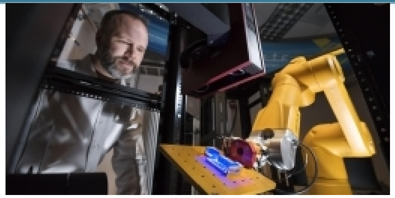
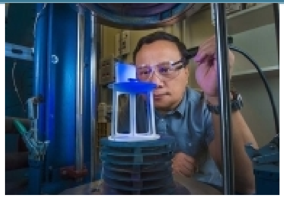
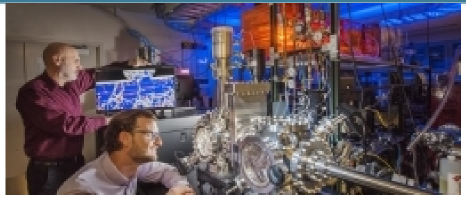
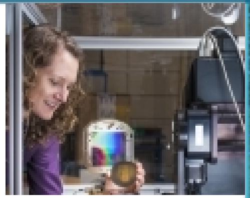
SAND2024-02084C

Sandia National Laboratories

Materials Innovation: Making the Future Possible

MATERIALS SCIENCE & ENGINEERING

David Montes de Oca Zapiain[1]

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U.S. DEPARTMENT OF ENERGY NNSA

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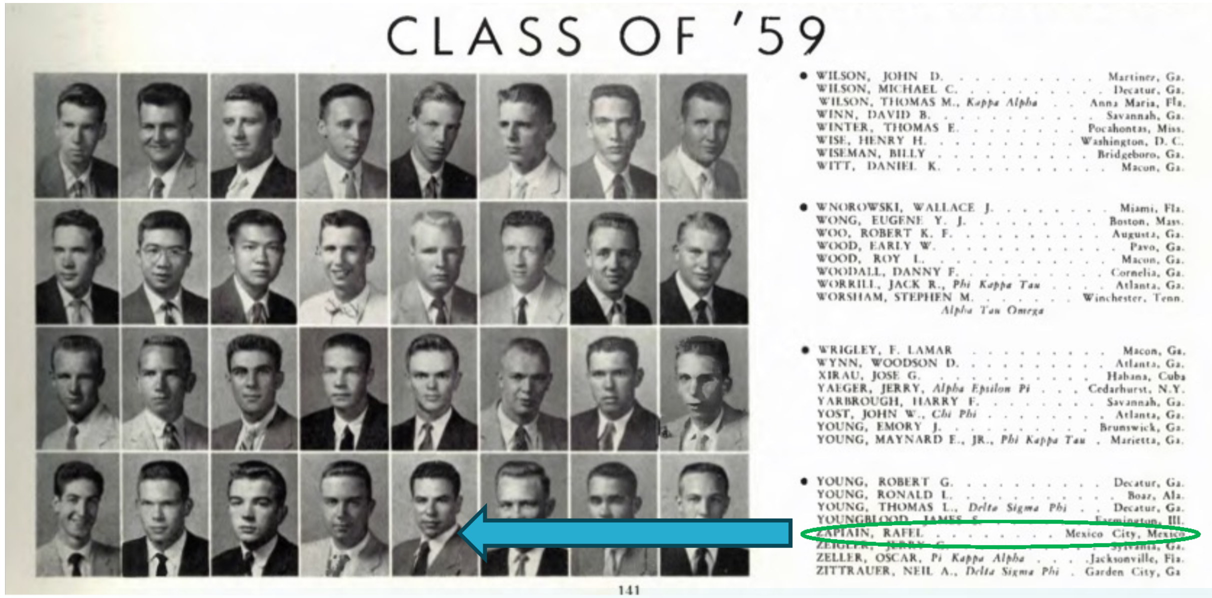
SAND No.

Personal Introduction: Who is David?

Personal Introduction: Rambling Wreck all the Way!



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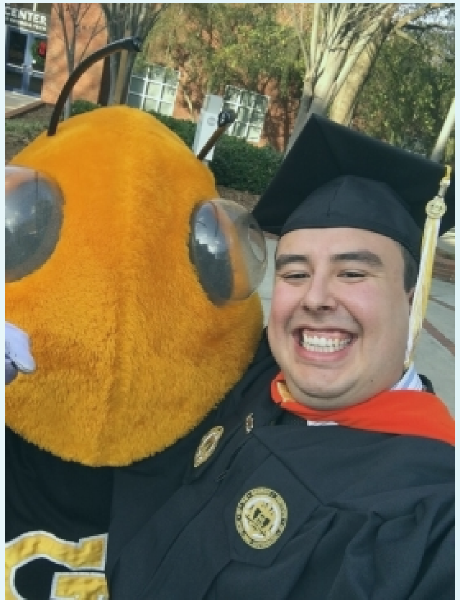
<u>BSME 2014</u>

<u>Ph.D. in ME 2019</u>



<u>MSME 2015</u>

Introduction: What is Innovation?

- The introduction of something new that addresses the most pressing challenges.

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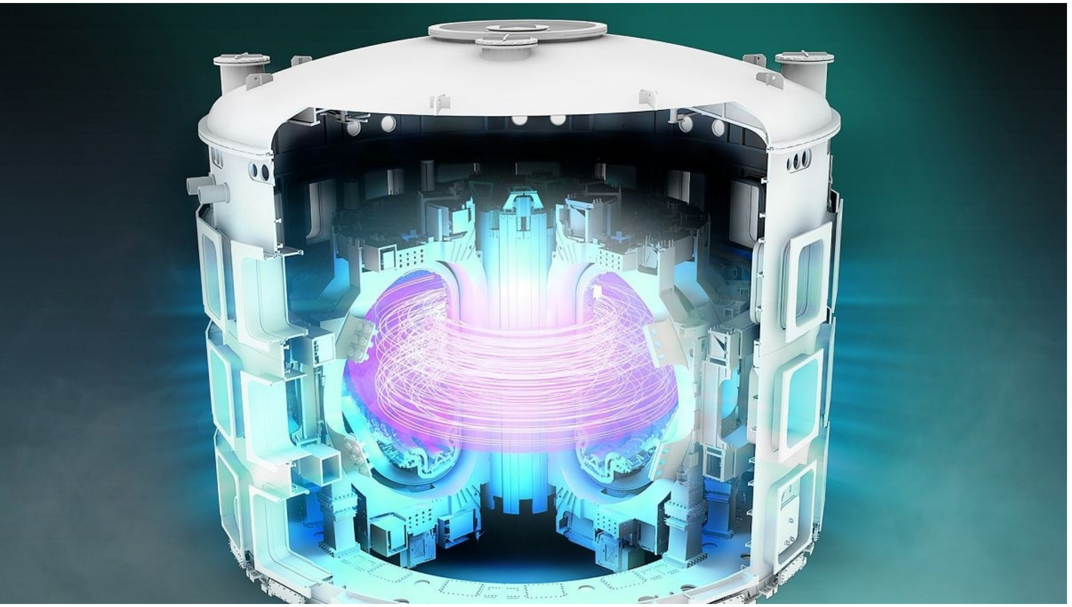
4 international students invent an automatic keg tap that fills a pitcher in 3 seconds. #GTExpo

5:14 PM · Dec 4, 2014

- Solving a tough problem by expanding/adopting skills from many different fields.

