

# THE INNOVATIVE FORCE OF HIGH-PERFORMANCE COMPUTING IN MATERIALS SCIENCE



**MATERIALS DESIGN, INC.**



**nVIDIA®**

# Topics

- ▶ The unprecedented global challenges
- ▶ The most powerful tools ever created by human ingenuity
- ▶ Industrial practice of materials modeling
- ▶ HPC in action – illustrative examples
- ▶ The future



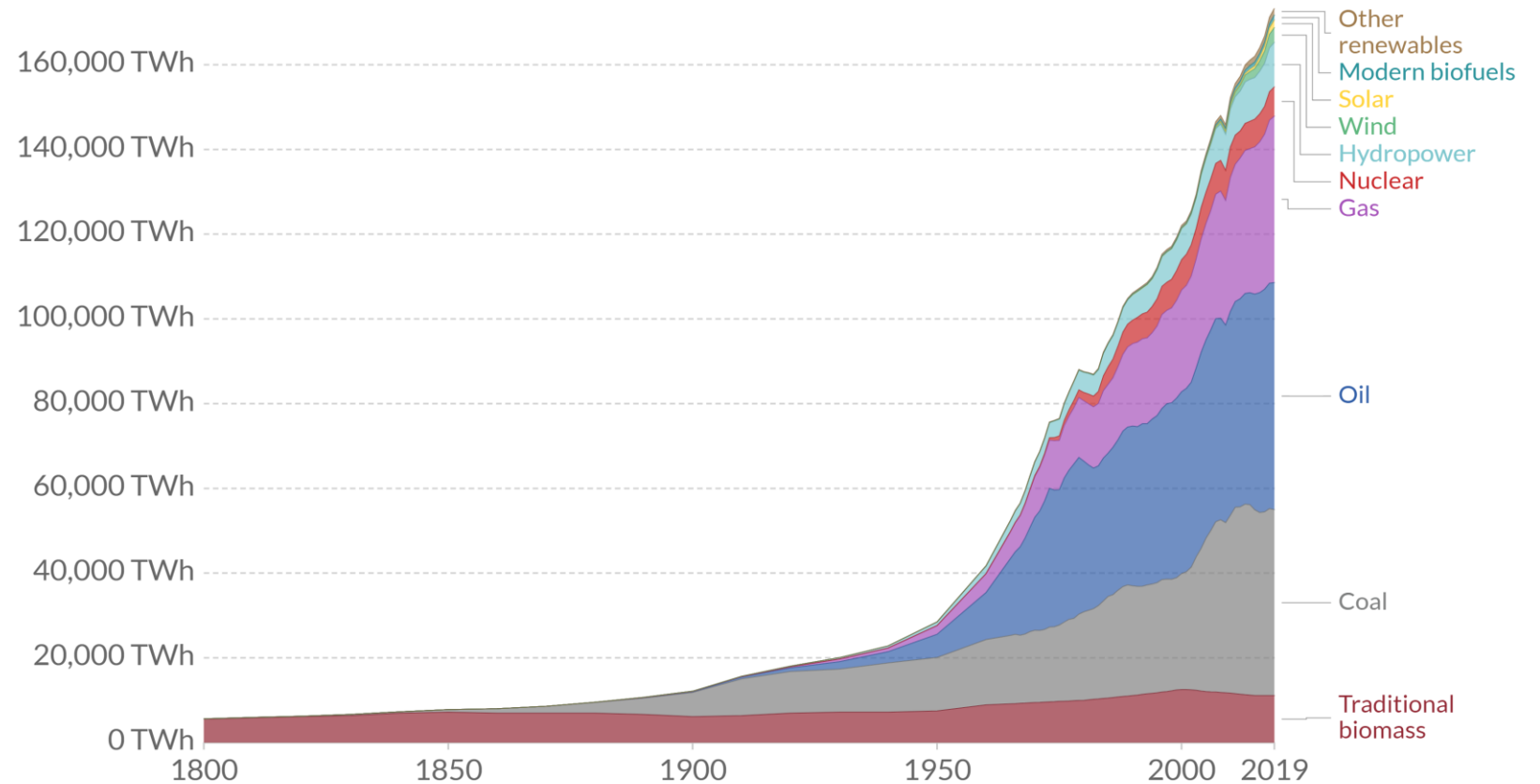
# Global Challenges

- ▶ Clean air
- ▶ Clean water
- ▶ Food
- ▶ Housing
- ▶ Health
- ▶ Communication
- ▶ Transportation
- ▶ Climate change

## Global primary energy consumption by source

Primary energy is calculated based on the 'substitution method' which takes account of the inefficiencies in fossil fuel production by converting non-fossil energy into the energy inputs required if they had the same conversion losses as fossil fuels.

Our World  
in Data



Source: Vaclav Smil (2017) & BP Statistical Review of World Energy

OurWorldInData.org/energy • CC BY

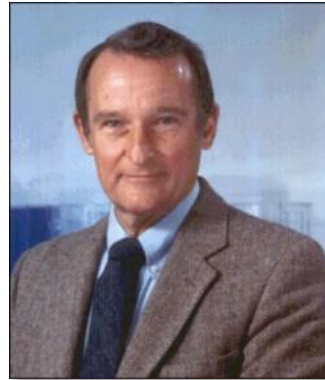


# Human Ingenuity and Entrepreneurship

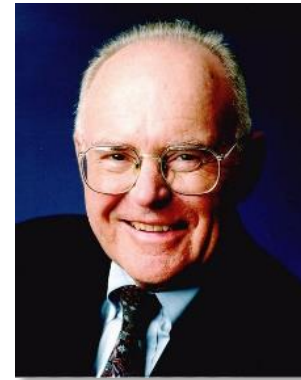
## Computers



John von Neumann



Seymour Cray



Gordon Moore

## Theory



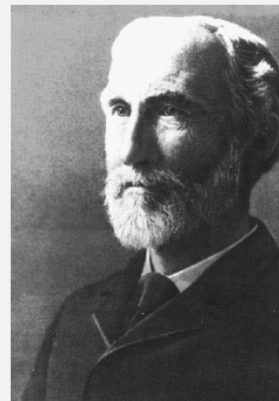
Isaac Newton  
1687



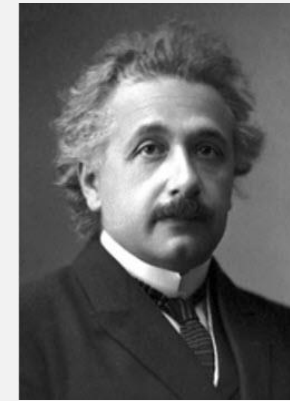
James C Maxwell  
1864



Ludwig Boltzmann  
1871



Josiah Willard Gibbs  
1876



Albert Einstein  
1905



Erwin Schrödinger  
1926





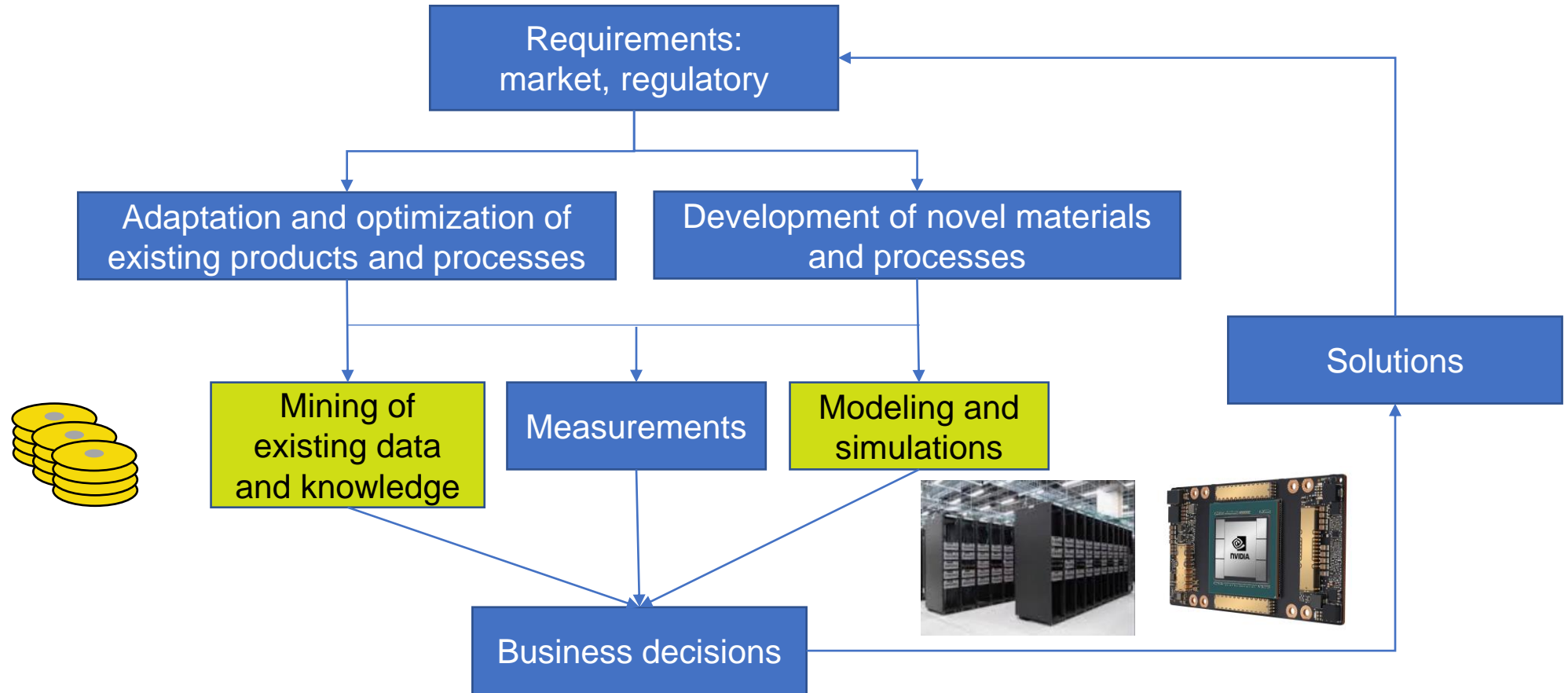
# INDUSTRIAL APPLICATIONS AND R&D WORKFLOW

# Industrial Application Areas

- ▶ Energy: oil, gas, nuclear, solar, wind
- ▶ Automotive: light-weight materials, batteries, electronics
- ▶ Chemical: catalysts, polymers
- ▶ Pharmaceuticals
- ▶ Electronics
- ▶ Metallurgy
- ▶ Glass and ceramics
- ▶ Other



