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Maximize your GPU Utilization: AI Chemistry as a Case Study

Fusion of HPC & AI: A New Computational Paradigm

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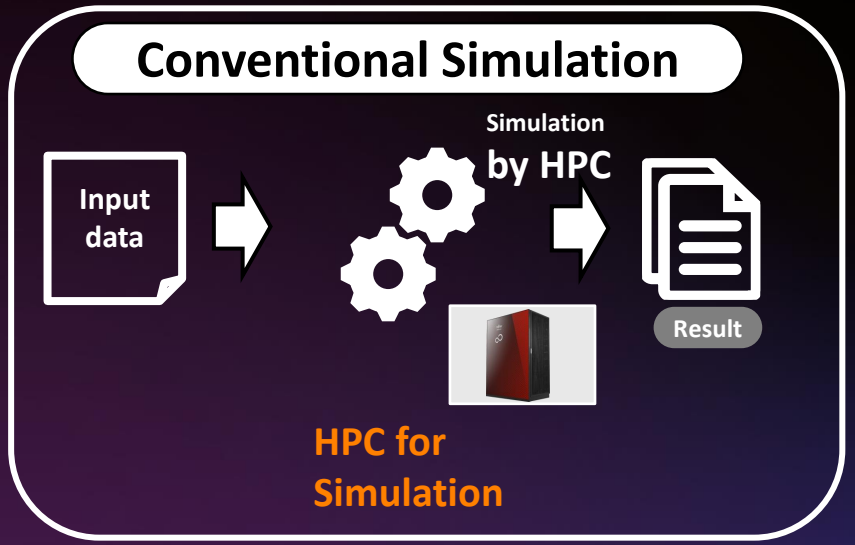
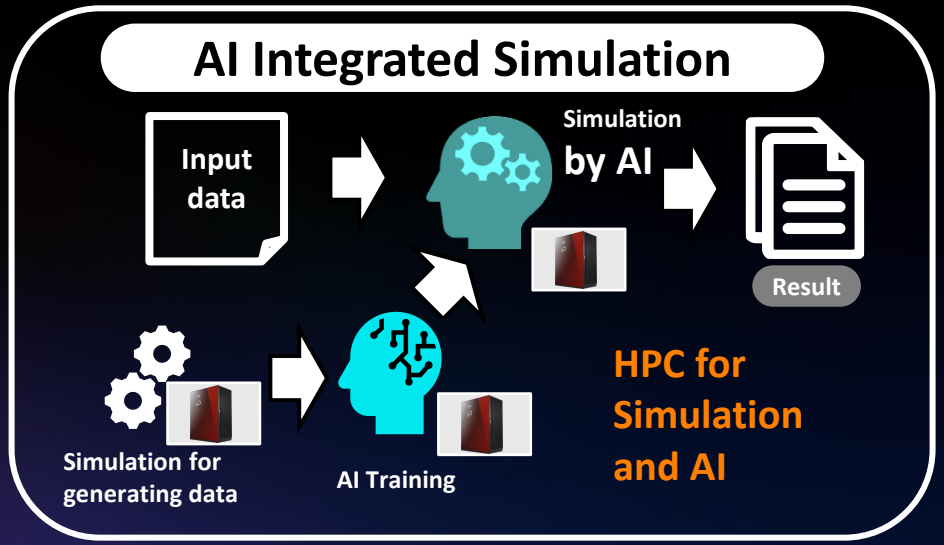
- **HPC systems are expected to accelerate not only traditional simulations but also AI workloads**
  - Integrating AI into simulations enables significant speedup
  - Achieving a seamless connection between HPC and AI has become a critical challenge





Material Design

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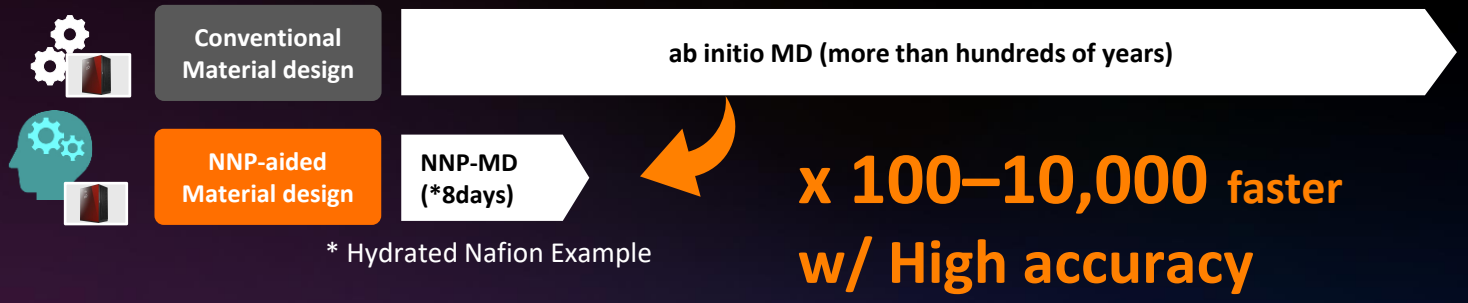
Molecular Dynamics Simulation:
For understanding dynamic characteristics of the target material