[Harvard Business Review (2017), McKinsey & Company (2022)]

Introduction: How does the Future Look Like?



- Design of new materials that can withstand the intense heat from the plasma.

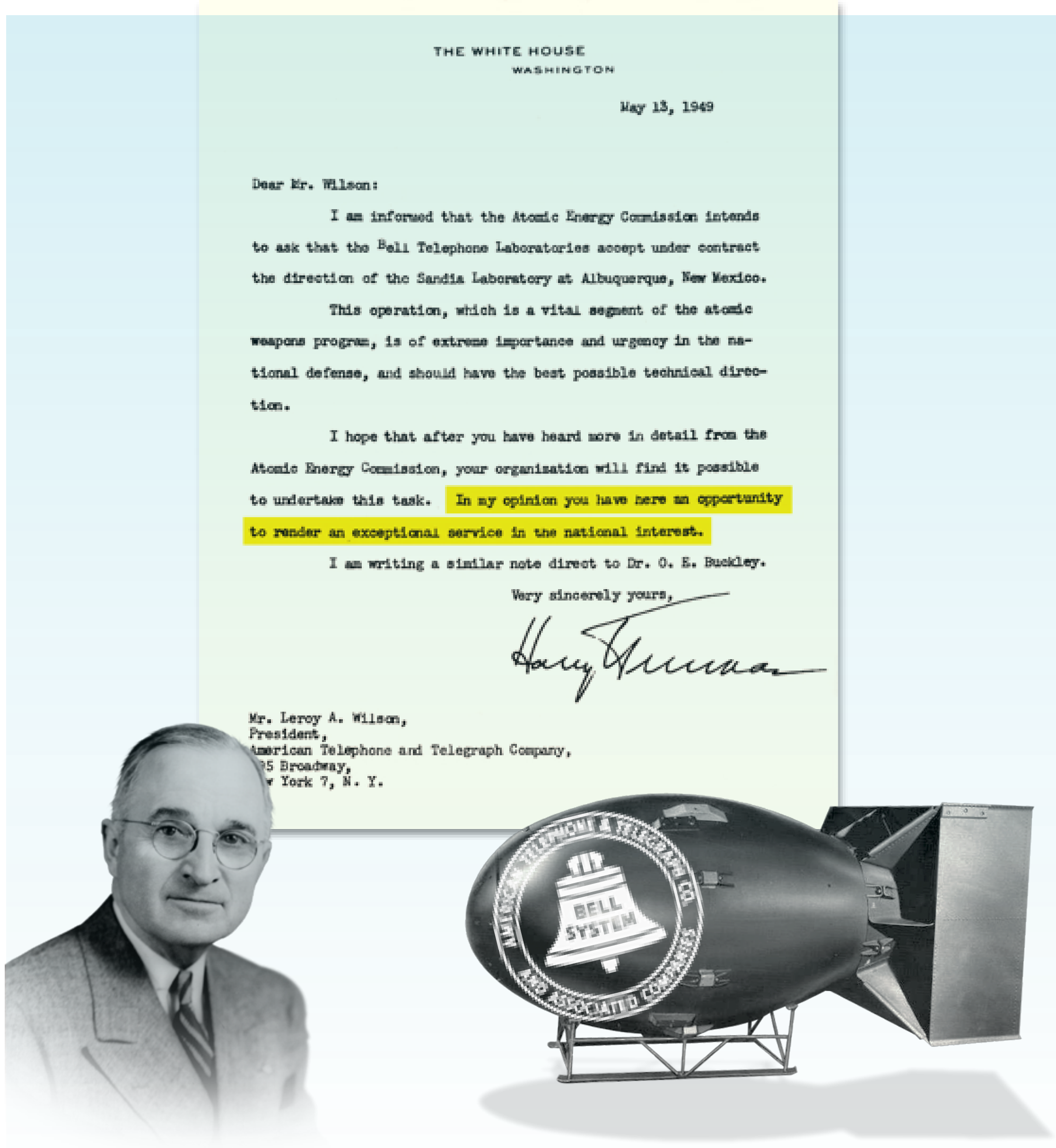
- Ultra-thin optical technologies for next-generation screens and monitors.

- Advanced manufacturing that can process and shape new materials.

Introduction: How are Innovation and Sandia Connected?

Sandia National Laboratories is an Engineering Lab.

- Our origins can be traced to the Manhattan Project and Los Alamos.
- In July 1945, J. Robert Oppenheimer established "Z Division" at Sandia Base to perform stockpile development activities and non-nuclear component engineering.
- Our ethos is: "Exceptional service in the national interest."
- This is the Lab to which the nation (and the world) turn to solve the toughest and most complex engineering challenges.



THE WHITE HOUSE
WASHINGTON

May 13, 1949

Dear Mr. Wilson:

I am informed that the Atomic Energy Commission intends to ask that the Bell Telephone Laboratories accept under contract the direction of the Sandia Laboratory at Albuquerque, New Mexico.

This operation, which is a vital segment of the atomic weapons program, is of extreme importance and urgency in the national defense, and should have the best possible technical direction.

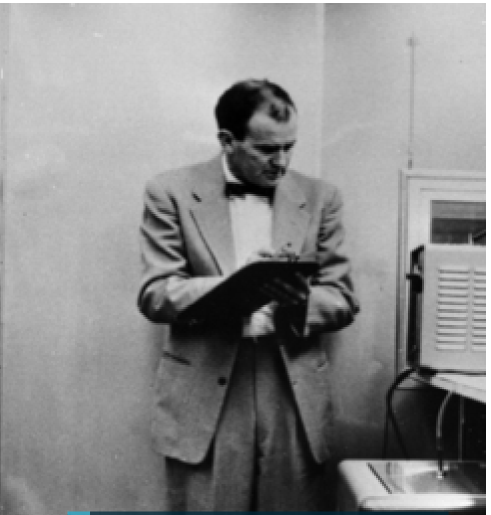
I hope that after you have heard more in detail from the Atomic Energy Commission, your organization will find it possible to undertake this task. In my opinion you have here an opportunity to render an exceptional service in the national interest.

I am writing a similar note direct to Dr. O. E. Buckley.

Very sincerely yours,

Mr. Leroy A. Wilson,
President,
merican Telephone and Telegraph Company,
5 Broadway,
York 7, N. Y.

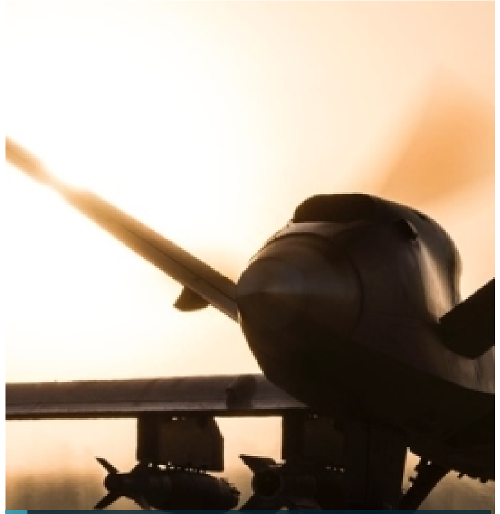
Introduction: Historic Impact of Sandia's Innovations



Sandia pioneered clean room technology to protect the circuitry that controls nuclear weapons.
It went on to be used in hospitals, computers and smartphones.