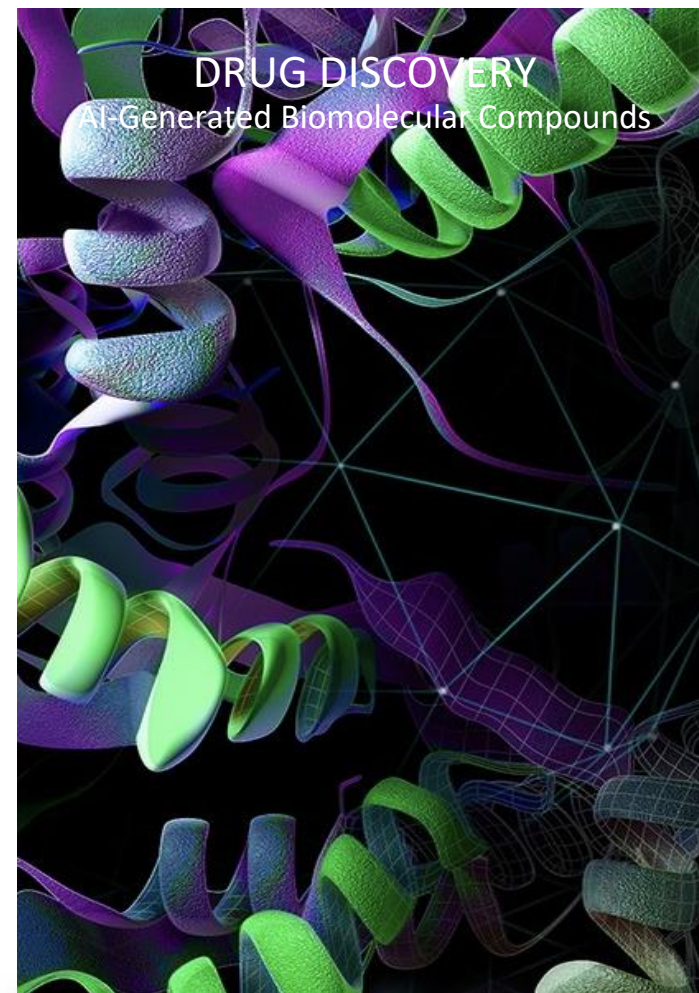
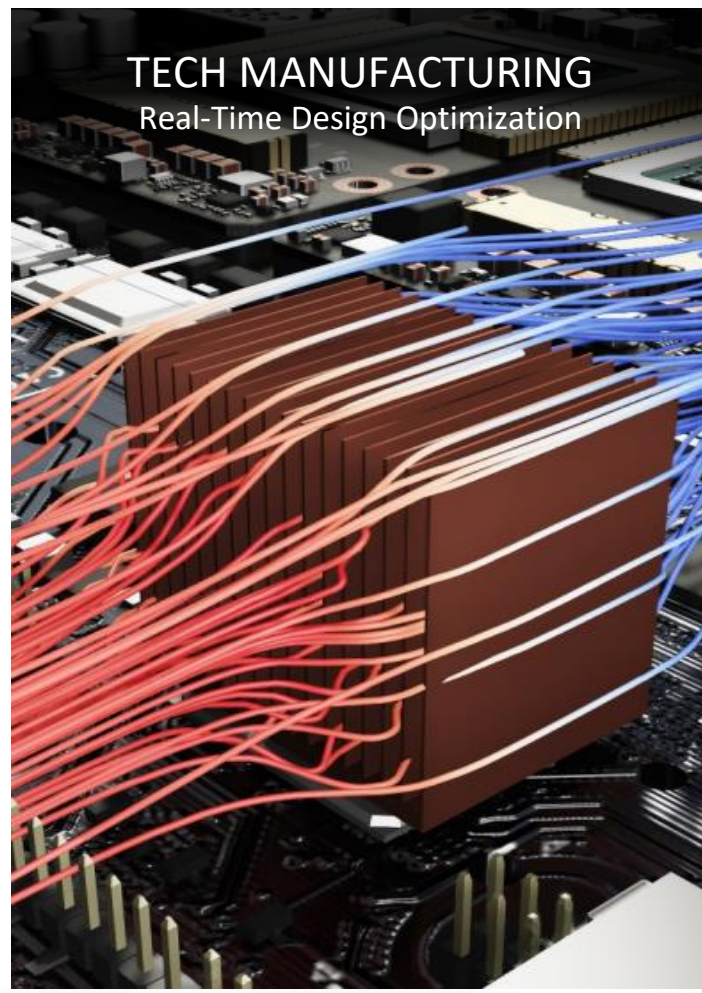
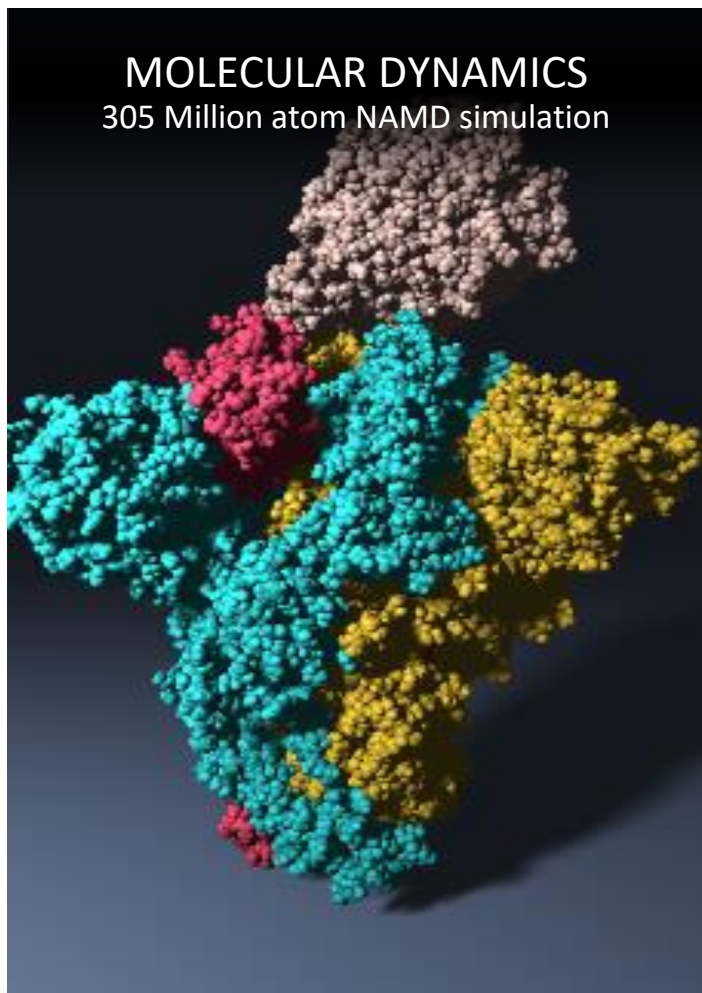
# R&D Workflow



## *Impact of HPC*

- ▶ Improved and new materials and processes through **faster** and **more accurate** simulations
- ▶ Shorter time to market of innovative products
- ▶ More efficient processes

# INDUSTRIAL HPC DELIVERS TRANSFORMATIONAL BREAKTHROUGHS

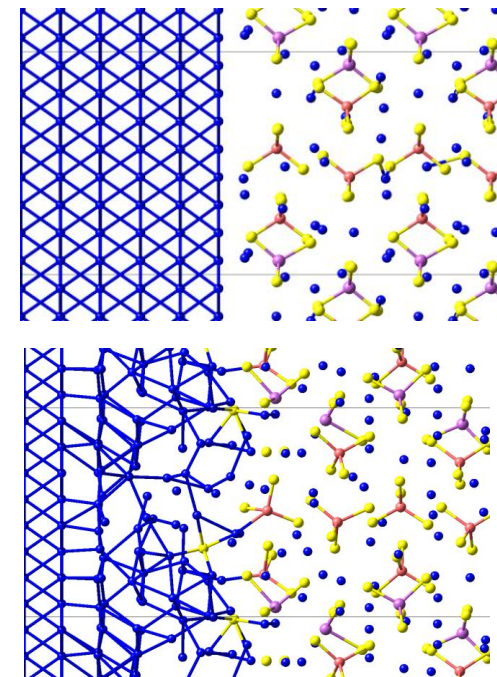
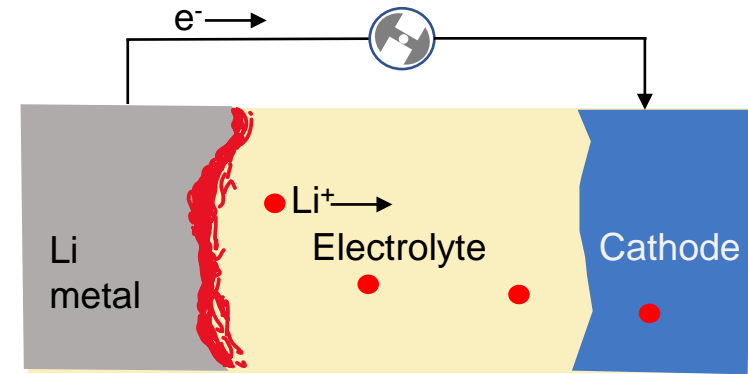




# EXAMPLES

# Batteries with High Power Density

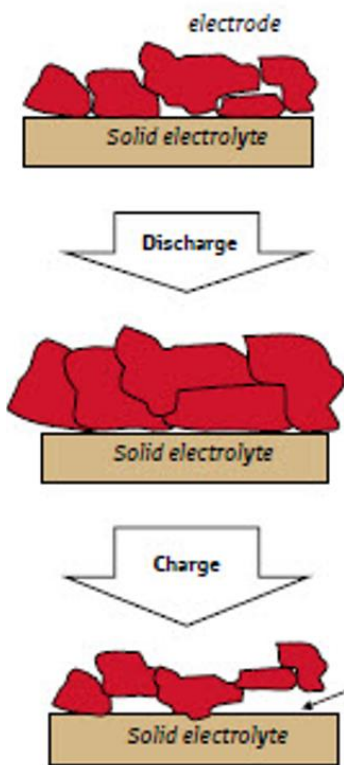
- ▶ The Challenge: increase the capacity of batteries while maintaining rigorous safety requirements
- ▶ Approach
  - Use Li metal rather than Li in graphite
  - Replace liquid electrolytes by solid state electrolytes
- ▶ The bottlenecks
  - Find solid state electrolytes with high ionic conductivity
  - Control the reaction of Li metal with the electrolyte
  - Find cathode materials with good mechanical match with solid state electrolytes
- ▶ The solution
  - Use large-scale accurate atomistic simulations to find optimal materials
  - Use quantum chemical calculations to understand and control the chemical reactions at interfaces



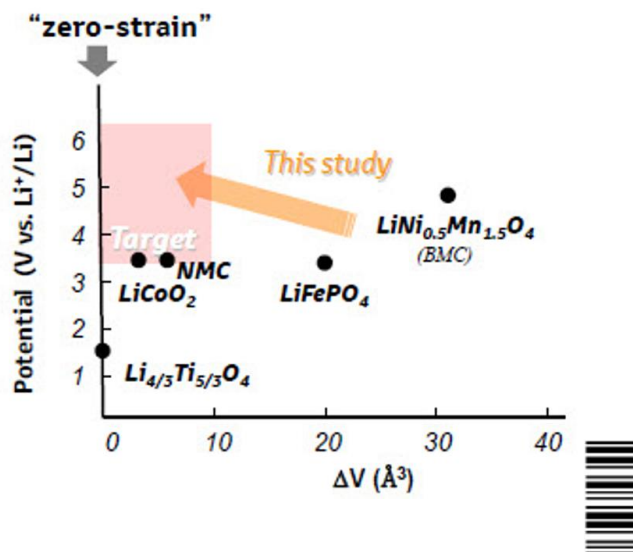
Ab initio molecular dynamics calculations are computationally highly demanding



# Batteries with High Power Density



- ▶ Computational screening of candidates with *MedeA VASP*



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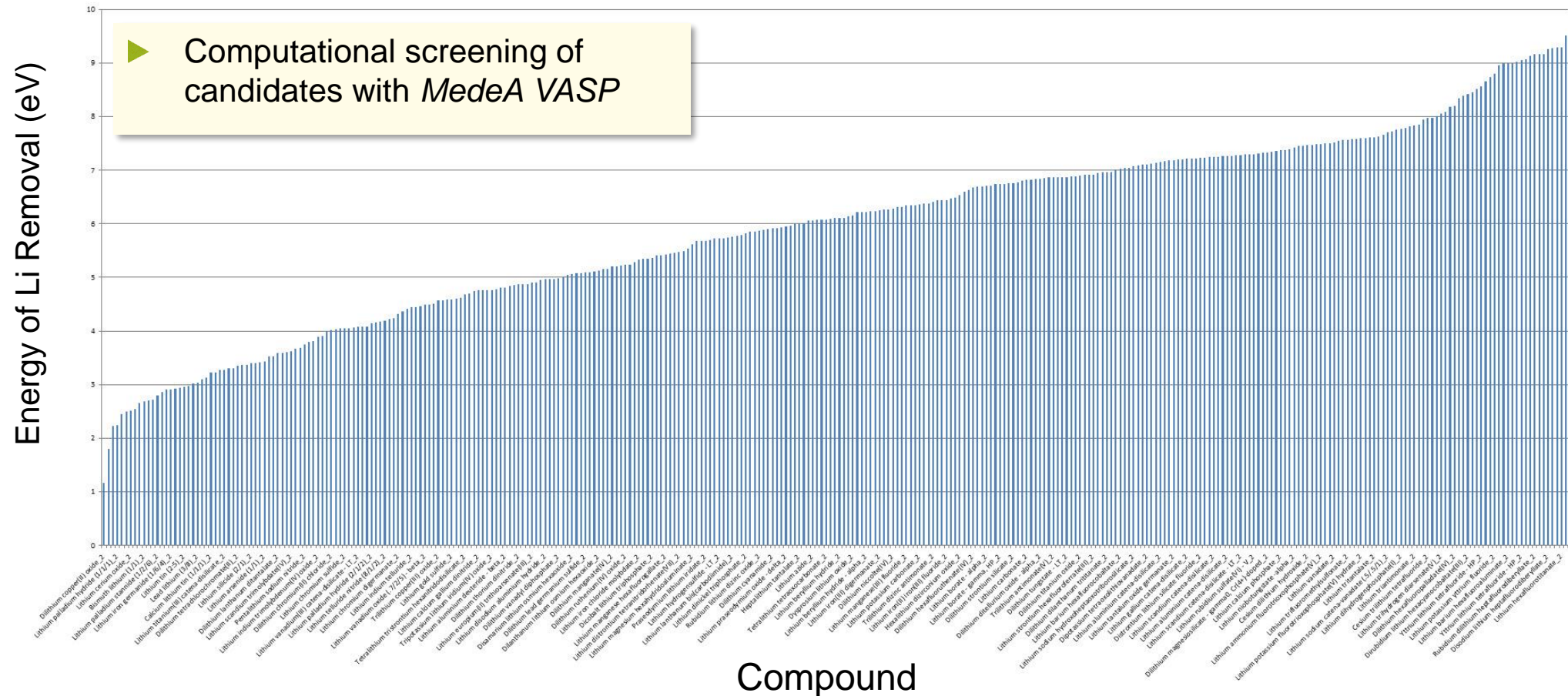
Published:

