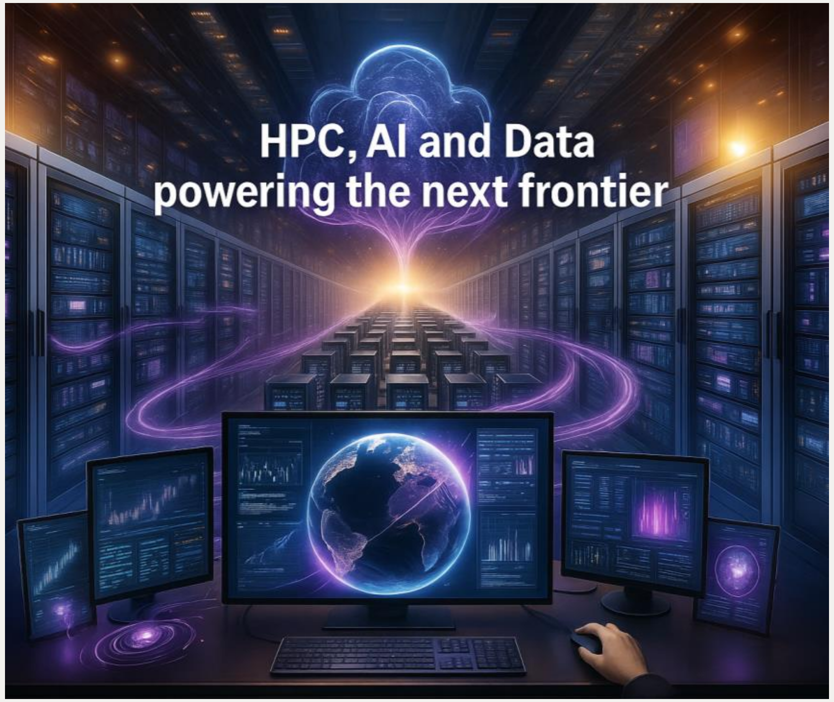
Accelerating Material Science using HPC and AI



By

Jayanth Mohan

Agenda

01 Introduction

What is HPC?

clusters of powerful processors that work in parallel to process massive, multidimensional data sets and solve complex problems at extremely high speeds.