Sandia's mobile SpinDX diagnostic device can test for viruses, bacteria and active toxins in less than an hour while the microneedles technique extracts interstitial fluid to quickly diagnose major illnesses or measure exposure to chemical or biological agents

Sandia found it was possible to build and operate a high-speed passenger ferry and research vessel powered solely by zero-emission hydrogen fuel cells. **The research led to the first fuel cell vessel built in the U.S. and the world's first commercial fuel cell ferry.**

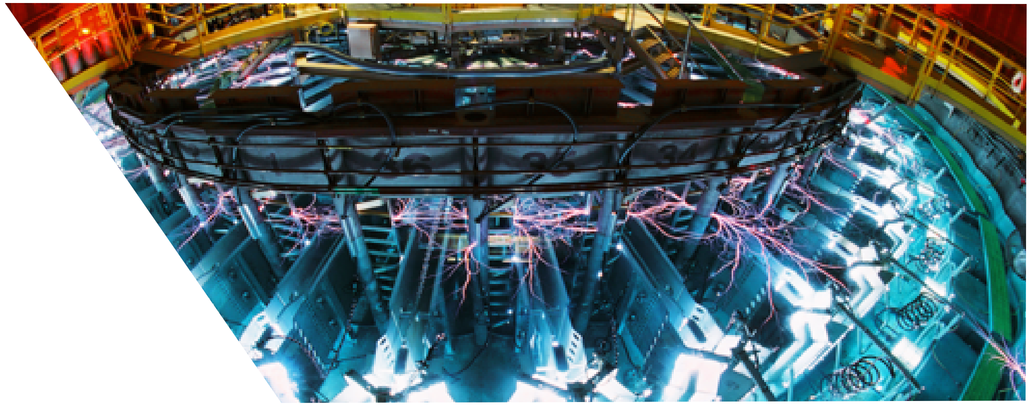


Sandia is a leader in research for Unmanned Aerial Vehicles and associated countermeasures building off our robotics legacy. **Our robotics have been used to reach trapped miners, demilitarize submunitions and disable IEDs.**

An innovative, 27.5-meter wind turbine blade developed by Sandia and industry **produces up to 10 percent more energy** than traditional linear blade designs without increasing wear and tear on the machine

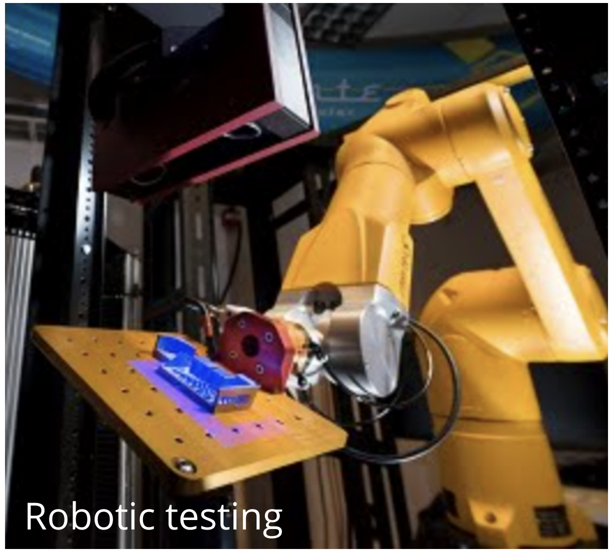
Introduction: How is Innovation Fostered?

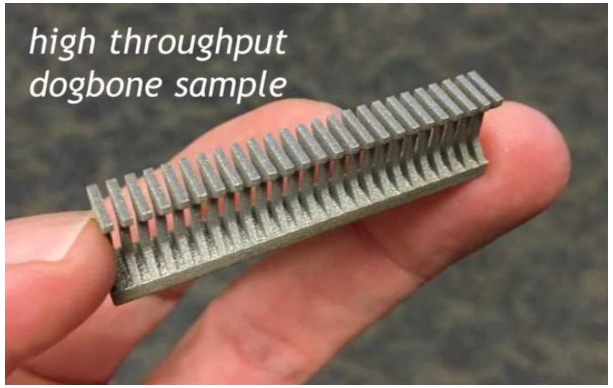
- The Labs **integrate state-of-the-art facilities** with a **highly specialized interdisciplinary technical experts.**