— with international search report (Art. 21(3))



# High-Throughput Screening of Materials

## Search of compounds with optimal Li binding energy



# VASP and OpenACC

- ▶ Complete rewrite of GPU acceleration in VASP 6
- ▶ Collaboration between VASP Software GmbH and NVIDIA



Prof. Georg Kresse

CEO of VASP Software GmbH

Computational Materials Physics  
University of Vienna

*“ For VASP, OpenACC is the way forward for GPU acceleration. Performance is similar and in some cases better than CUDA C, and OpenACC dramatically decreases GPU development and maintenance efforts.”*

# FEATURES AVAILABLE AND ACCELERATED IN VASP 6.2

## LEVELS OF THEORY

Standard DFT (incl. meta-GGA, vdW-DFT)  
Hybrid DFT (double buffered)  
Cubic-scaling RPA (ACFDT, GW)  
Bethe-Salpeter Equations (BSE)

## SOLVERS / MAIN ALGORITHM

Davidson (+Adaptively Compressed Exch.)  
RMM-DIIS  
Davidson+RMM-DIIS  
Direct optimizers (Damped, All)  
Linear response

## PROJECTION SCHEME

Real space  
Reciprocal space

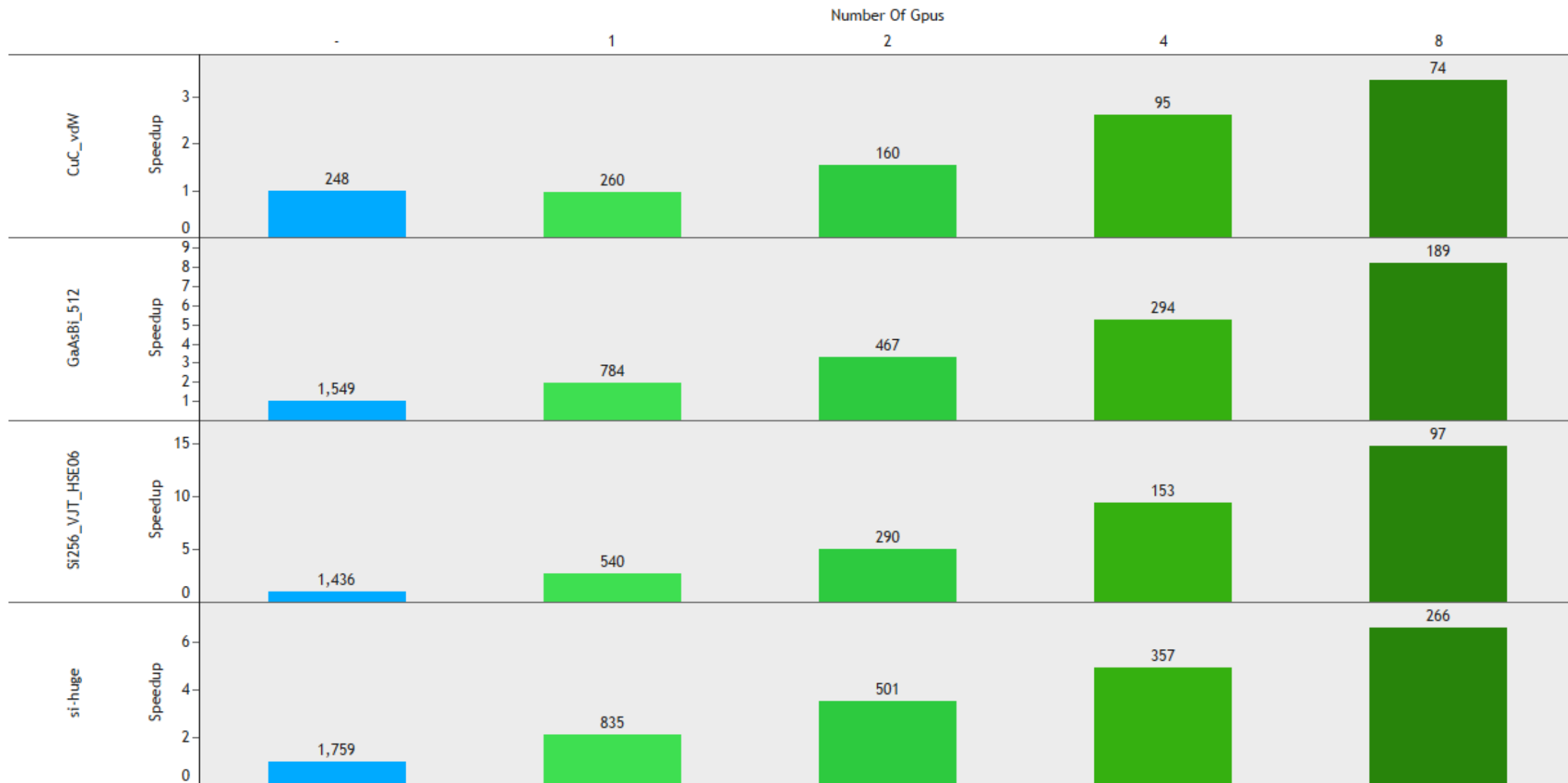
## EXECUTABLE FLAVORS

Standard variant  
Gamma-point simplification variant  
Non-collinear spin variant

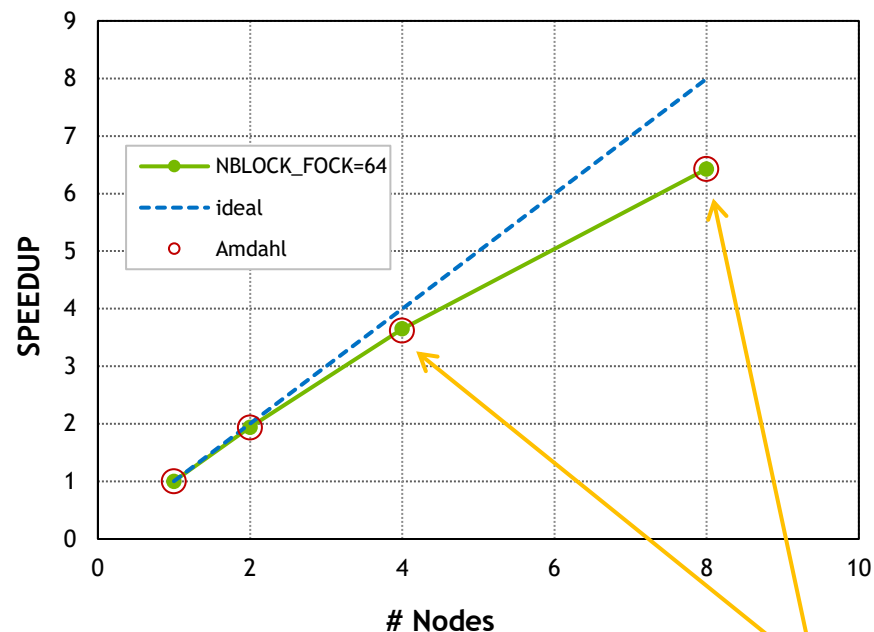
- Existing acceleration in VASP 6
- **New acceleration**
- Acceleration work in progress
- [On acceleration roadmap](#)

# VASP - 6.2.0

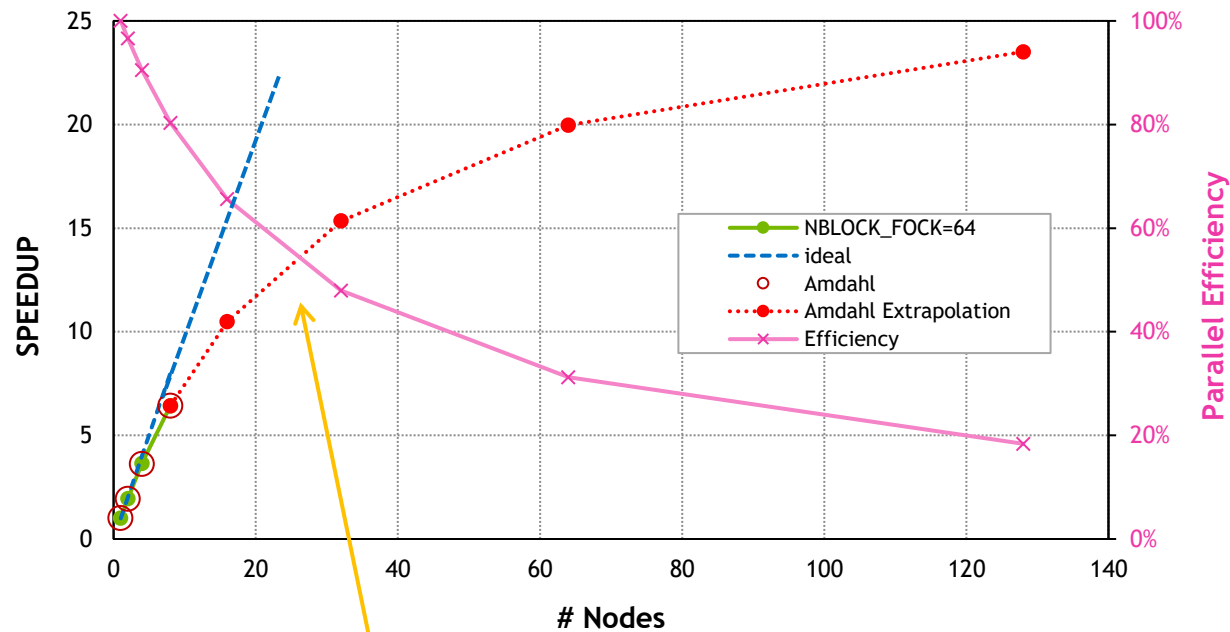
CPU-only: 2xEPYC 7742 GPUs: A100-SXM4-80GB with HPC SDK 21.2 and CUDA 11.0



# VASP strong-scaling hybrid DFT



With an Amdahl's law numerical fit the approximation is quite good



50% Scaling efficiency occurs at 30 nodes in this example

Dataset: Si256\_VJT\_HSE06

Hardware: DGX1 (8xV100 GPUs per node) connected with HDR Infiniband

# VASP Recommended Configuration

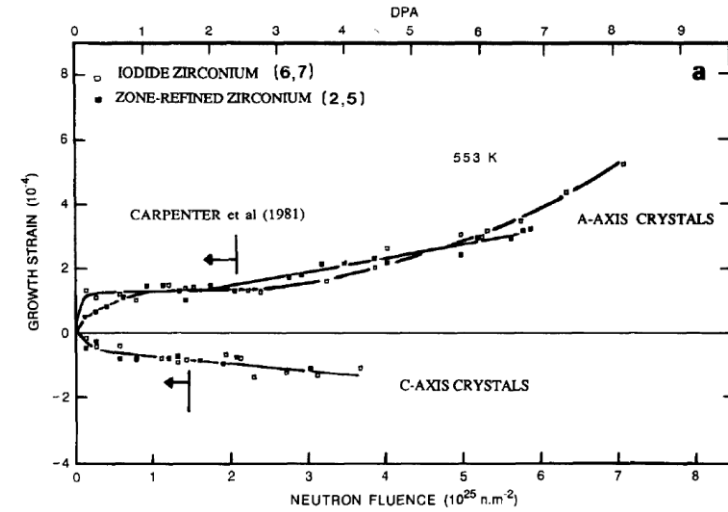
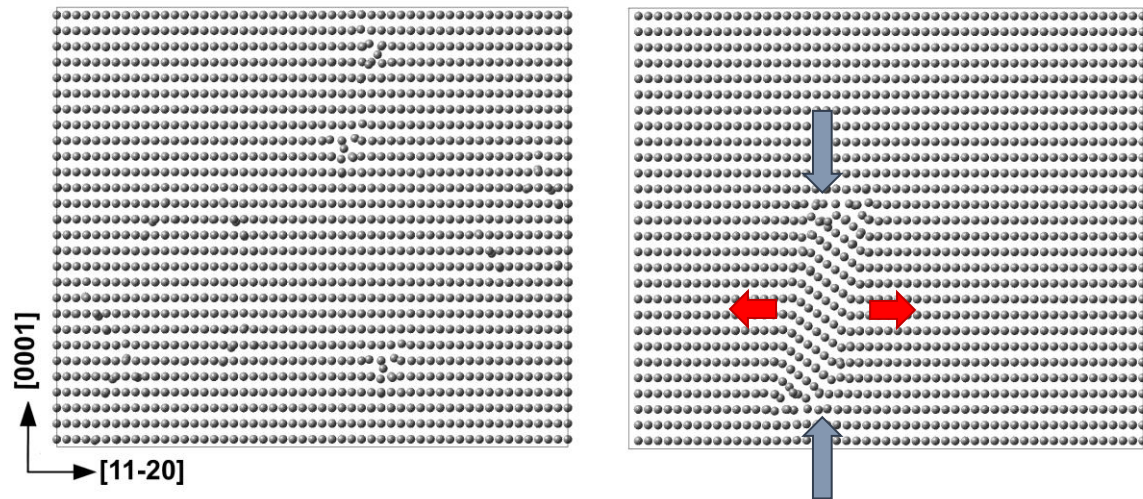
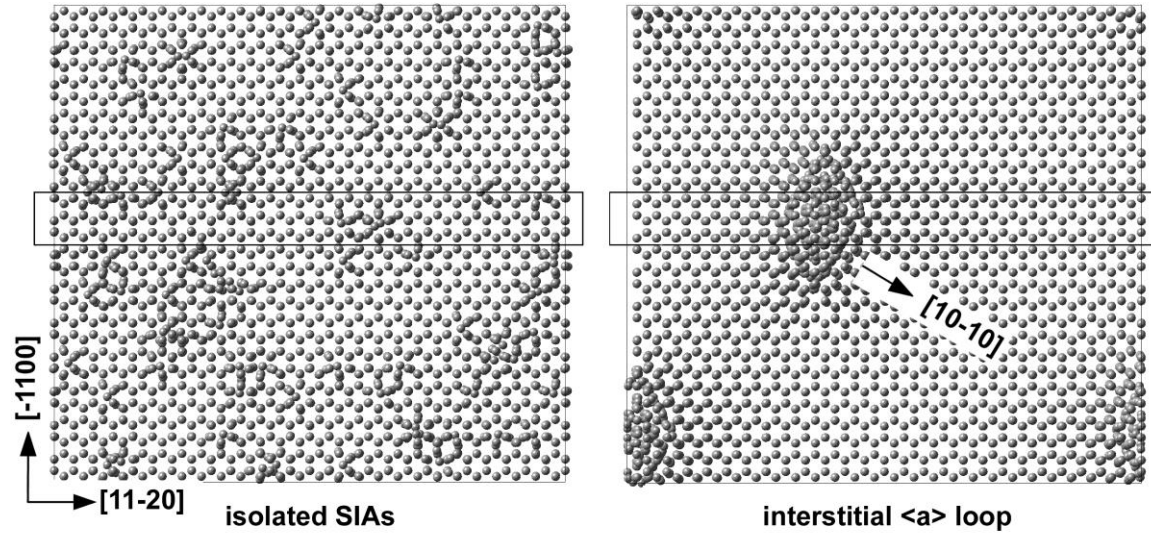
<b>Motherboard and CPU</b>	Any CPU
<b>System memory</b>	$\geq 128$ GB
<b>GPUs</b>	A30 and A100 (NVLink preferred)
<b>GPUs per socket</b>	1 to 8 (dense nodes preferred)
<b>GPUs per job</b>	All
<b>Multi-node</b>	Yes - Mellanox Infiniband