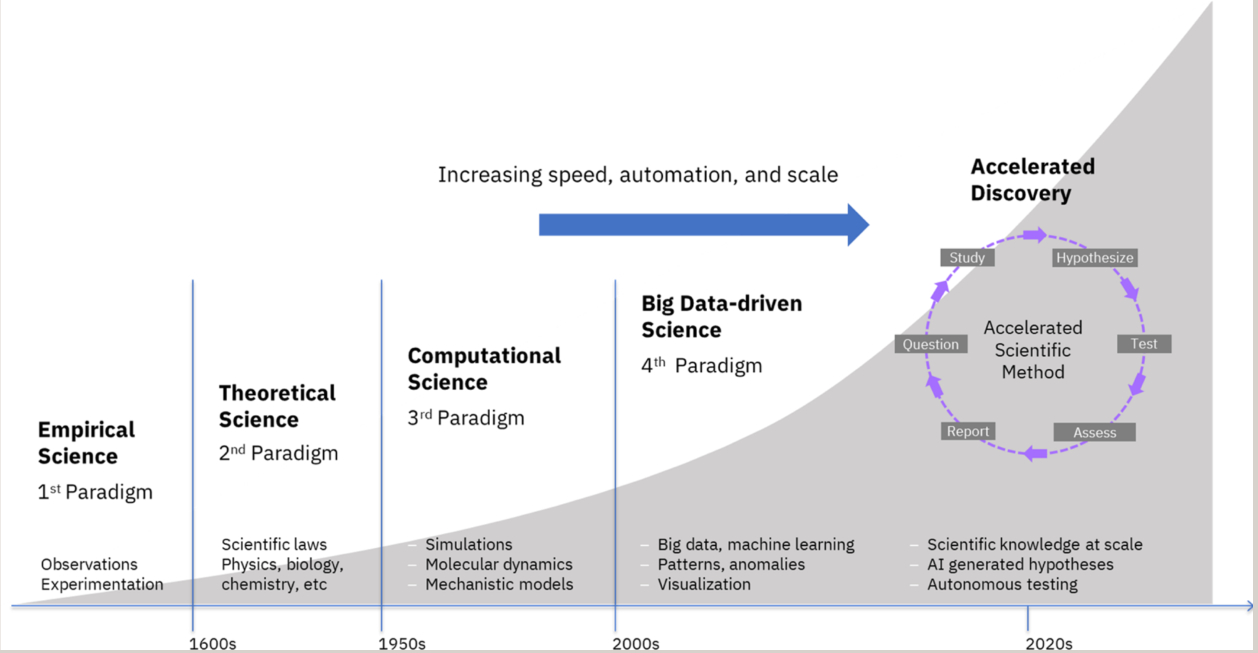
01

Introduction

What Role does it play in Simulations?

01

AI in Material Science



How AI complements HPC?

- Predictive modeling
- Rapid material screening
- Optimization and surrogate models

02

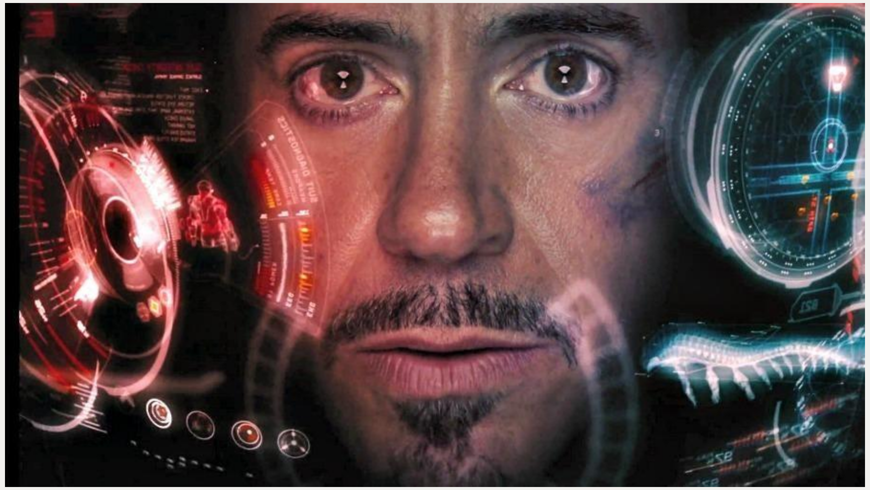
Iron Man's Arc Reactor – Fiction Meets Science

Do you Remember How Iron Man Discovered an Alternative to Palladium ?

Jarvis – AI and HPC in Fiction

Jarvis as an AI-enabled HPC system:

