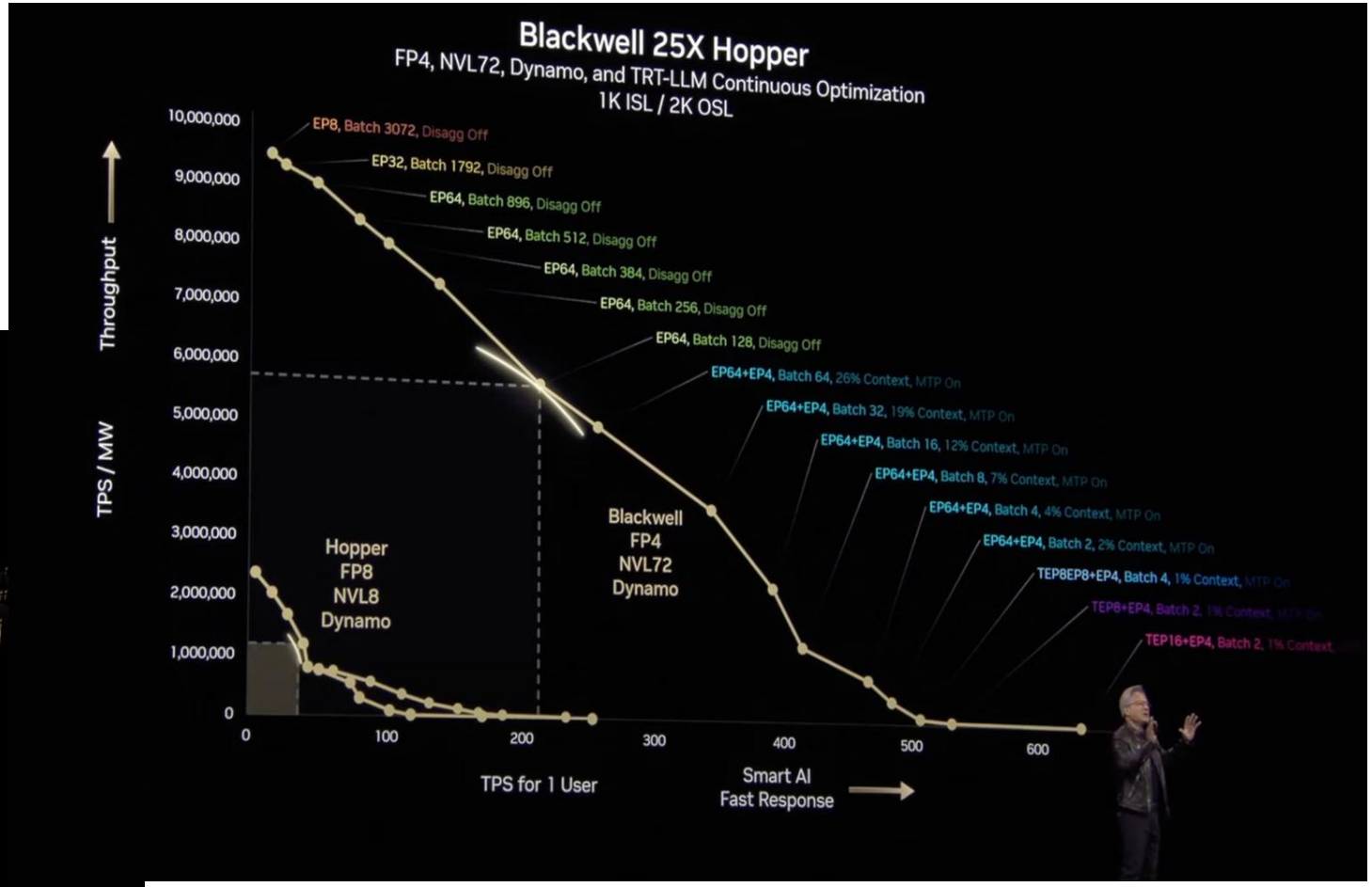
InPEx 2025 Japan: GenAI Breakout






GenAI: Platforms

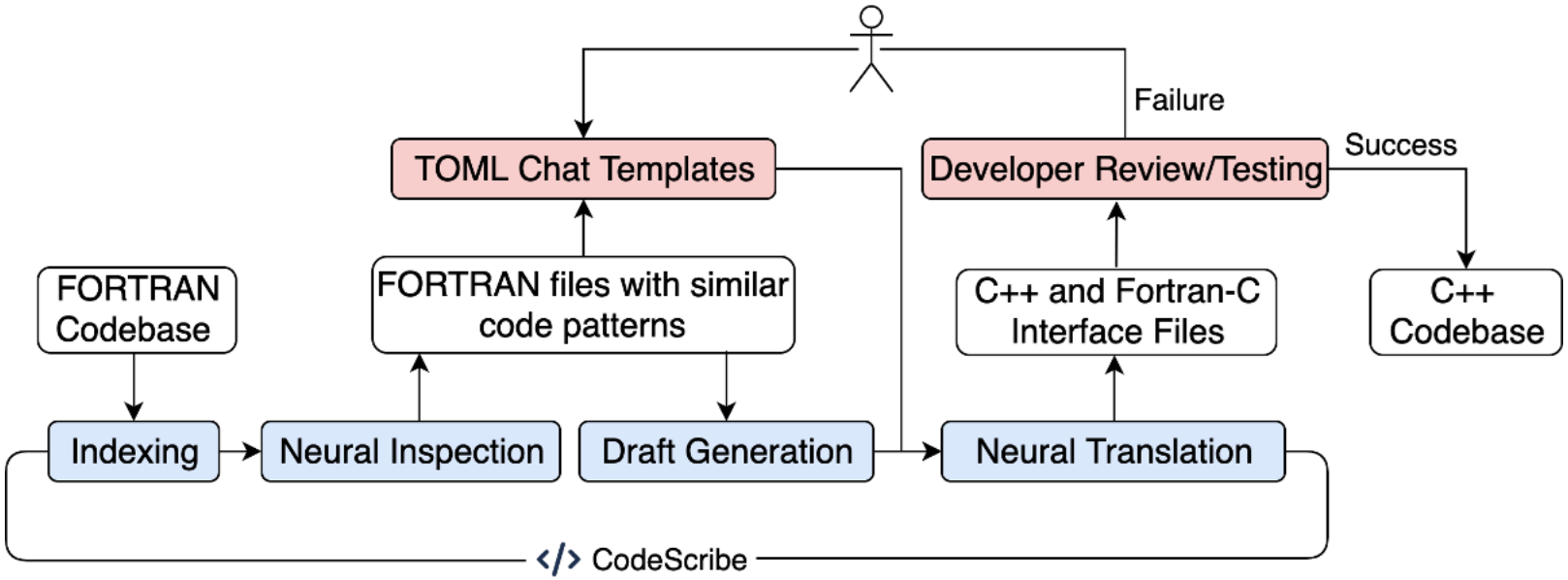




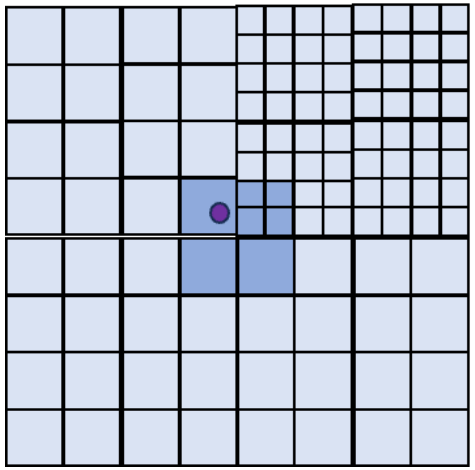
Key Insights: Future AI/HPC Architectures

- **Divergence vs. Integration?**: HPC remains unique due to precision and storage. AI brings low-precision inference and training demands—opportunities arise at the intersection.
- **Opportunities for Innovation**: Most innovation expected on the software stack, while hardware is vendor-driven. Emulated FP64, edge computing, and chiplet ecosystems were highlighted.
- **Portability & Sharing**: Emphasis on portability across platforms — especially for hybrid HPC+AI environments.
- **Operational Shifts**: Agents and inference are shaping new operational paradigms– we should address this with a working group
- **Global Coordination**: Strong sentiment: balance industrial AI trends and scientific HPC needs.

GenAI: Code



Monte Carlo code for LHC interactions

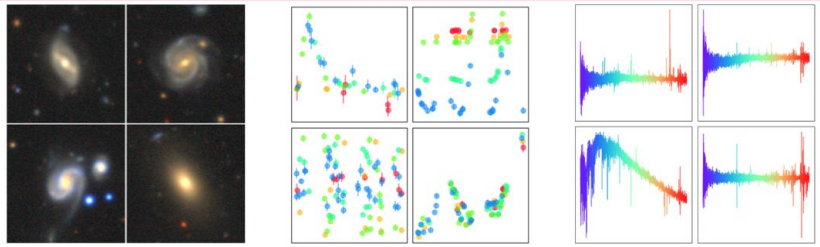


An algorithm for depositing from particle to mesh - decomposition, prompts and test-driven development, debugging – everything happening in (what should be) very precise English