# Advanced Materials for Nuclear Power

- ▶ The Challenge: increase the life-time of materials in the reactor while maintaining their safe operation
- ▶ Approach
  - Use materials modeling to identify the key degradation mechanisms under irradiation
  - Develop a predictive computational approach
  - Predict the performance of improved and new materials prior to experimental testing which is expensive and time consuming
- ▶ The bottleneck
  - Highly accurate multi-scale models
  - 3D simulations require large-scale simulations
- ▶ The solution
  - HPC enables simulations of high complexity and accuracy with predictive power, thus accelerating the development and certification of advanced materials.



# Simulation of Materials for Nuclear Power Plants

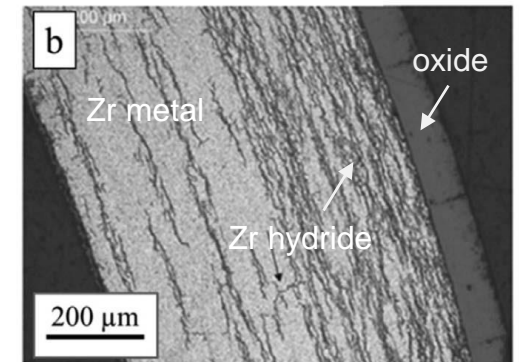
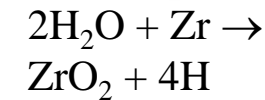


- ▶ Under irradiation, zirconium alloys deform anisotropically
- ▶ Molecular dynamics simulations provide atomistic understanding of the underlying atomic-scale phenomena



# Corrosion of Zirconium Alloys

- ▶ Hot water and irradiation in the reactor cause oxidation of the zirconium cladding and hydrogen pickup. Both phenomena reduce the life-time of the alloy.
- ▶ The Challenge: reduce the rate of corrosion and hydrogen pickup
- ▶ Approach
  - Use materials modeling to identify the oxidation mechanisms and the effect of alloying elements such as Sn, Fe, Cr, Ni, and Nb.
- ▶ The bottleneck
  - Large-scale quantum mechanical calculations are needed for a large variety of systems, e.g., water/oxide interfaces, vacancies, surfaces, interfaces, second-phase particles Zr(Fe,Cr) for a large number of conditions
- ▶ The solution
  - HPC enables simulations of high complexity and accuracy with predictive power, thus creating a large and consistent set of critical materials properties, e.g. elastic coefficients, diffusion barriers, surface energies, serving as input into meso-scale models



*A.T. Motta et al. / Journal of Nuclear Materials 518 (2019) 440–460*

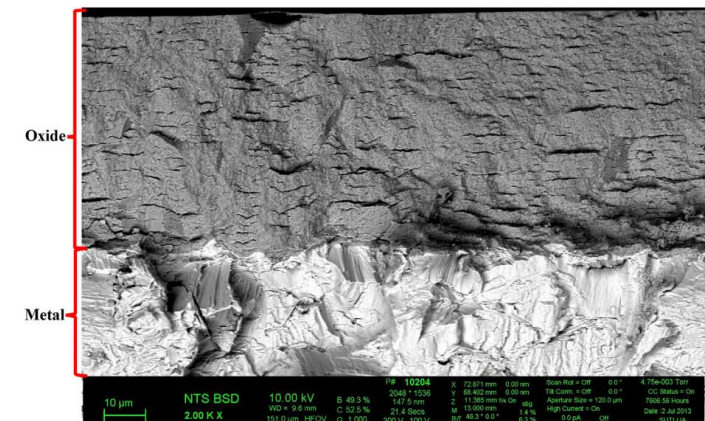
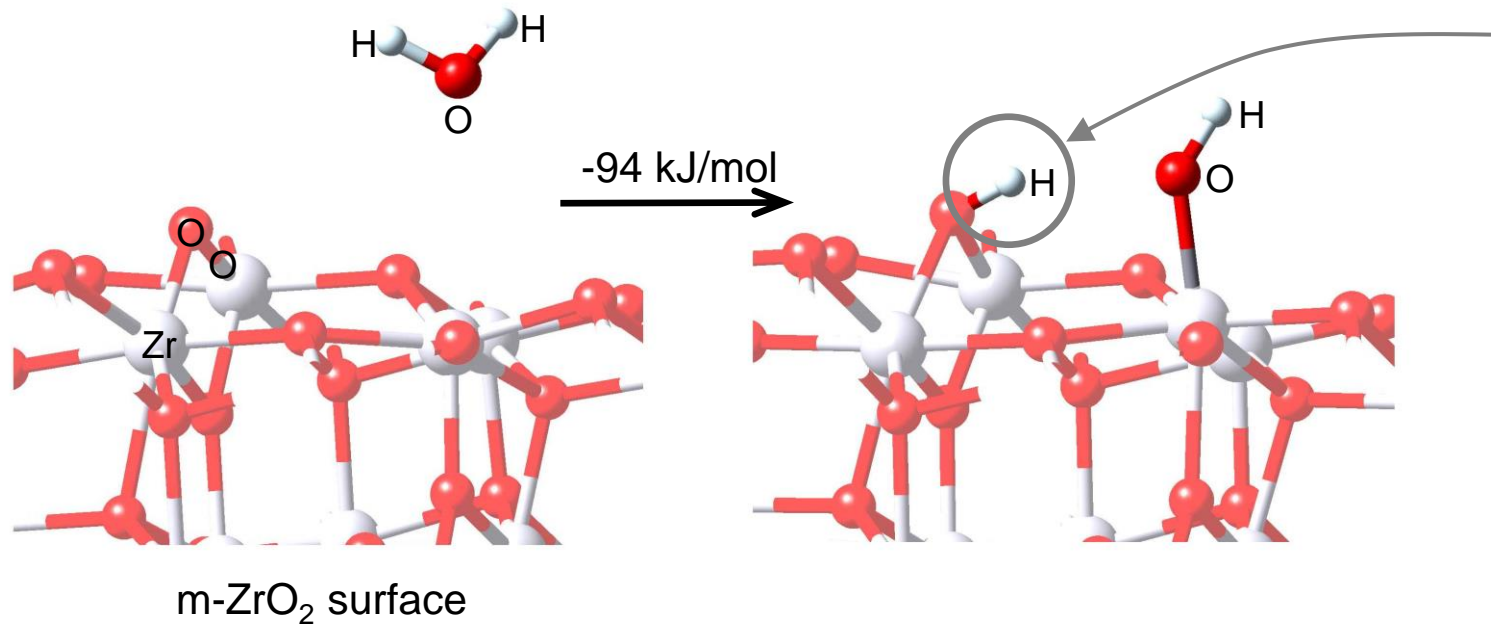


Fig. 15. SEM image of a fatigue fractured Zircaloy-4360 °C autoclave corrosion coupon 100032, 779 wt ppm H.

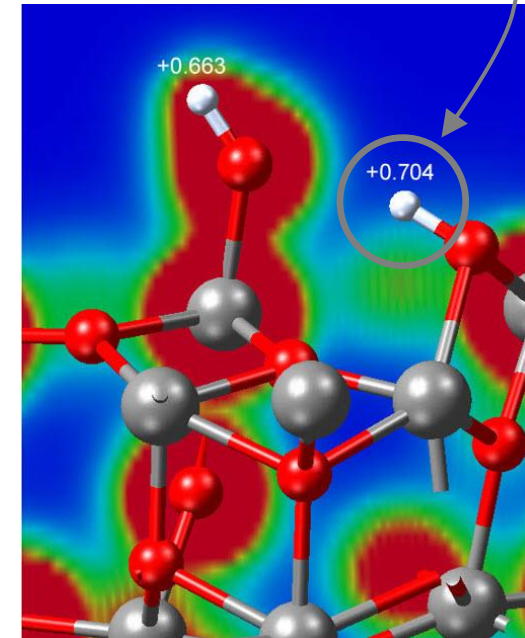


# Zr Corrosion



Water molecules dissociate on monoclinic ZrO<sub>2</sub>(1-1-1) surfaces releasing 94 kJ/mol, similar to dissociation on tetragonal ZrO<sub>2</sub>(001) surfaces (102 kJ/mol).

These H atoms are positively charged and can migrate to the metal/oxide interface by “proton hopping” or by diffusion through the oxide.



# Zr Corrosion - Video



# GPU accelerated features in LAMMPS

LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) is an open-source molecular dynamics simulation application for materials modeling both solid-state and soft matter. It also supports coarse grained simulations for larger particles. Development is funded by DOE and the primary developers are at Sandia National Laboratory, though it benefits from a rich community engagement.

Many features in LAMMPS are accelerated on NVIDIA GPUs using [Kokkos](#) with strong performance.