- Simulating elemental configurations rapidly
- Identifying viable new element

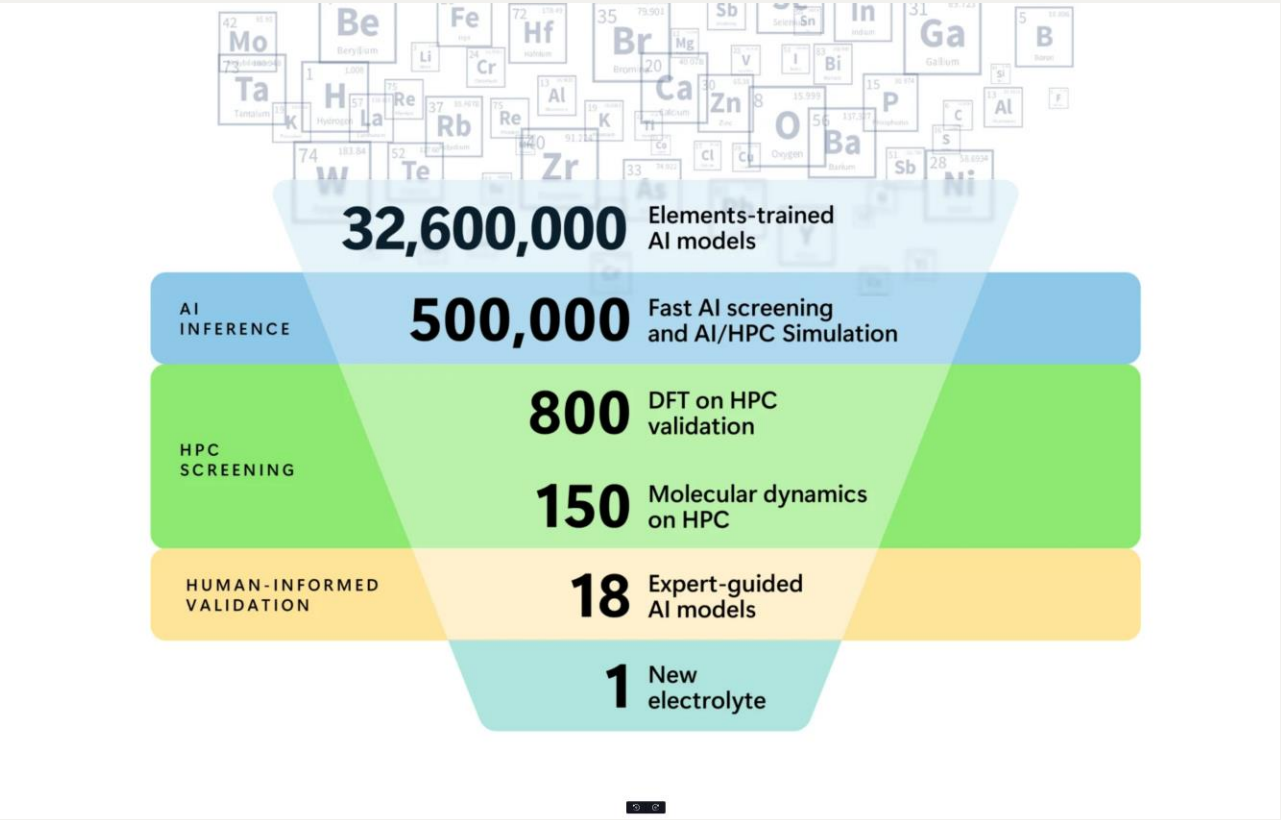


case study 1 – Microsoft and PNNL

Overview:

32.6 million candidates screened for battery electrolyte

- AI narrowed down materials; HPC simulations validated predictions
- Result: Discovery of a novel solid-state electrolyte (70% less lithium)



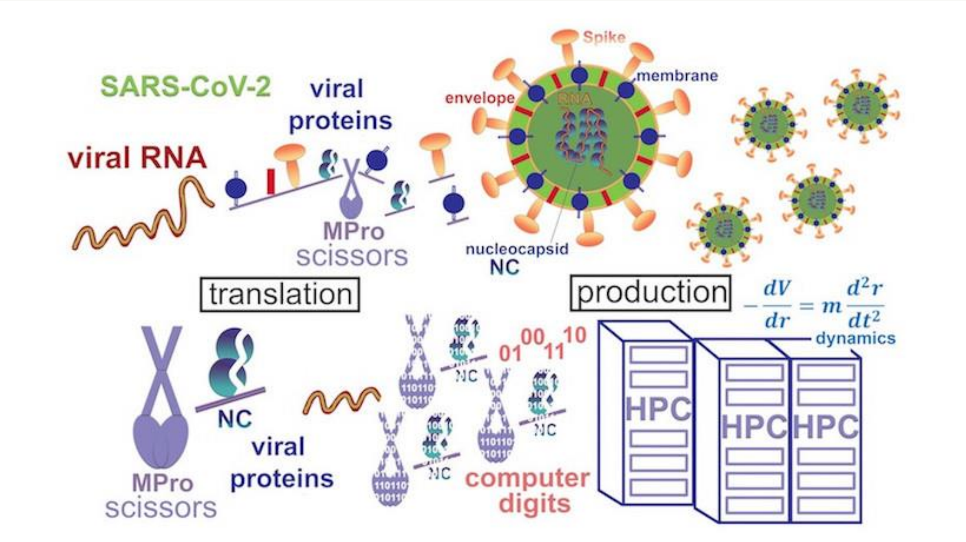
https://news.microsoft.com/source/features/innovation/how-ai-and-hpc-are-speeding-up-scientific-discovery/