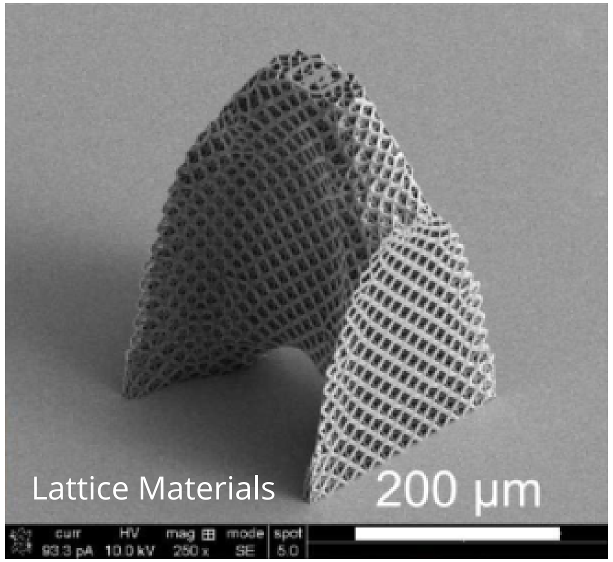


Innovation in Materials: A pathway to Advanced Manufacturing

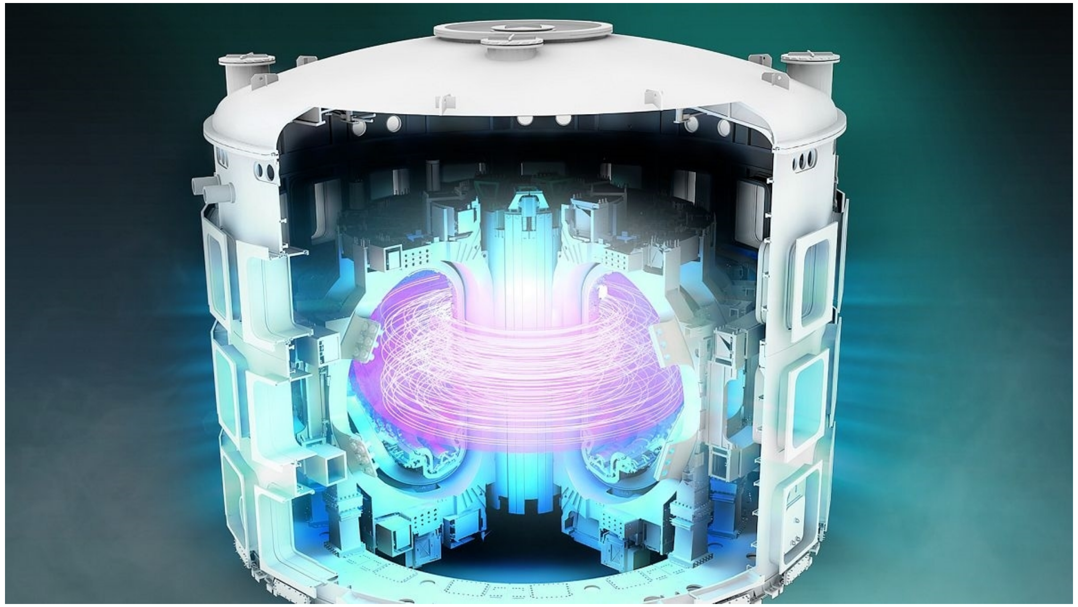
Sandia's National Security Mission





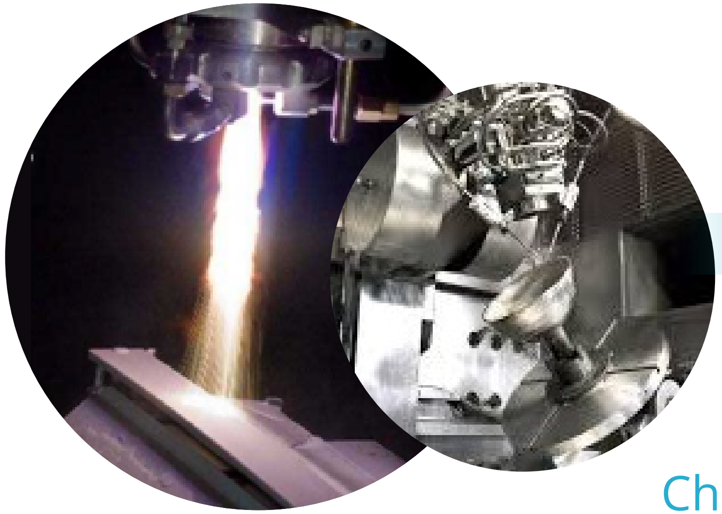


DOE and Industry Common Challenges

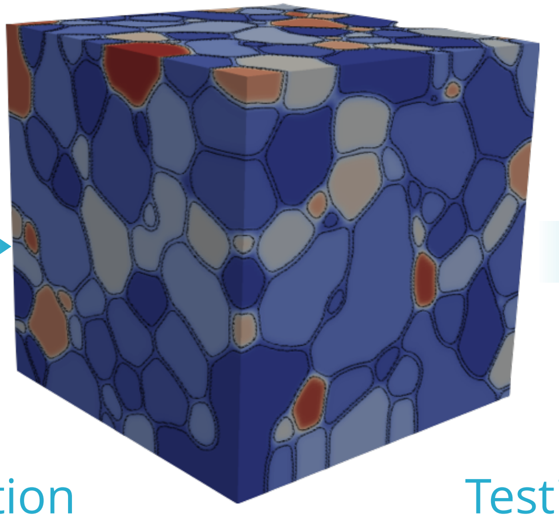


Motivation: Traditional Manufacturing is not Agile

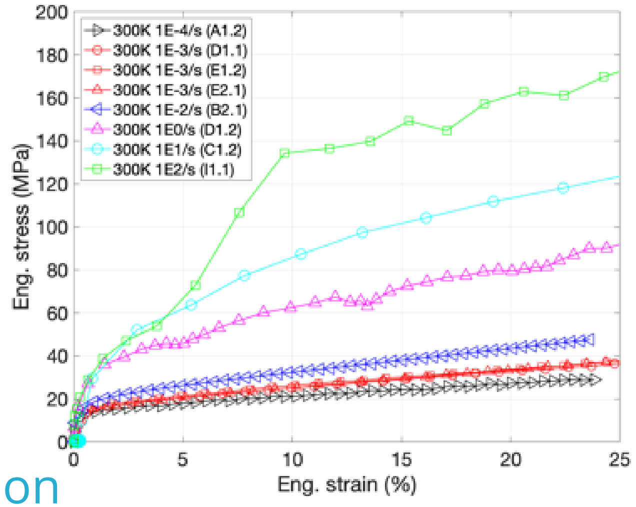
SYNTHESIS PROCESS



MATERIAL STRUCTURE

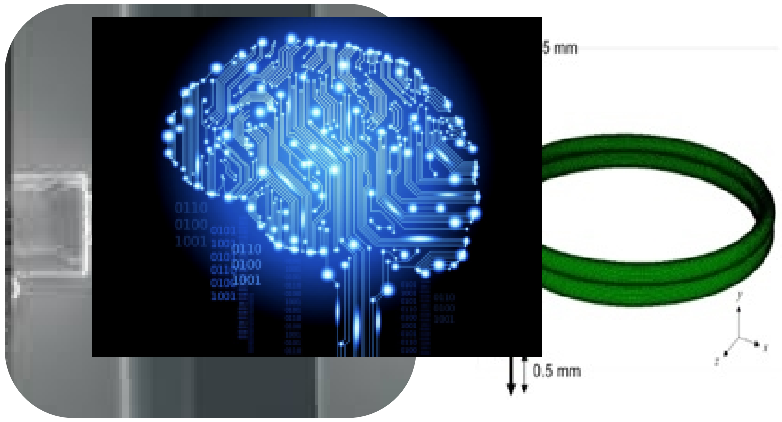


PROPERTY

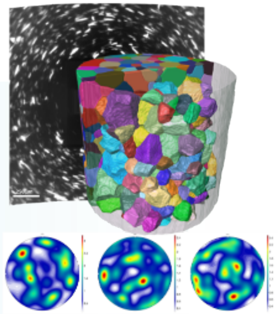


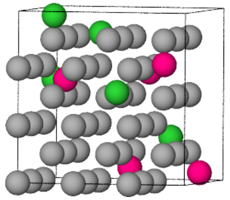
Characterization

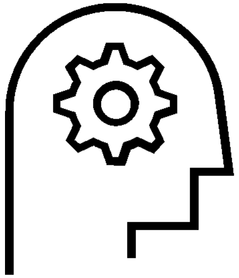
Testing / Simulation



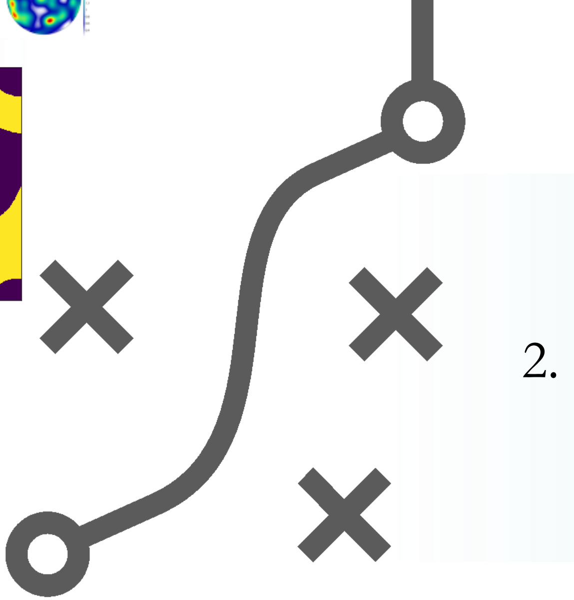
Innovation in Materials: How can it be done?