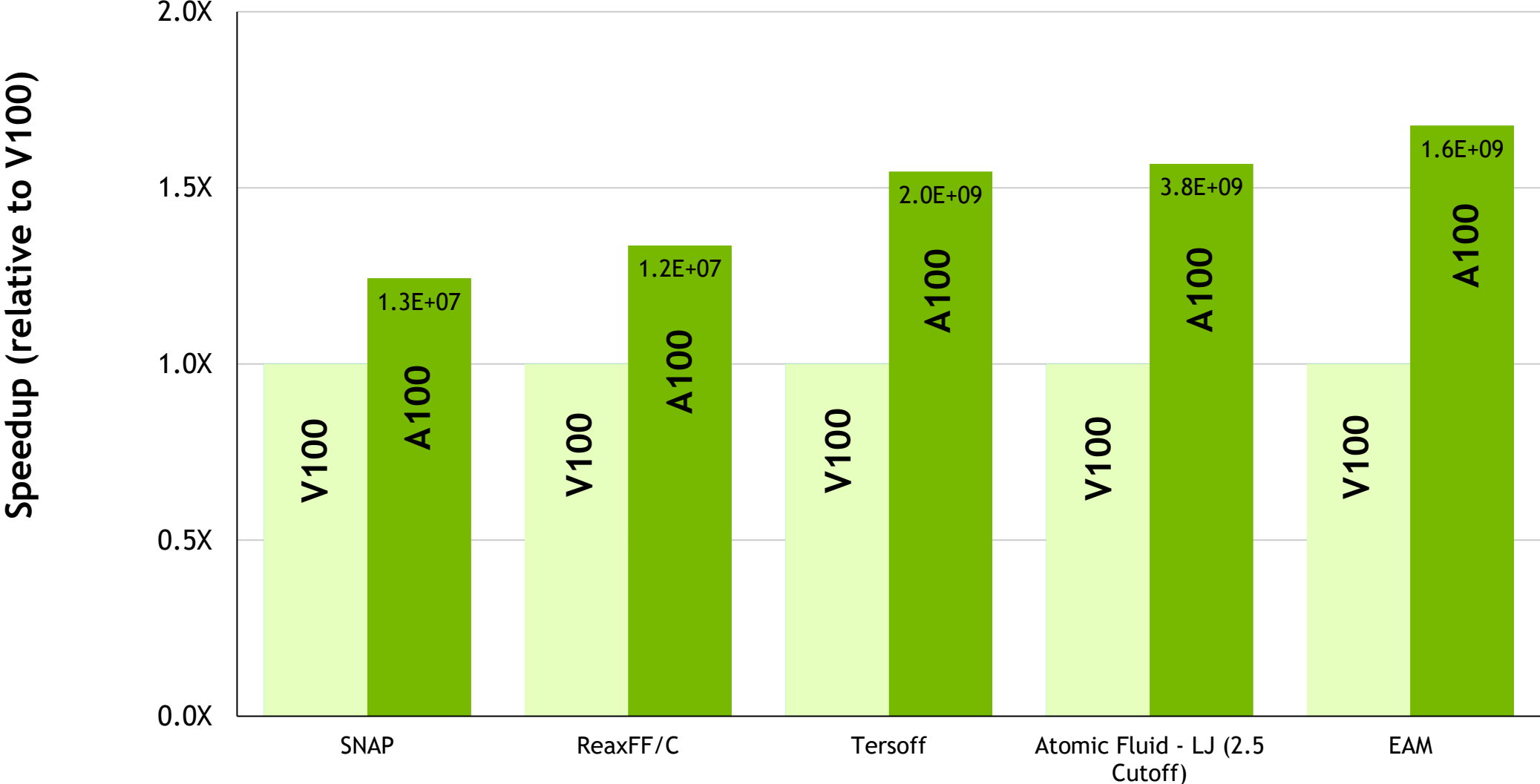
This includes many common “[interatomic potentials](#)” such as:

- Pairwise potentials: Lennard-Jones
- Many-body potentials: EAM, Tersoff, ReaxFF
- Machine learning potentials: SNAP
- Long-range interactions: PPPM for Ewald / particle mesh Ewald
- Compatibility with force fields from CHARMM, AMBER, GROMACS, COMPASS, pcff+

NVIDIA GPU performance is always improving due to a partnership between LAMMPS developers and NVIDIA Devtech organization. Each release has additional enhancements – so keep a look out for these updates.

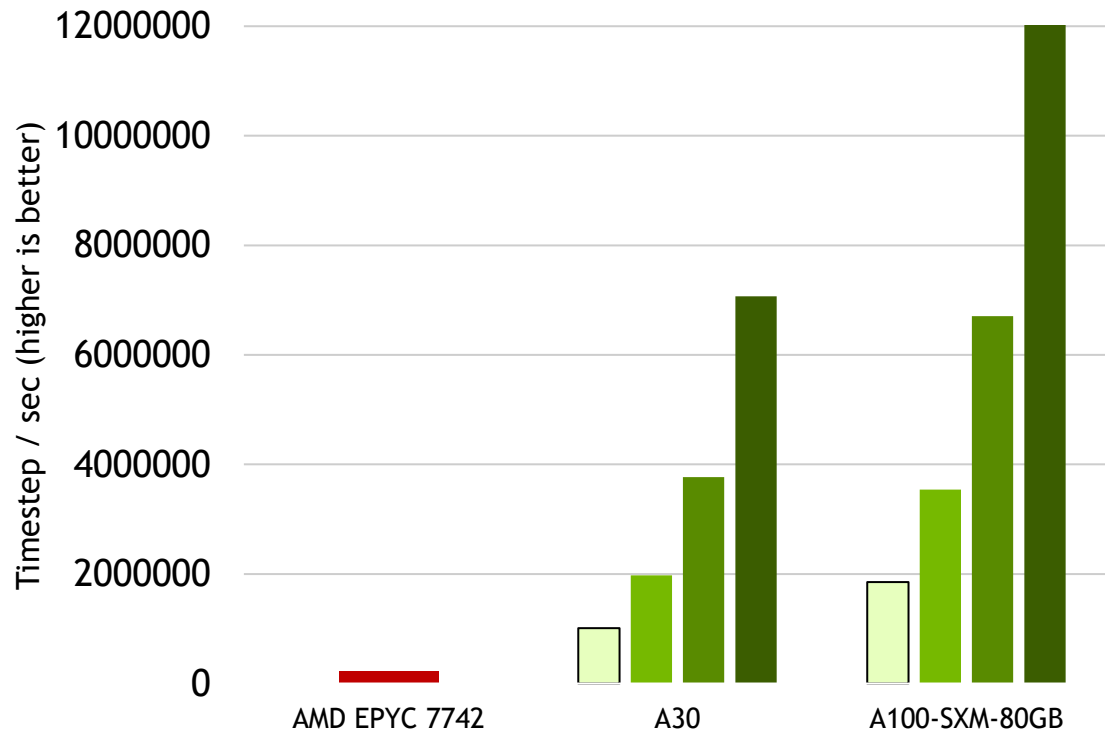
# LAMMPS SPEEDUP OVER GPU GENERATIONS

LAMMPS - Speed up from V100 to A100 - 8X GPU scaling



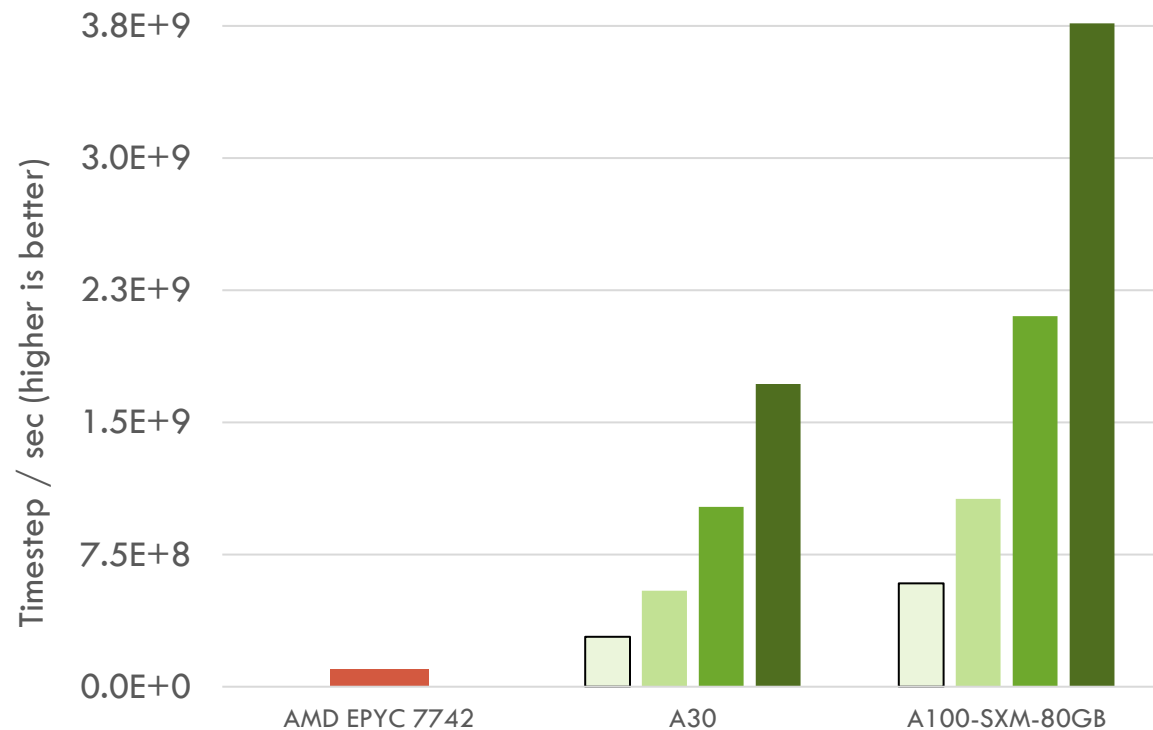
# LAMMPS GPU COMPARISON

LAMMPS patch\_10Feb2021  
Dataset: SNAP



Number of GPUs  
□ 1 ■ 2 ■ 4 ■ 8 ■ 0

LAMMPS patch\_10Feb2021  
Dataset: Atomic Fluid Lennard-Jones 2.5 cutoff

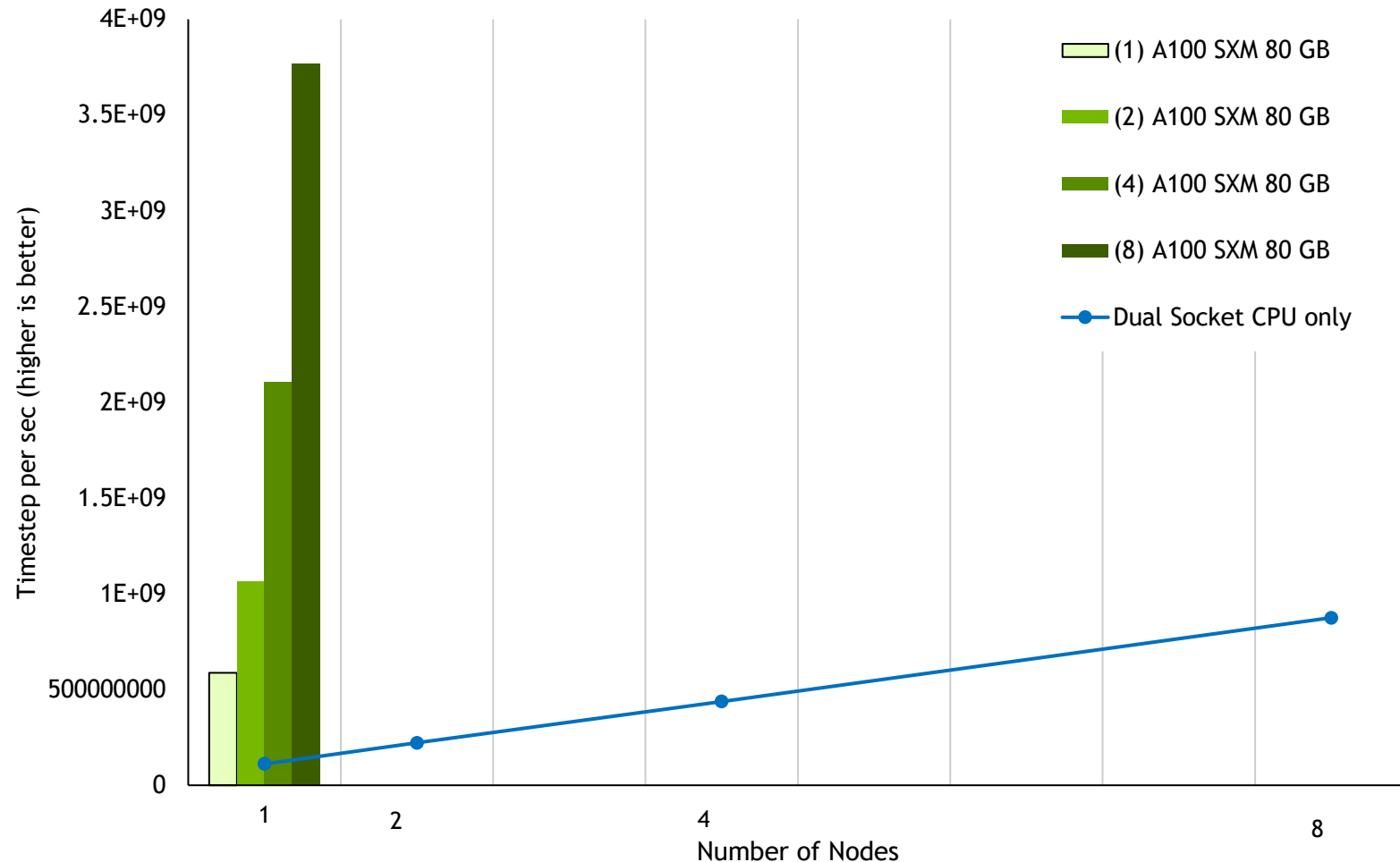


Number of GPUs  
□ 1 ■ 2 ■ 4 ■ 8 ■ 0

# LAMMPS PERFORMANCE COMPARISONS

## MULTI-NODE CPU VS. SINGLE NODE MULTI-GPU

LAMMPS patch\_10Feb2021  
Dataset: Atomic Fluid Lennard-Jones 2.5 cutoff



Assuming perfect scaling  
CPU Only **requires 34 nodes**  
to reach the performance  
of one 8 GPU A100 node