Classical MD:	Computation time ✓	Accuracy ✗
ab initio MD:	Computation time ✗	Accuracy ✓

→ The best of both worlds: **MD using Neural Network Potentials**



Fujitsu provides a generator of NNP for MD

MD Simulation Case Study

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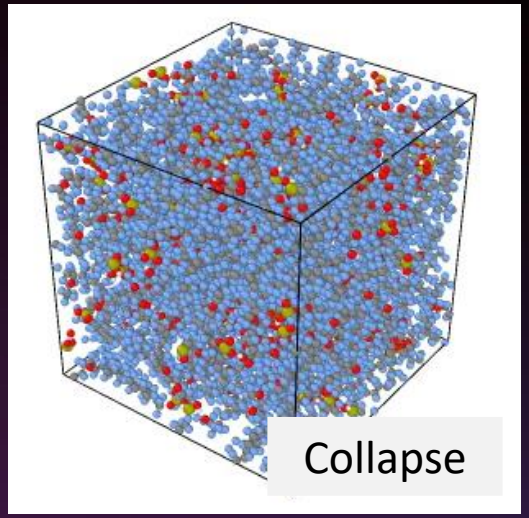
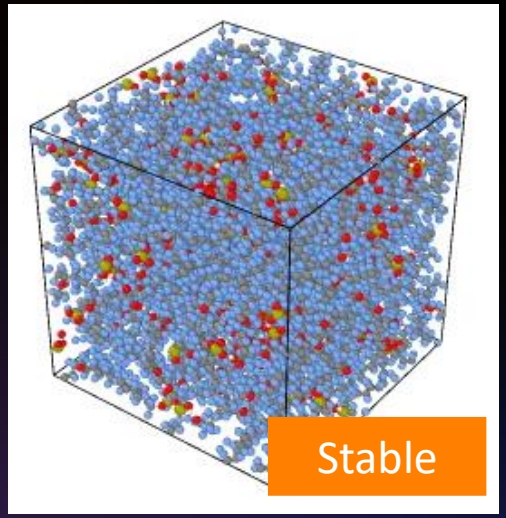
MD Simulation Breakthrough: 20,000 Atoms, 30 ns (60M steps) in 8 Days, cutting simulation time from hundreds of years！

w/o Our Technology



w/ Our technology



Note: Running 30 ns of MD takes 1.5 days

Hydrated Nafion (19,670 atoms)

Achieved sufficient performance for practical use

10k-atoms: Large enough to design entire devices

10M-steps: Reproducible chemical reactions

1-week: Acceptable computation time for developers

Feature of Our NNP Generator

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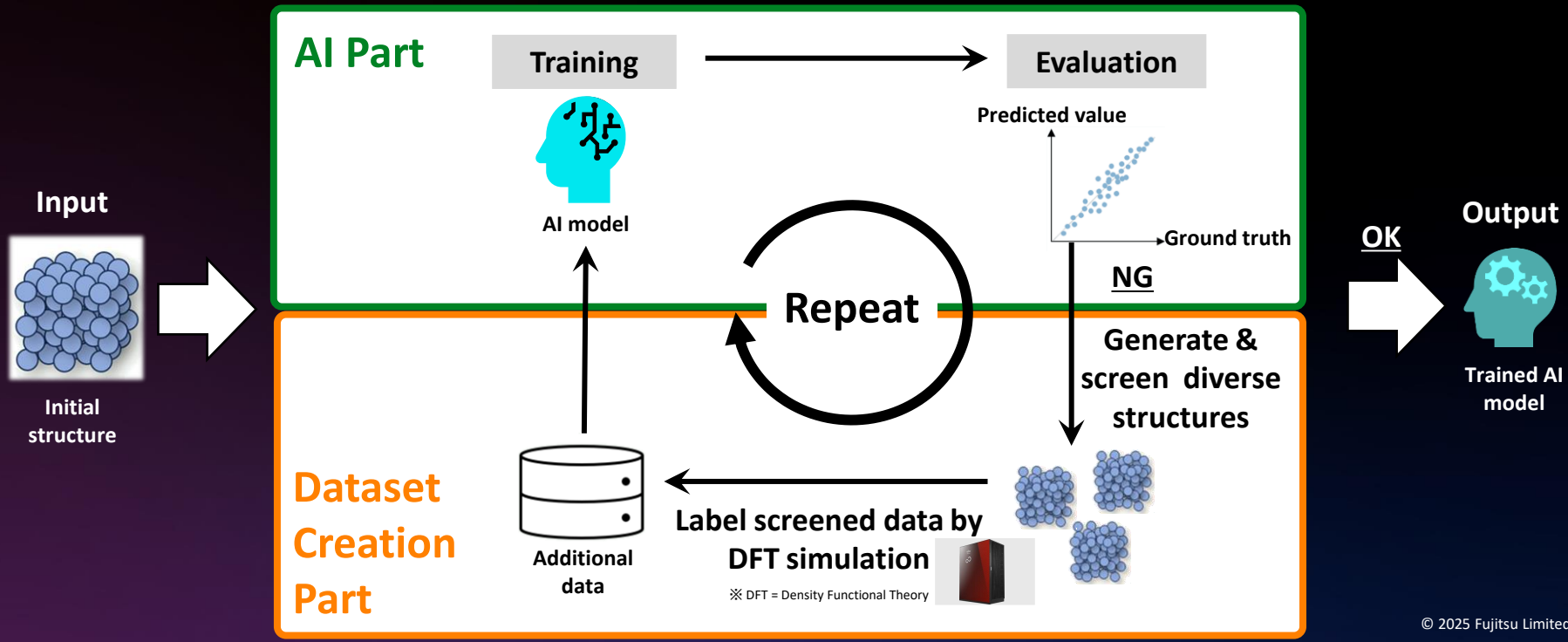
Generate NNP with high accuracy, high speed, and high MD stability with our unique training data generation technology (Active Learning)