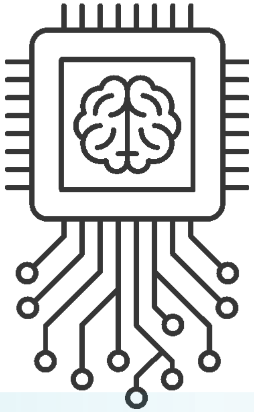






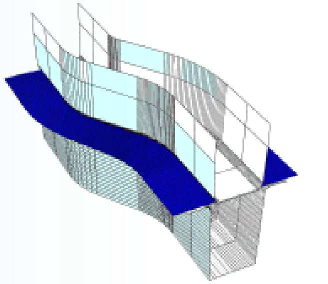
1. Generate a diverse training set on which the model will be trained.

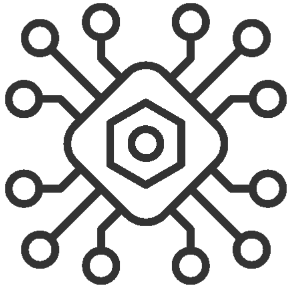




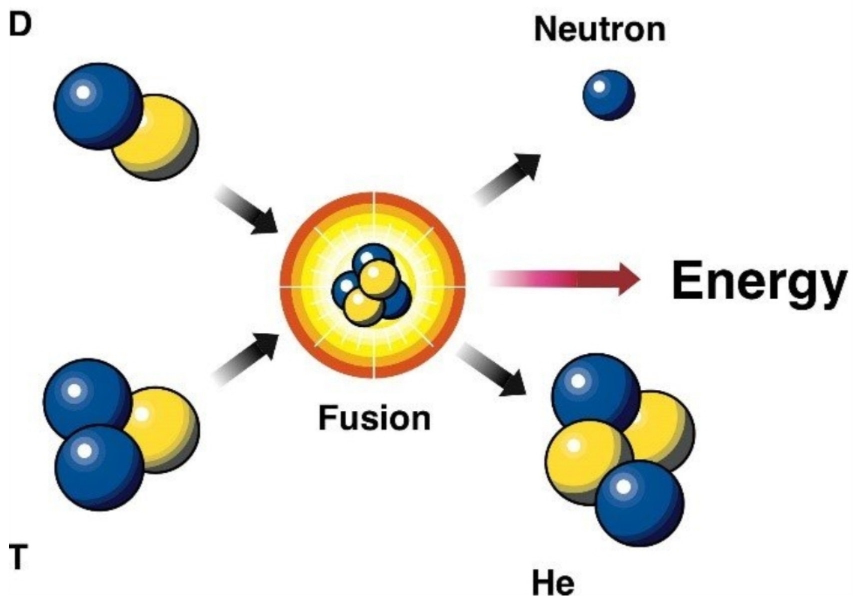
2. Obtain a unique fingerprint descriptor of the structure.

3. Integrate Machine Learning to develop Linkage.



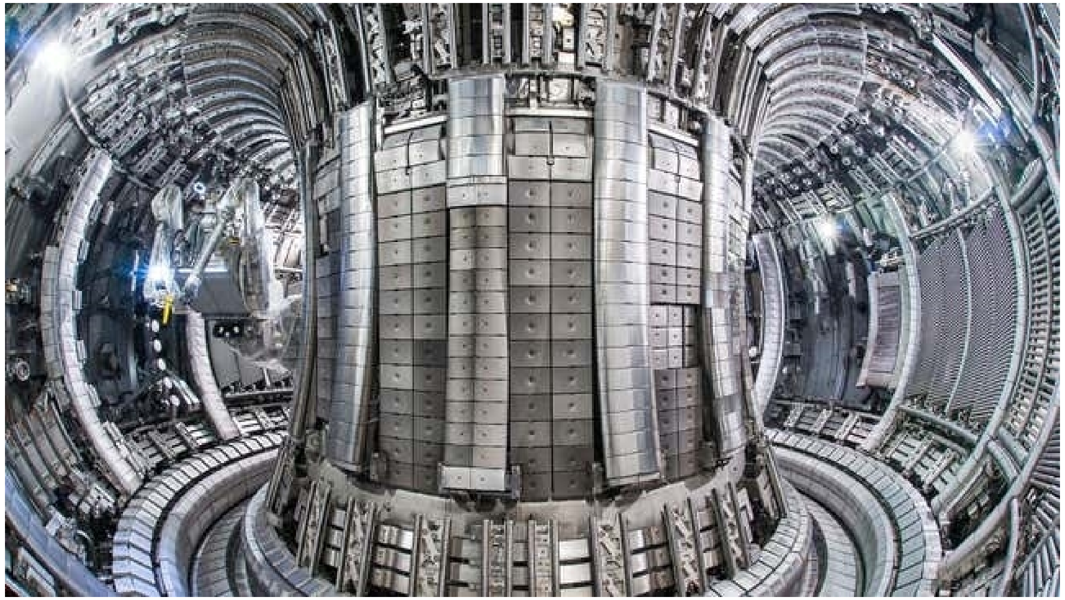


Innovation in Materials: Small Particles, Big Effects



[https://www.energy.gov/science/doe-explainsnuclear-fusion-reactions]

- Massively energetic process where two light nuclei merge to form a single heavier nucleus.
- Energy/Plasma generated needs to be contained in a reactor.
- Metal of the surface facing parts are heavily bombarded by energetic particles and massive amount of heat/energy.



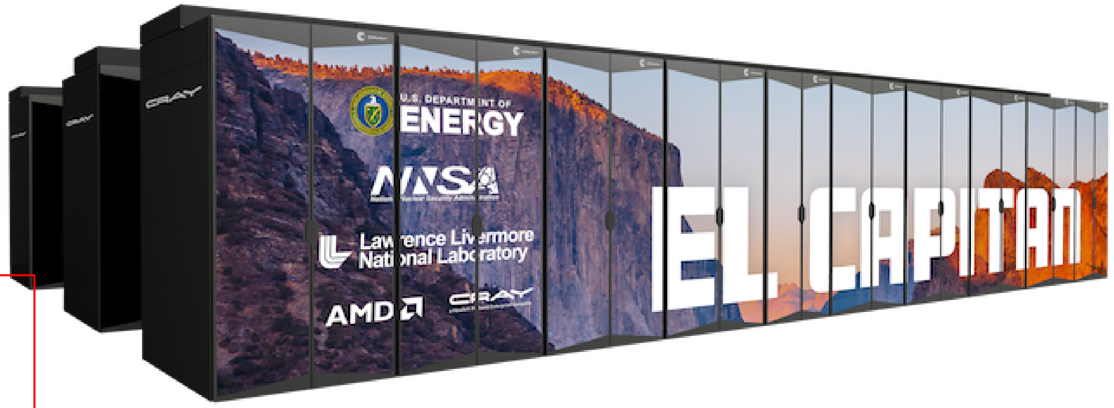
- How do material react to these conditions?
- What is the fundamental behavior/response of a material to an impact from these particles?