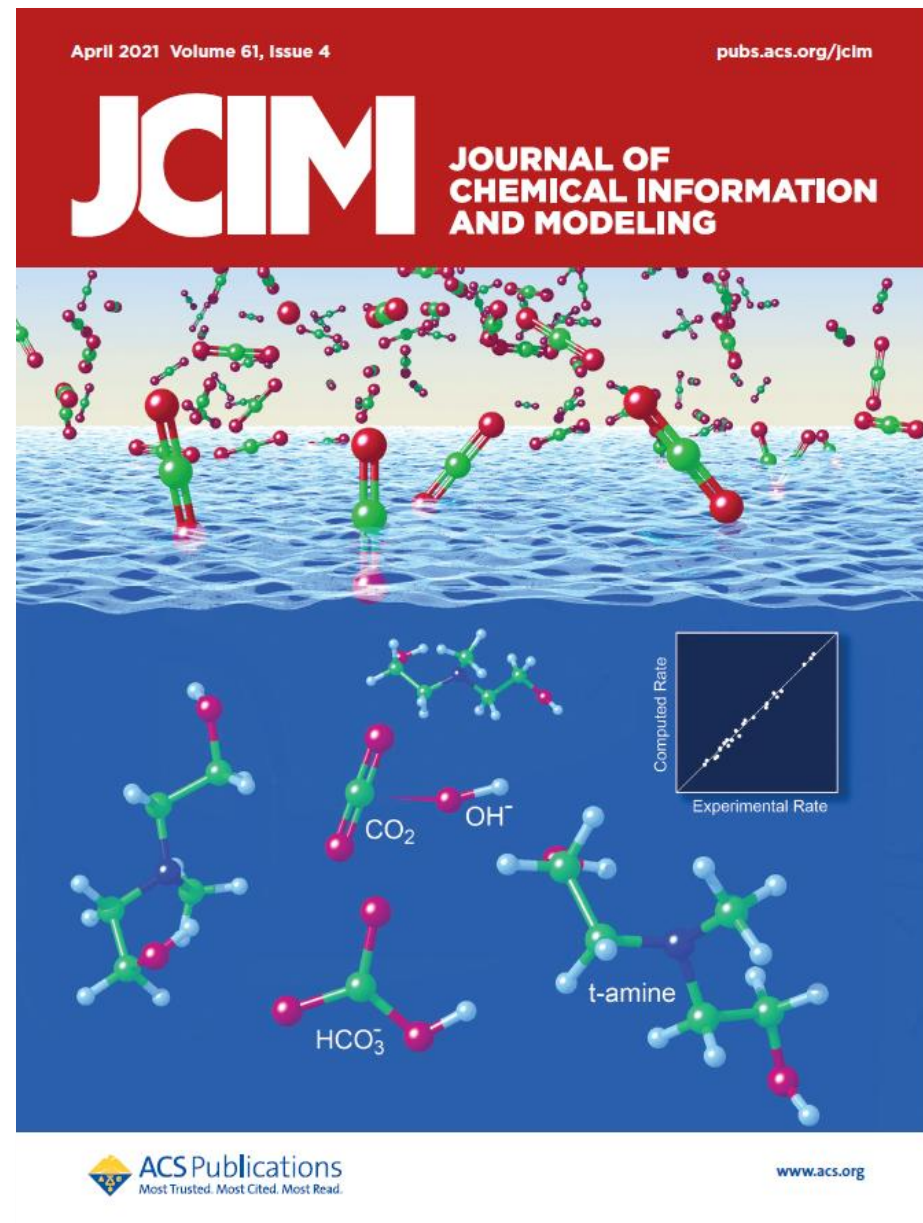
# LAMMPS Recommended Configuration

<b>Motherboard and CPU</b>	Dual-socket CPU
<b>System memory</b>	$\geq 150\text{GB}$
<b>GPUs</b>	A30 and A100
<b>GPUs per socket</b>	1 to 8
<b>GPUs per job</b>	All
<b>Multi-node</b>	Yes - Mellanox Infiniband

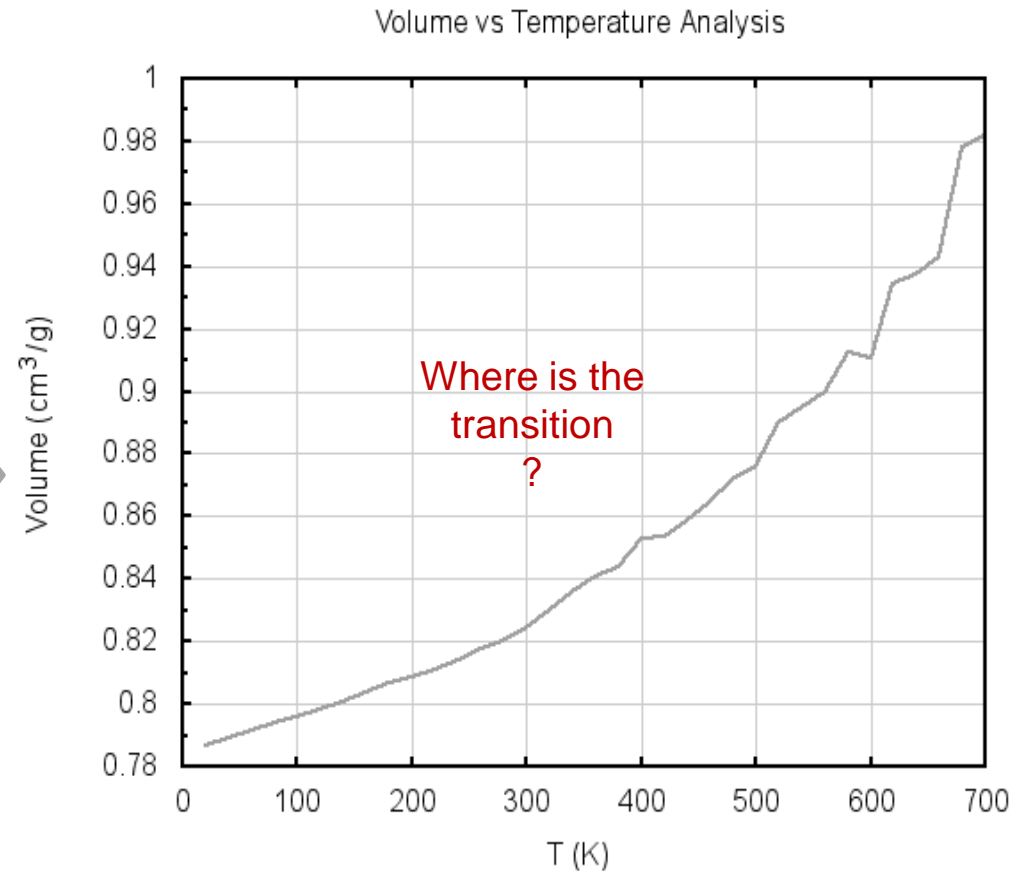
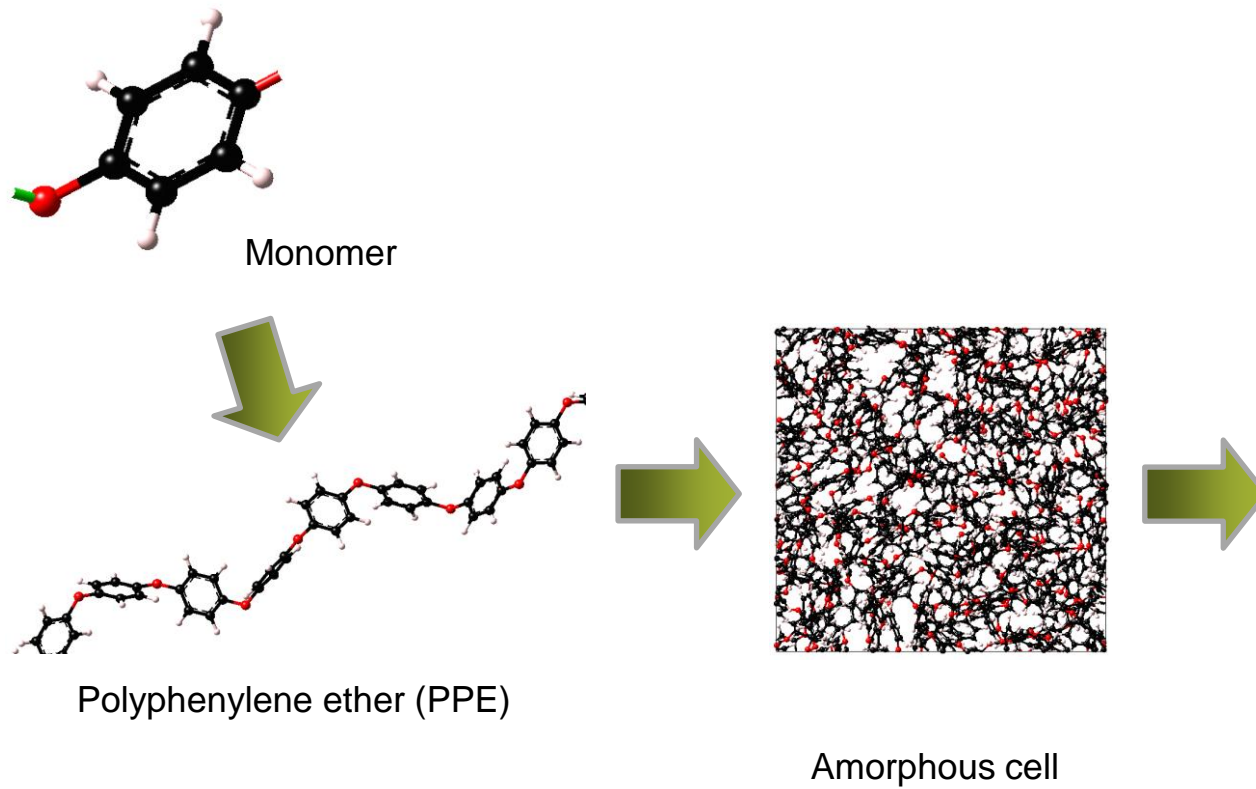
# More Efficient CO<sub>2</sub> Capture

- ▶ The Challenge: improve the efficiency and flexibility of existing chemical processes
- ▶ Approach
  - Use molecular modeling to find the key chemical reaction mechanisms
  - Develop a predictive computational approach
  - Predict the performance of new molecules prior to their synthesis and experimental testing
- ▶ The bottleneck
  - Highly accurate models require large-scale molecular dynamics simulations (evaluate several thousands of interatomic interactions in each of 100 million molecular dynamics steps)
- ▶ The solution
  - HPC enables faster screening of potential candidates, thus gaining time and a competitive advantage

Work performed in collaboration with the energy company TOTAL and published: "Quantitative Kinetic Model of CO<sub>2</sub> Absorption in Aqueous Tertiary Amine Solvents", X. Rozanska, E. Wimmer, and Frédéric de Meyer, J. Chem. Inf. Model. **61**, 1814-1824 (2021)



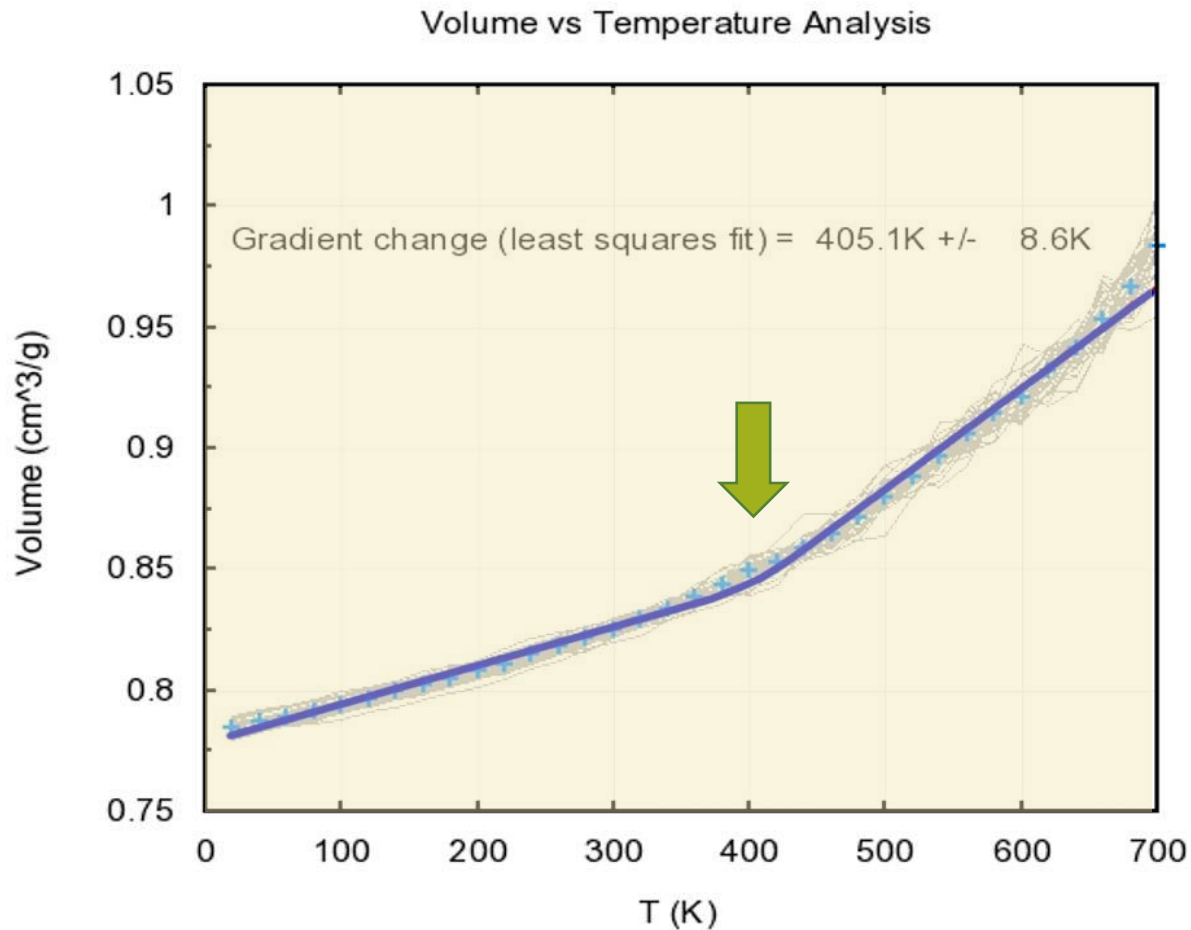
# Polymers: Glass Transition Temperature