Molecular Dynamics Simulations

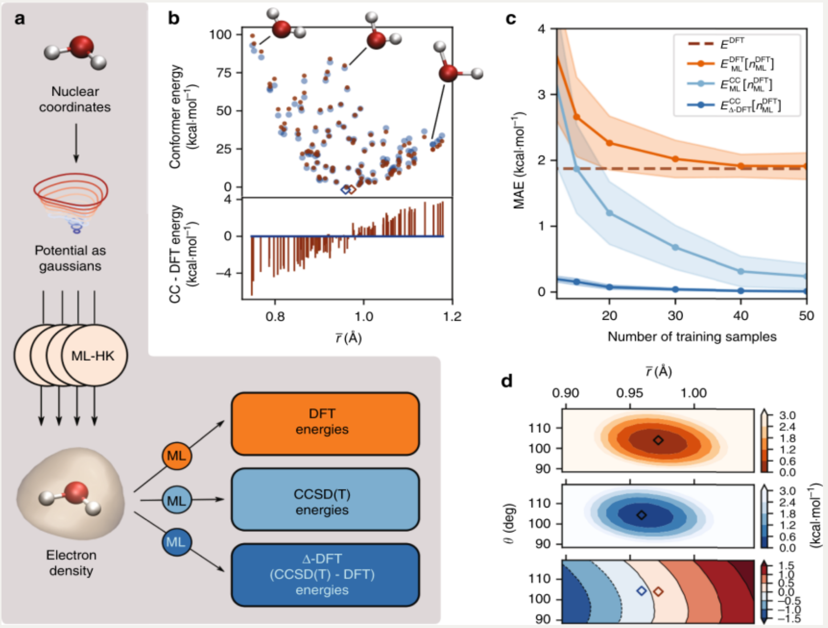
What is MD? And Why it matters now ?

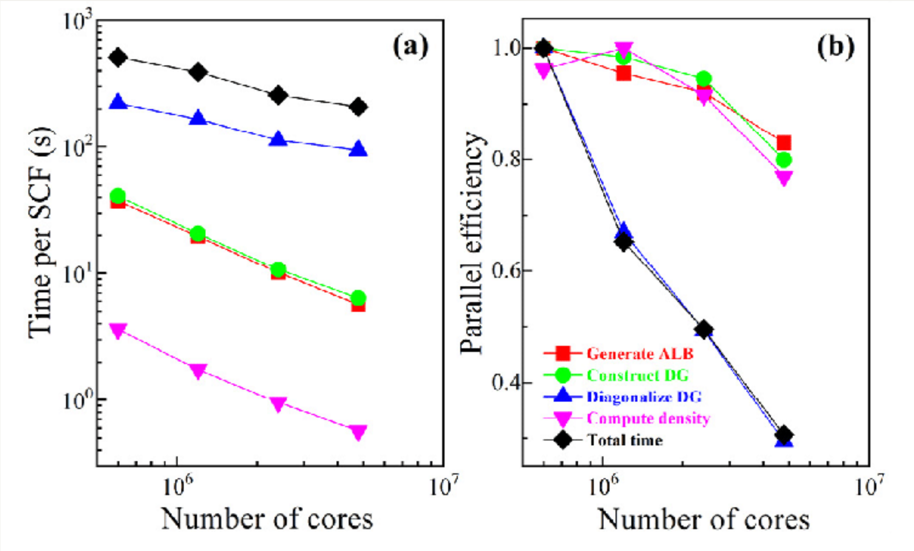
Key Applications:

•Self-healing polymers
•Drug delivery nanocarriers
•Polymer chain behavior



Quantum Mechanics & DFT Calculations





What is DFT?
A quantum mechanical method to calculate electronic properties of materials from first principles.