Answers to these questions are not easily obtained experimentally.

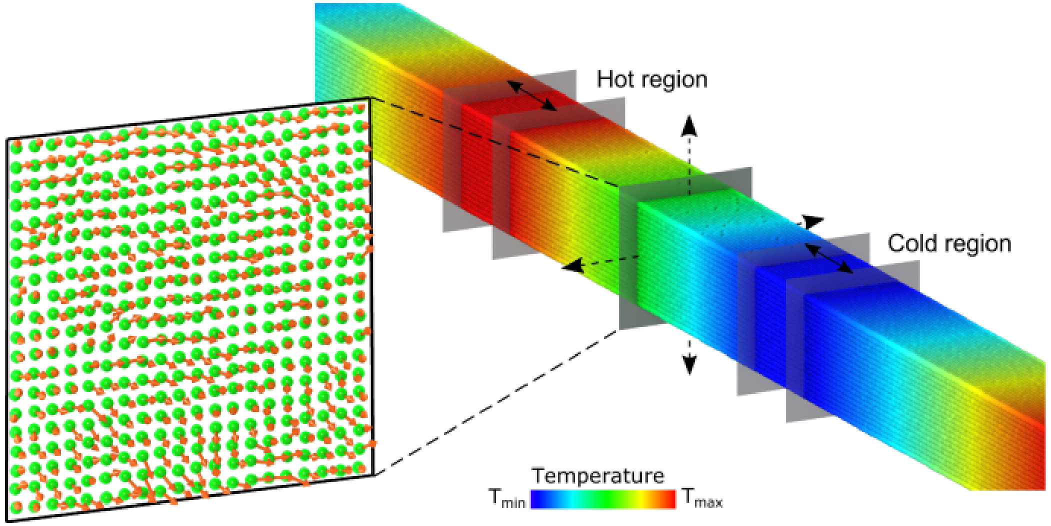
Traditional Simulation Process: Cannot Meet Demand

- These interactions can be described with quantum mechanics and accurately modeled using density functional theory.
- Really complex equations that require specialized computers.

Can only model couple tens of thousand atoms for short time scales.

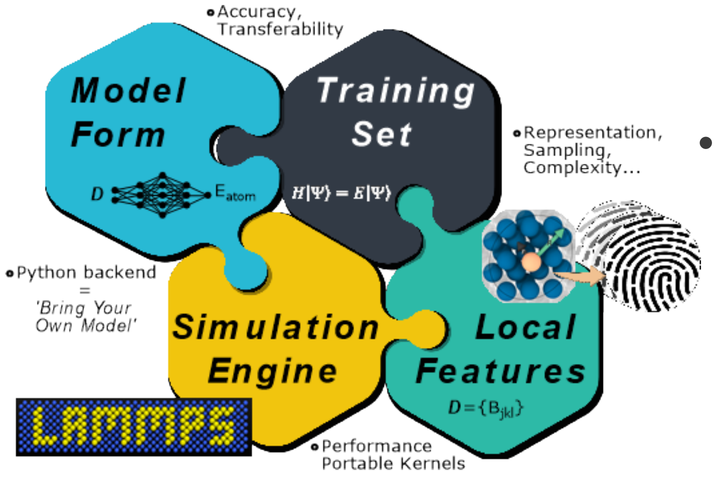


Large-Scale MD Simulation



[Nikolov et al. 2022]

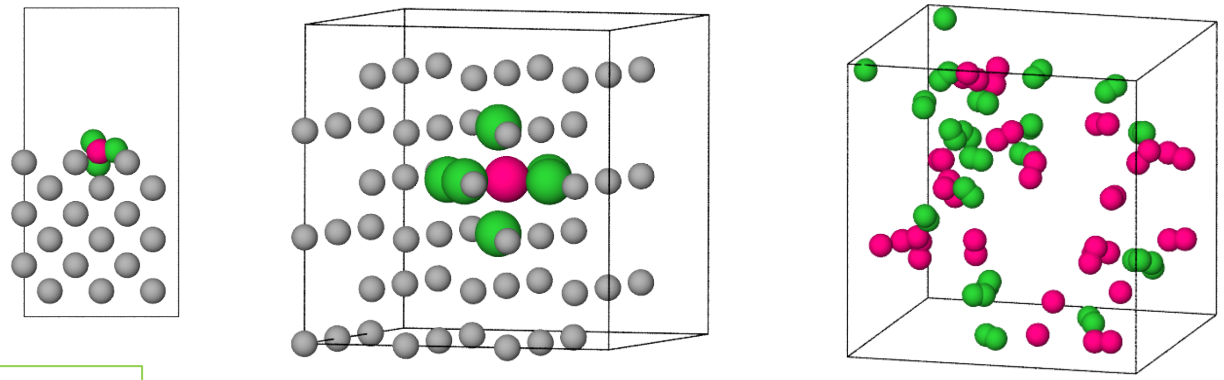
- The interatomic potential (IAP) serves as a surrogate to model atomic environments to energies and forces and are fitted to a reference set of training quantum calculations.



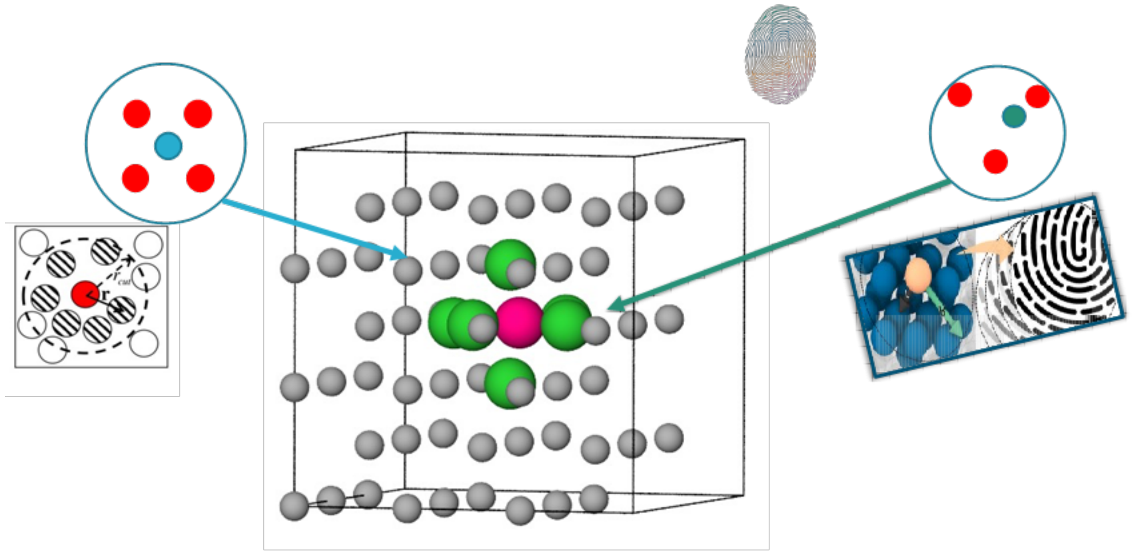
- Resultant models are not transferable and only work for the situations where they were trained.