Key Insights:
Code Generation, Precision, Debugging

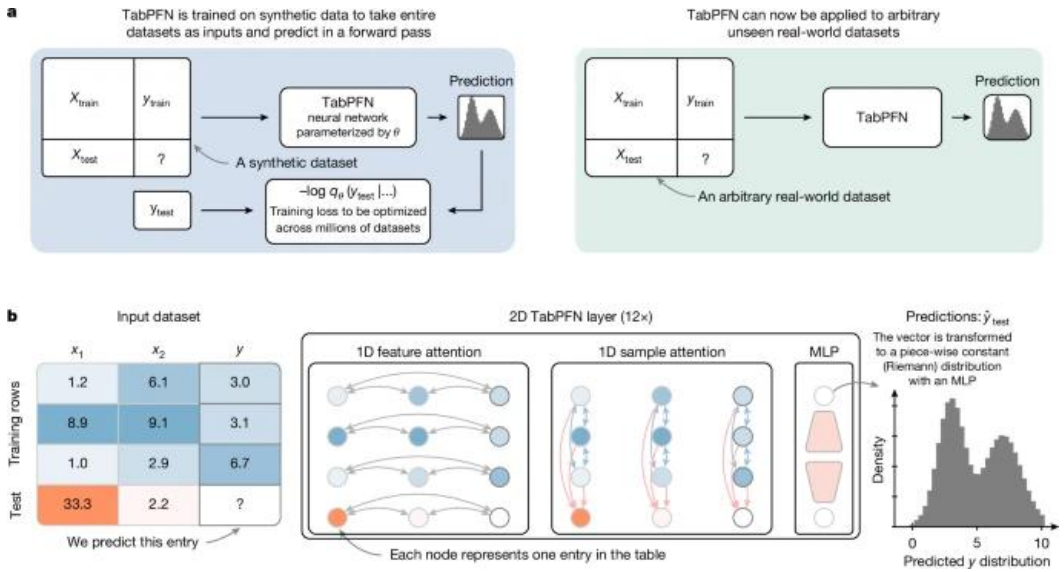
- **AI Helps:** LLMs assist well with simple tasks and boilerplate code; fail more often on complex, hybrid, or algorithmic logic.
- **Prompting ≠ Programming**: Prompt engineering seen as inadequate pedagogy. Better for experienced developers, not a replacement for formal programming education.
- **Trust & Validation**: Consensus on the need for (more) robust test harnesses (unit tests, integration) and human-in-the-loop practices for validation.
- **Scientific Intuition**: (current) AI lacks intuition; safe precision reduction must remain scientist-guided, though AI can support validation and testing.
- **Path Forward: (FAST!)** International repositories (e.g., prompt libraries, agent systems) and shared fine-tuned models for HPC contexts.

GenAI: Data

	Images	Time-Series	Spectra
# examples	140M	4.5M	225M
Description	images in a variety of wavelength ranges, including optical and infrared	multivariate time-series of flux + uncertainty in different wavelength ranges	flux as a function of wavelength
Tasks	galaxy classification, physical property estimation	time-series classification, redshift estimation	physical property estimation
Examples			

The Multimodal Universe Collaboration, 2024

100M synthetic datasets



Hollman et al, 2024

>= 1T tokens

The Well: 15TB of Physics Simulations

Ohana et al, 2024

Key Insights: Data Curation & Generation

- **Data Complexity Problem**: Each community has unique formats. There is a great need for AI to help make scientific data available for training.
- **Local Storage**: (a key difference in AI/HPC platforms): Supercomputing centers could support in-situ AI processing before discarding intermediate data.
- **Workflow Innovation**: Need for shared pipelines to load, preprocess, and stream data—especially for large GenAI models.
- **Access**: Social and political barriers limit data access.. This is difficult. We must continue to improve availability. Some fields (e.g., structural biology) are ahead; others lag behind.
- **Future:** Clear plan for improving, not just talking about, scientific data for AI

GenAI: Truth

AI for Science: 5 Lessons from my PhD

#1: AI usage doesn't imply AI usefulness

#2: AI will benefit some areas of science but not others

#3: Evaluating whether AI is accelerating science is extremely difficult

#4: Conflicts of interest and researcher degrees of freedom make AI-for-science overoptimistic

#5: AI-for-science is often a solution looking for a problem

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Weak baselines and reporting biases lead to overoptimism in machine learning for fluid-related partial differential equations

Nick McGreivy ✉ & Ammar Hakim

Nature Machine Intelligence **6**, 1256–1269 (2024) | Cite this article

Key Insights: GenAI for Science

(Is AI Improving Scientific Progress?)

- **Impact Metrics**: Track *time to discovery*, *scientific output*, *human effort saved*, *community uptake*, and *cross-disciplinary impact*. Use both *quantitative* (e.g., citations, speedups) and *qualitative* (e.g., novelty, utility) measures.
- **Practical Benefits**: GenAI is best at supporting *tedious, complex, or repetitive tasks* like literature review, hypothesis generation, debugging, and code maintenance – freeing up human creativity.
- **ModSim vs AI**: GenAI can enable science in *data-rich domains* (e.g., astrophysics, protein folding) and assist where *first-principle models fall short*.
- **Best Practices**: Avoid biases (e.g., cherry-picking, weak baselines) via *provenance tracking*, *peer review*, and *international frameworks*.
- **Global Collaboration**: 1000 Scientist Jam – repeated in many places. Build *REAL* experience. Foster trust through transparency and reproducibility.

Thank You