Why Use It?
Predicts band structure, total energy, magnetic behavior, and stability — crucial for designing semiconductors and quantum materials

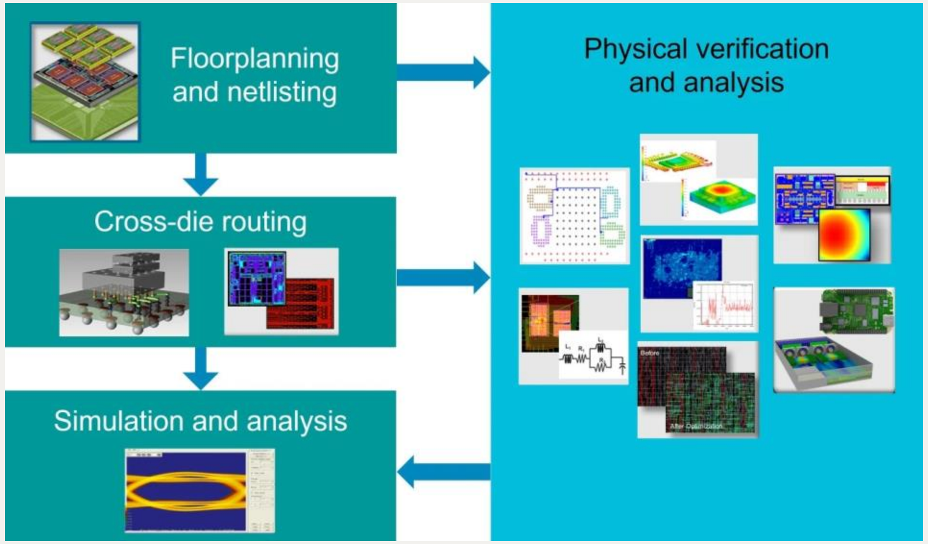
Multiphysics Simulations

- **What Is It?**
  Combines multiple physical phenomena — mechanical, thermal, electrical — into one simulation framework.

- **Why It Matters:**
  Materials in real devices undergo complex, interacting conditions. Simulating them together gives realistic performance insights.

Applications:

- Solid-state batteries (ion flow + heat + stress)
- Microchips (thermal dissipation)
- Carbon capture membranes



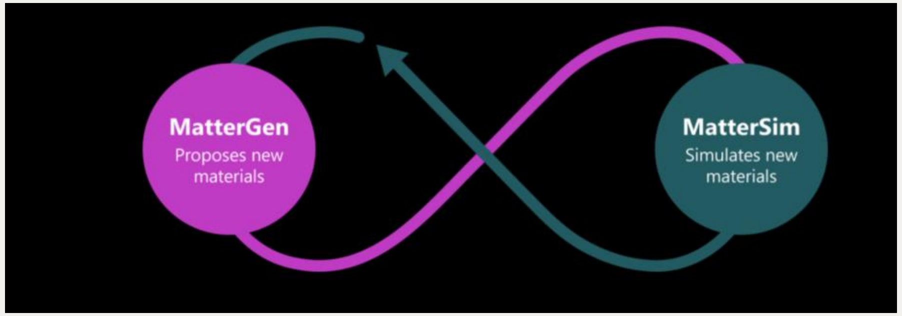
Case Study 2:
Heat dissipation simulations in stacked microchips helped engineers avoid thermal hotspots — improving reliability and lifespan.

AI-Enhanced Material Discovery

AI models learn patterns from HPC simulation data, then predict properties or outcomes — fast and at scale.

What It Enables:

- Surrogate models for quantum simulations
- Smart screening of materials
- Data-driven design rules



Benefits:

=> Reduces simulation time from hours to milliseconds

=> Explores millions of compositions virtually

https://www.microsoft.com/en-us/research/story/ai-meets-materials-discovery/

Real-World Applications of HPC in Materials Science

1.) Energy Storage (Batteries):

- HPC accelerates the discovery of safer, longer-lasting battery materials through atomic-level simulations.

2.) Aerospace & Defense

- Simulations predict material performance under extreme heat and stress, enabling next-gen flight and defense systems.

3.) Electronics & Semiconductors

- HPC models thermal and electronic behavior in chips, driving faster, smaller, and more efficient devices.

4.) Nuclear & Fusion Energy

- High-fidelity simulations guide the design of radiation-resistant materials for reactors of the future.

5.) Climate & Clean Tech

- HPC helps develop advanced materials for carbon capture, hydrogen storage, and green infrastructure.

Conclusion & Future Vision

HPC + AI Are Revolutionizing Materials Science

=>Faster discovery cycles

=>Less trial-and-error

=>Deeper atomic-scale insights

Looking Ahead:

AI-guided HPC is becoming our scientific "Jarvis" — capable of automating experiments, simulations, and discovery.

Thank You !!