Innovation in Materials: Enabling High-Fidelity Simulations

- Therefore, the choice of training data becomes critical for the development of these models.
- Infinite space that complicates direct sampling and needs domain expert guidance.



Recast the problem to represent the atomic structure with a unique fingerprint descriptor that can be sampled.



- Sample the new descriptor base using an maximization algorithm.
- Enables to generate vast and diverse dataset that will enable models to be transferable.

[Karabin, M. & Perez, D (2020), Bartok et al. (2010)]

Innovation in Materials: Revolutionizing Computational Modeling of Nuclear Fusion

npj computational materials

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ARTICLE OPEN

Training data selection for accuracy and transferability of interatomic potentials

David Montes de Oca Zapiain[1], Mitchell A. Wood[1], Nicholas Lubbers[2], Carlos Z. Pereyra[3], Aidan P. Thompson[1] and Danny Perez[4]

Advances in machine learning (ML) have enabled the development of interatomic potentials that promise the accuracy of first principles methods and the low-cost, parallel efficiency of empirical potentials. However, ML-based potentials struggle to achieve transferability, i.e., provide consistent accuracy across configurations that differ from those used during training. In order to realize the promise of ML-based potentials, systematic and scalable approaches to generate diverse training sets need to be developed. This work creates a diverse training set for tungsten in an automated manner using an entropy optimization approach. Subsequently, multiple polynomial and neural network potentials are trained on the entropy-optimized dataset. A corresponding set of potentials are trained on an expert-curated dataset for tungsten for comparison. The models trained to the entropy-optimized data exhibited superior transferability compared to the expert-curated models. Furthermore, the models trained to the expert-curated set exhibited a significant decrease in performance when evaluated on out-of-sample configurations.

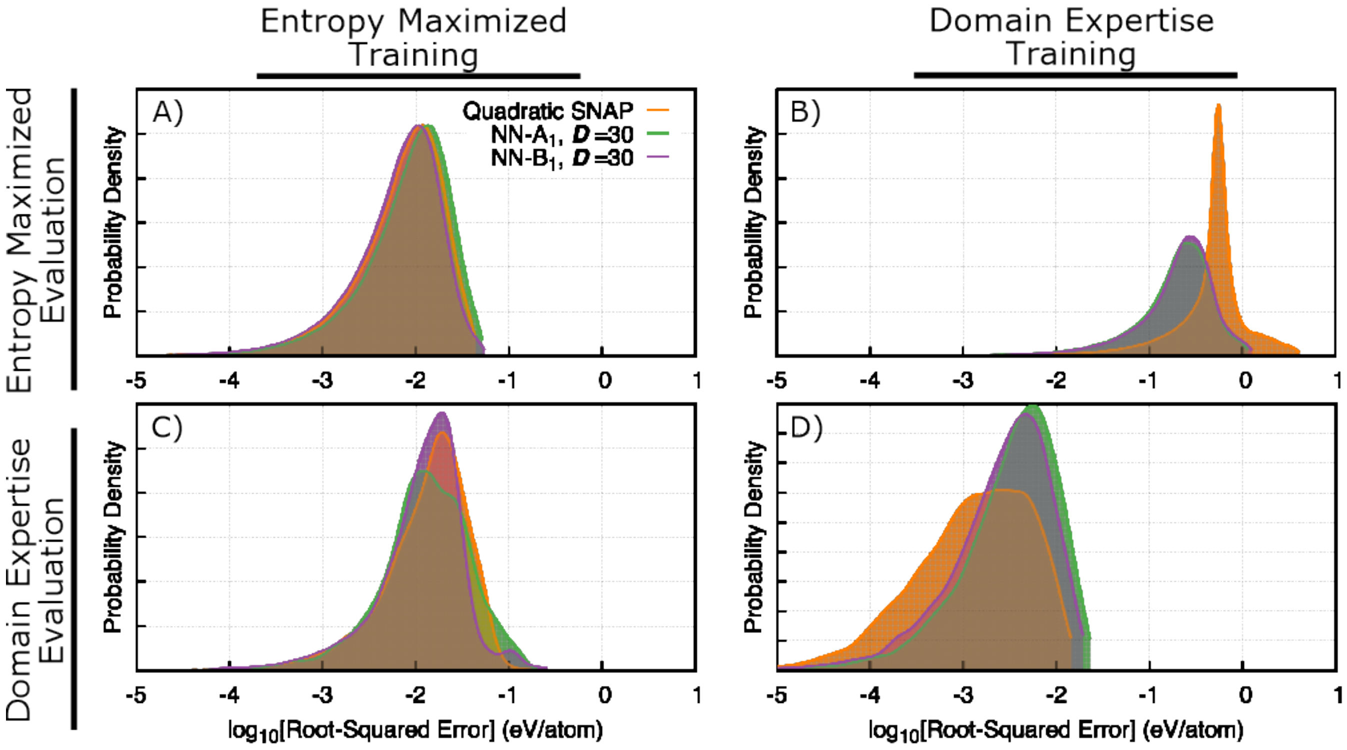
npj Computational Materials (2022)8:189 ; https://doi.org/10.1038/s41524-022-00872-x

INTRODUCTION

The rapid adoption of machine learning (ML) methods in virtually all domains of physical science has caused a disruptive shift in the expectations of accuracy versus computational expense of data-driven models. The diversity of applications arising from this swell of attention has brought about data-driven models that have accelerated pharmaceutical design[1–3], material design[4,5], the processing of observations of celestial objects[6], and enabled accurate surrogate models of traditional physical simulations[7–9]. While many of these models have proved extremely powerful, new questions and challenges have arisen due to the uncertainty in model predictions coined as extrapolations[10], i.e., when prediction occurs on input that are found outside of the support of the training data. Moreover, the accuracy of a machine-learned model can only be quantified using the training itself, or on a subset thereof, held out as validation. For that reason, it is often

thus enabling extremely large simulations[17,18] that would be impossible with direct quantum simulations. However, a critical limitation of empirical IAPs is that they are approximate models of true physics/chemistry and as such have to be fitted to reproduce reference data from experimental or quantum calculations. ML techniques have recently enabled the development of IAPs that are capable of maintaining an accuracy close to that of quantum calculations while retaining evaluation times that scale linearly, presenting significant computational savings over quantum mechanics. This is due to their inherent ability to learn complex, non-linear, functional mappings that link the inputs to the desired outputs[19–21]. Nevertheless, despite significant advances in the complexity of the behavior that can be captured with ML-based models, machine learning interatomic potentials (MLIAPs) often struggle to achieve broad transferability[22–24].