NPT Molecular dynamics

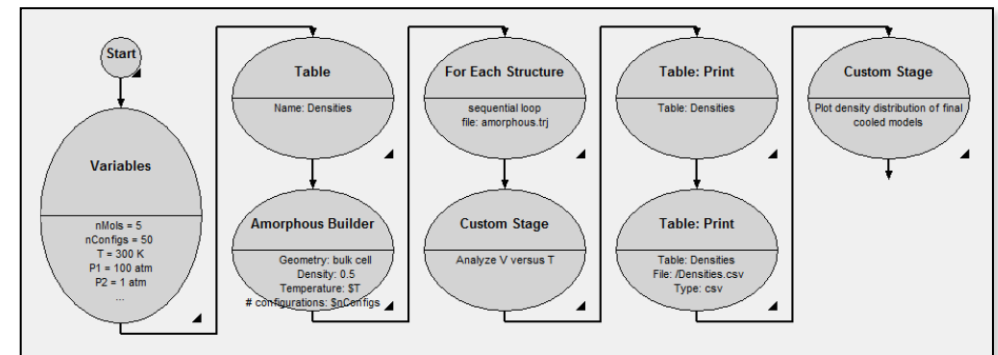


# High-Throughput: More is Different



Value of high throughput calculations:

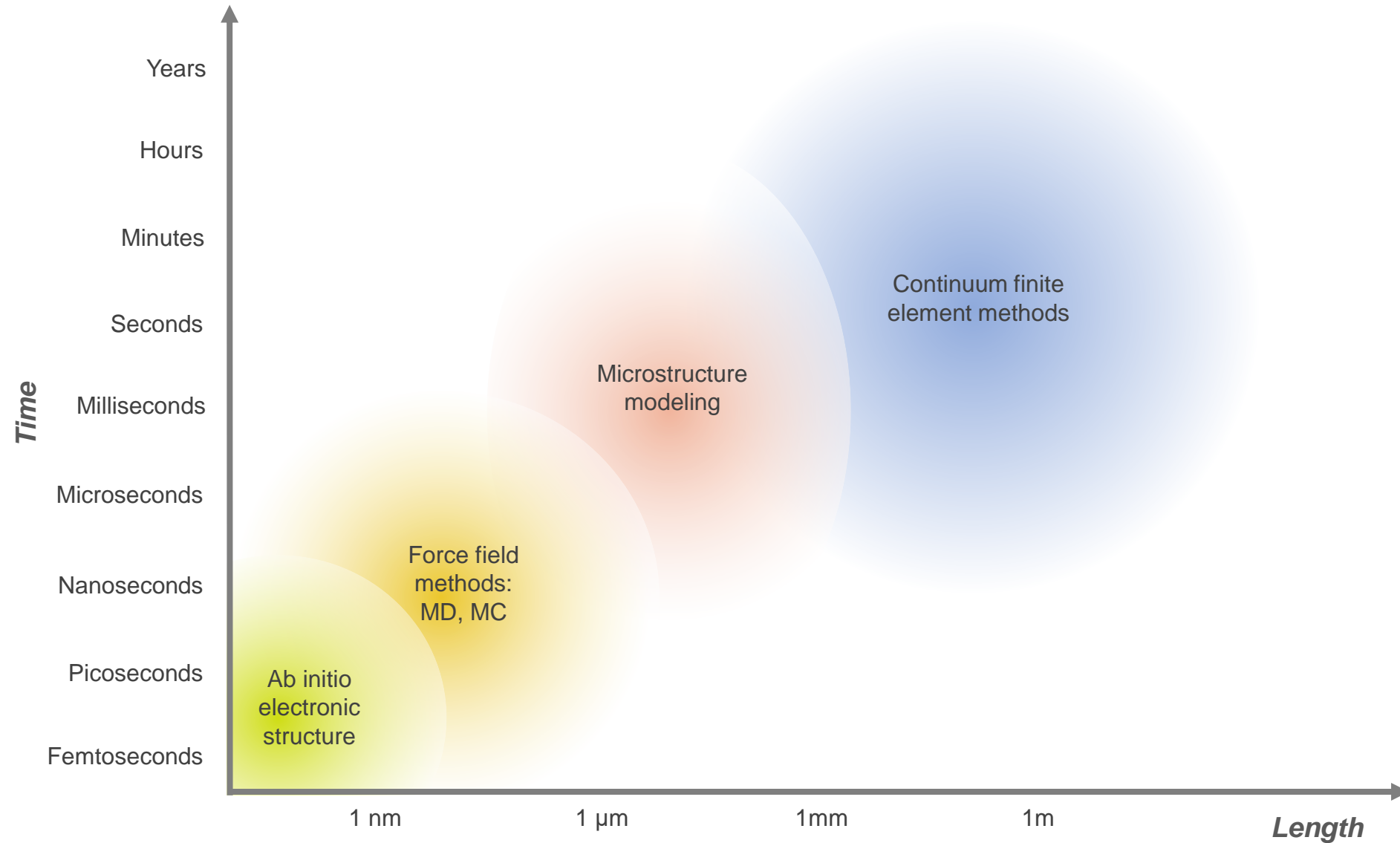
- ▶ Clear signal from noisy simulation data
- ▶ Variability in individual  $V$  vs.  $T$  curves (gray lines)
- ▶ Fit yields properties for the simulated system
- ▶ Automatic procedure: single high throughput flowchart



MedeA Flowchart



# Multiscale Simulations in Need of HPC



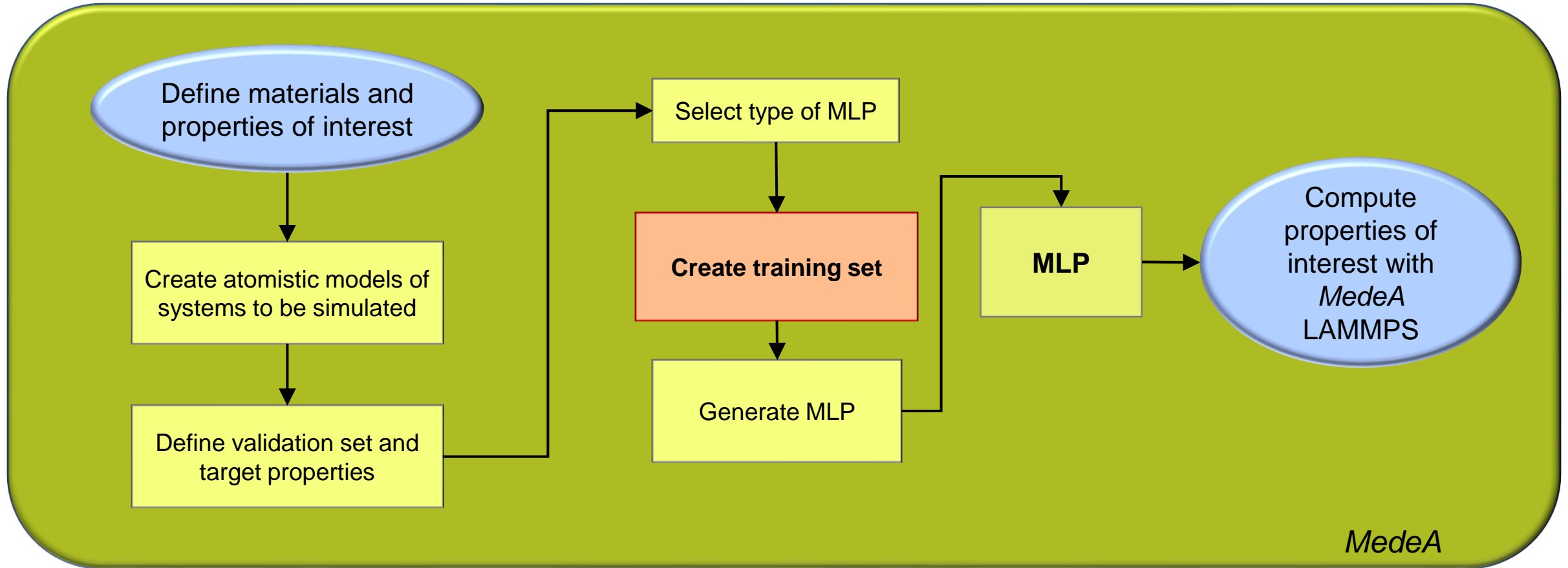
# Multiscale Simulations in Need of HPC

- ▶ Machine learning potentials (MLPs):
  - Ab initio accuracy
  - Speed of forcefield methods
  - Scales linearly with system size
- ▶ Need to generate potentials for each class of systems
- ▶ Bottleneck: generation of ab initio training sets
- ▶ Solution: HPC + Artificial Intelligence