Practical Use Case of NNP Generator

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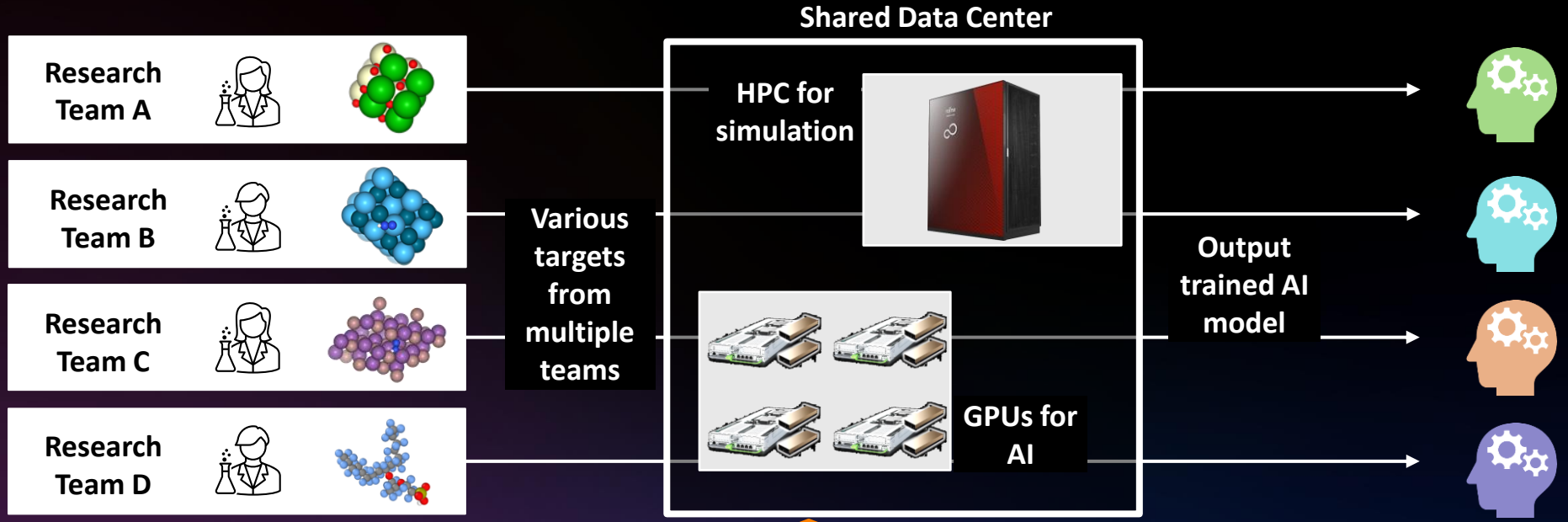
Multiple AI training for each target are running simultaneously on limited computing resource



Challenge: Heavy AI-training jobs monopolize GPU, delaying short jobs significantly

AI computing broker (ACB)

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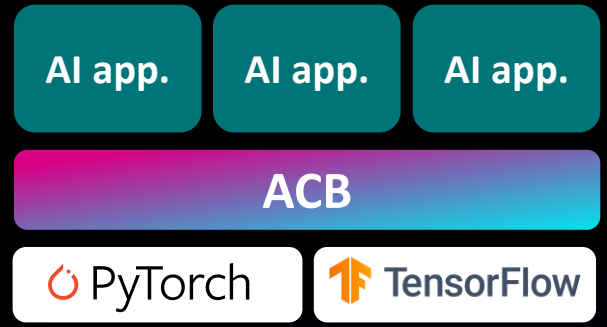
A middleware to share GPUs among AI apps.

Key Features

- Best-in-class GPU utilization efficiency
- Optimized memory management across various AI applications



“Doubled model training throughput!”

“Deploying multiple jobs beyond physical GPU memory capacity!”

Success stories from ACB users
Scan here for more detail!

Smarter Training
for NNP Generator with ACB!