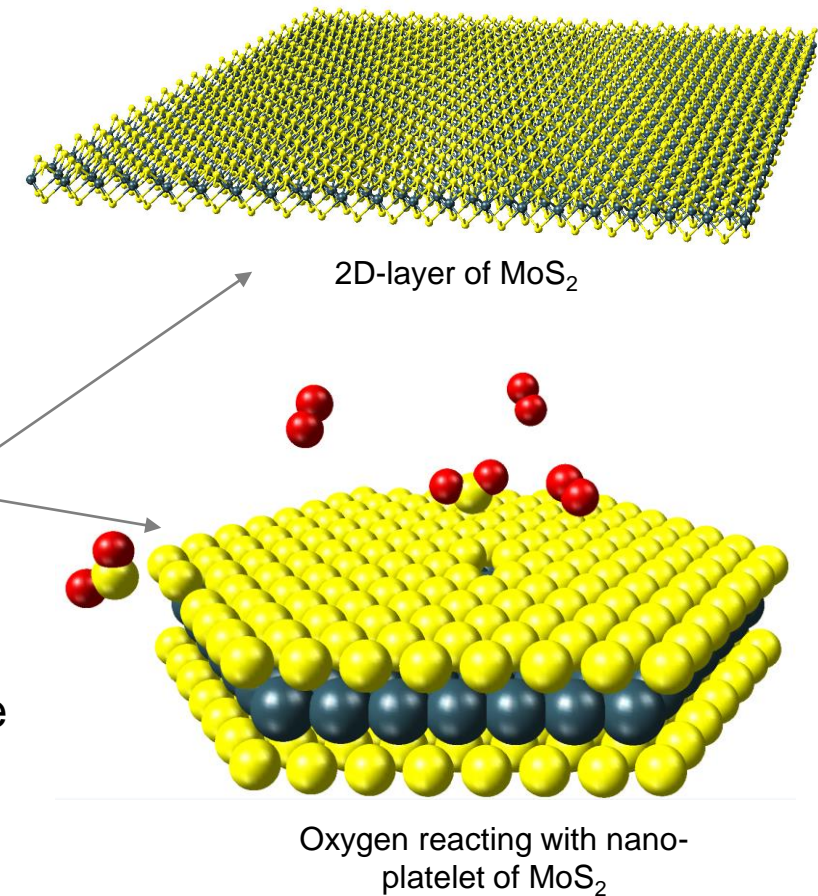
# MedeA MLP Generator

## Workflow

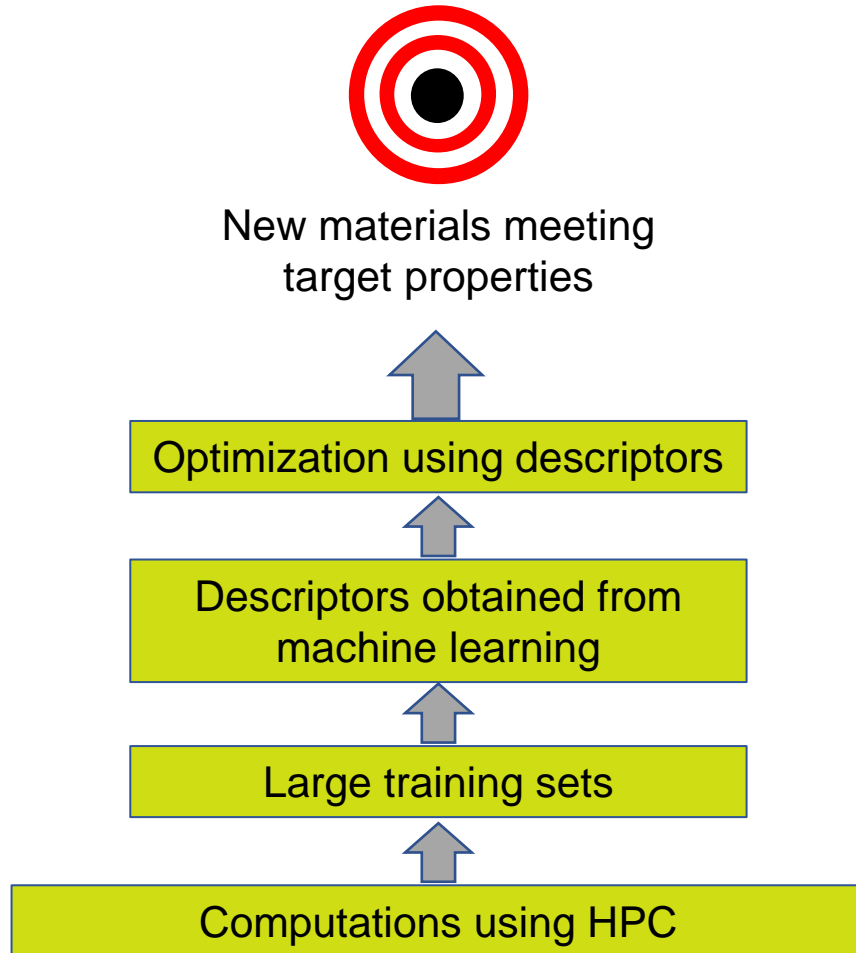


# Example of Generating Machine Learning Potentials

- ▶ System: MoS<sub>2</sub> layer with defects
- ▶ Property of interest: thermal vibrations, thermal conductivity
- ▶ Modeling steps:
  - Build models of: MoS<sub>2</sub> layer without and with defects including O<sub>2</sub> and SO<sub>2</sub> molecules
  - Create training set using *MedeA VASP* and store results in structure list
  - Create machine learning potential using *MedeA MLP Generator*
  - Use the new MLP to perform simulations with *MedeA LAMMPS*
- ▶ Time limiting steps:
  - Generation of training set with VASP
  - Large-scale molecular dynamics simulations with VASP – machine learning potentials are between one and two orders of magnitude more compute intensive than classical interatomic potentials.



# Machine Learning in Materials R&D



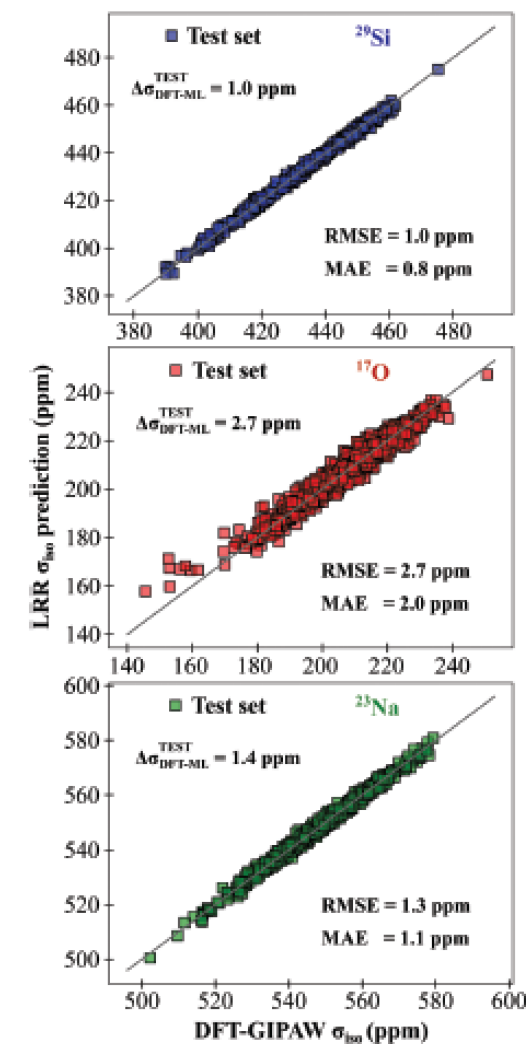
- ▶ The success of machine learning in materials science depends on the availability of extensive and consistent training sets connecting structure and properties.
- ▶ HPC with accurate and efficient approaches enables the creation of such training sets.



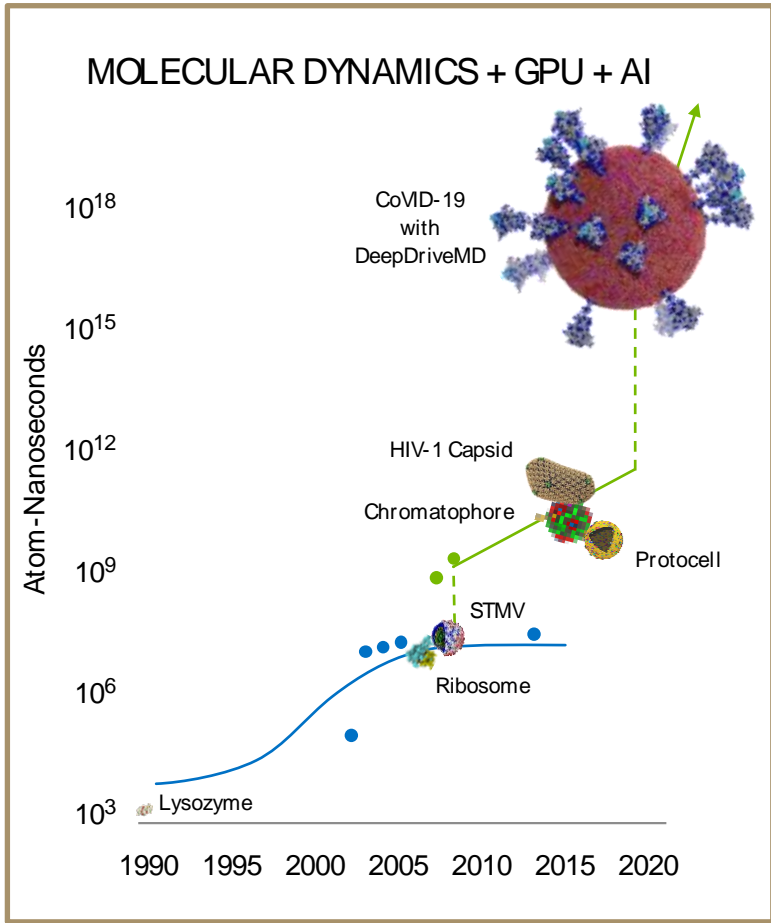
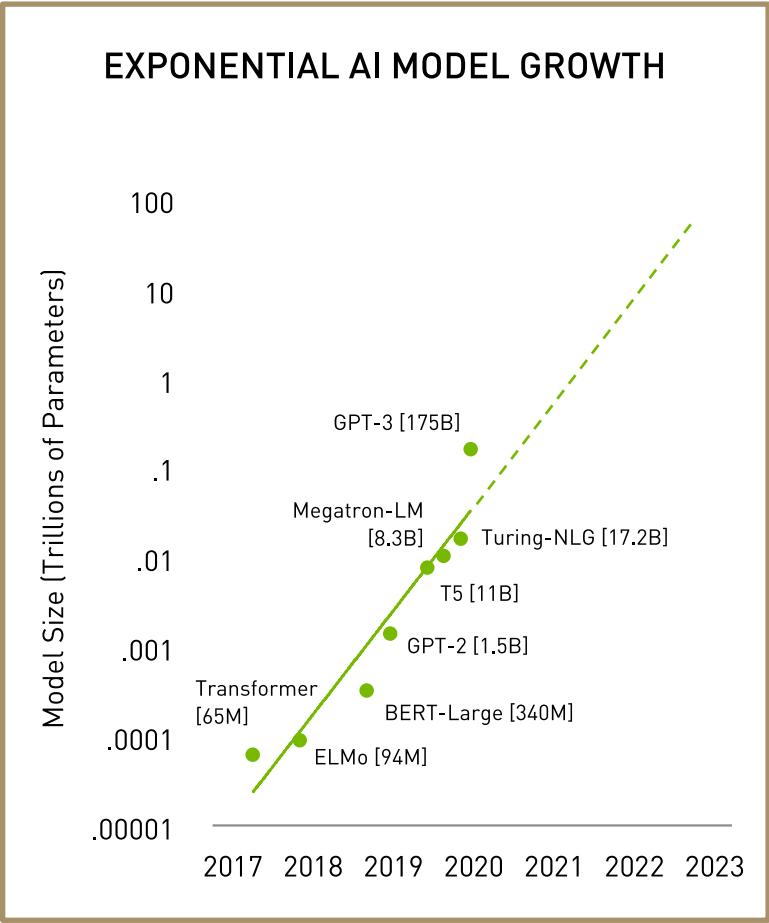
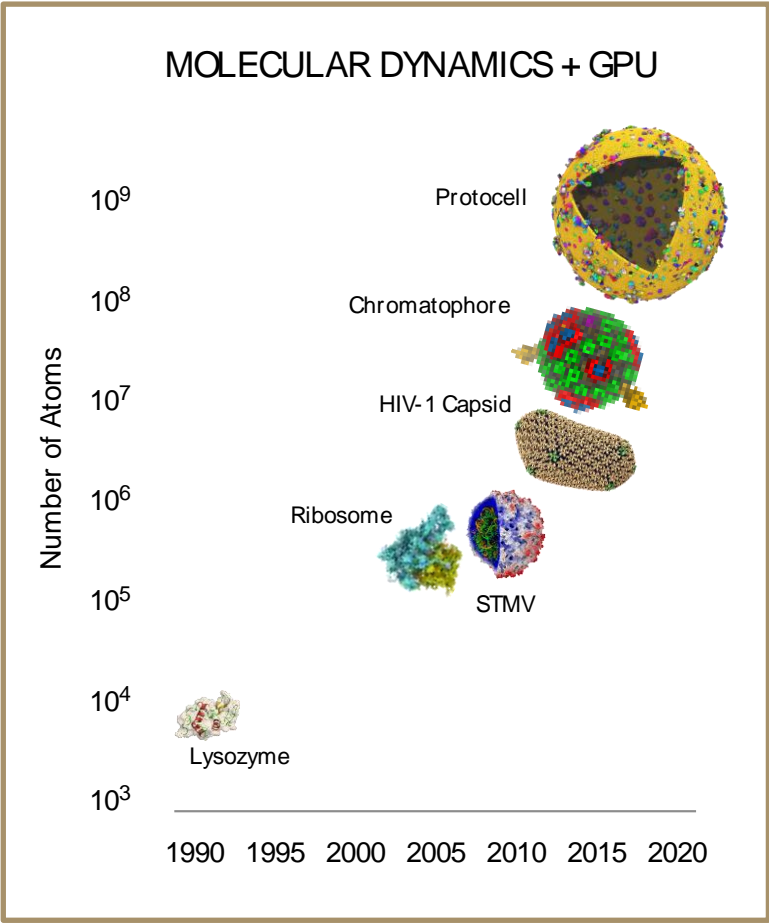
# Machine Learning in Materials R&D: NMR Predictions

- ▶ Objective: Rapid prediction of structural properties of glasses from solid-state nuclear magnetic resonance experiments
- ▶ Approach:
  - Use correlation between NMR shifts and structure
  - Obtain correlation using ML techniques
  - Train on ab initio calculations of NMR shifts using VASP
- ▶ Bottleneck: Highly accurate VASP calculations on large number of systems with many atoms
- ▶ Solution: Use VASP in HPC environment with GPUs

Z. Chaker, M. Salanne, J.-M. Delaye, and T. Charpentier, NMR shifts in aluminosilicate glasses via machine learning, Phys. Chem. Chem. Phys. **21**, 21709 (2019)



# INDUSTRIAL HPC AT THE TIPPING POINT



# Take-Home Messages

- ▶ Mankind is facing unprecedented global challenges.
- ▶ The combination of the fundamental theory of physics and chemistry, sophisticated software, and high-performance computing provide unprecedented capabilities helping to meet these challenges.
- ▶ Increasingly, industrial R&D will rely on accurate, large-scale simulations
- ▶ Illustrative examples are:
  - Improvement of the capacity and power density of batteries
  - Enhancing the capacity of generating safe and sustainable, primary energy
  - Improving the processes of CO<sub>2</sub> capture
  - Designing better polymers
  - Machine learning in materials science
- ▶ Multi-scale simulations using machine learning techniques require HPC+AI.
- ▶ The future of computational materials science with HPC+AI is bright and exciting.



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