Indeed, increasing the complexity of the ML models, while

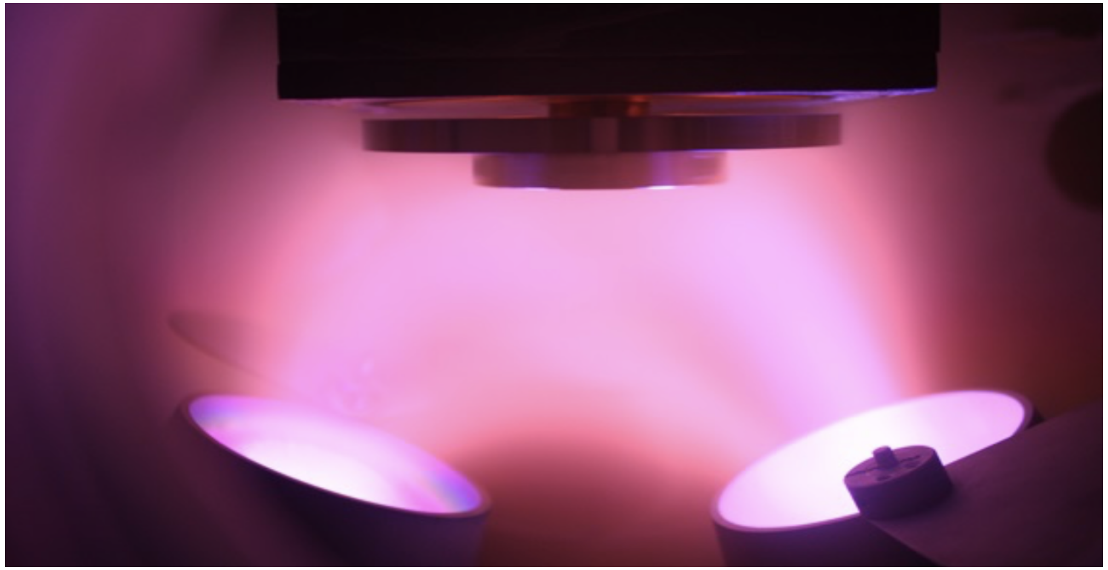


- Now we can train potentials that are transferable in a data-driven manner.
- This is a first step towards making large scale simulations that accurately describe at an atomic level the interactions of plasma and the reactor material.

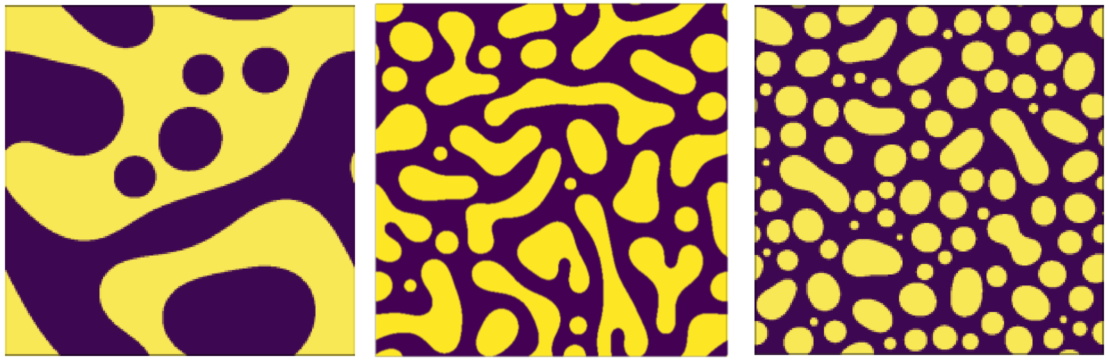
Innovation in Materials: Thin Films, Strong Implications

- Advanced optics which requires enhanced thin-film and coating processes.

Coating Process: Physical Vapor Deposition

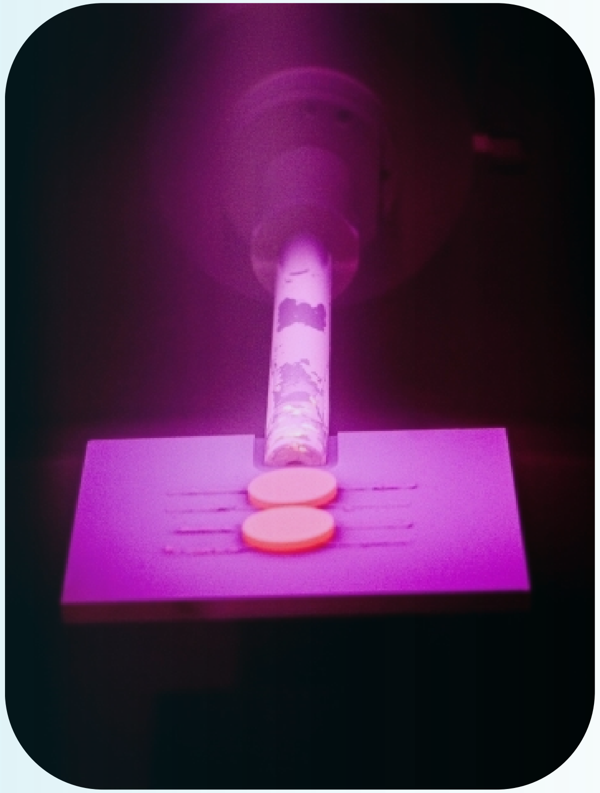


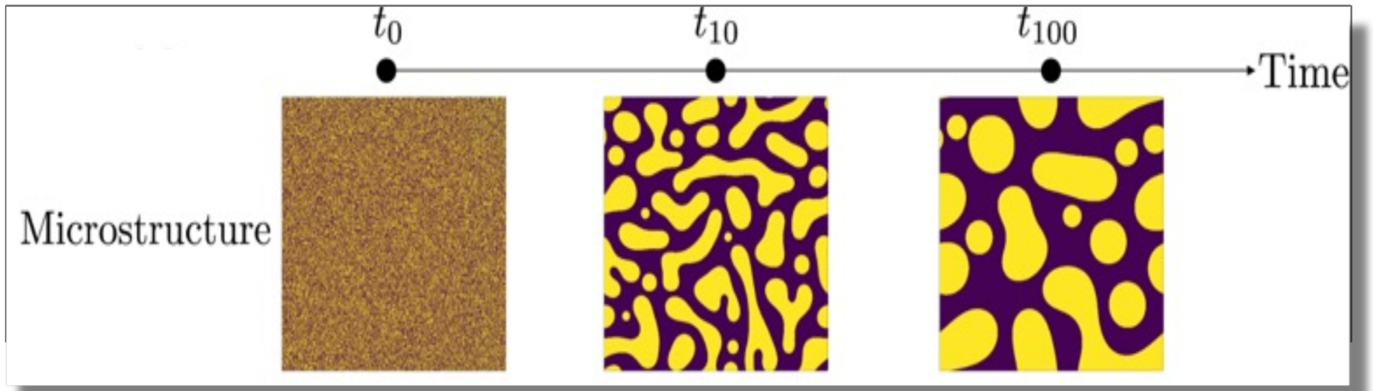
Phase-field simulations of thin-film microstructures.



Microstructure is dependent on large parameter space.

Existing Solutions: Force us to Make a Compromise





Computational Exploration and Characterization:

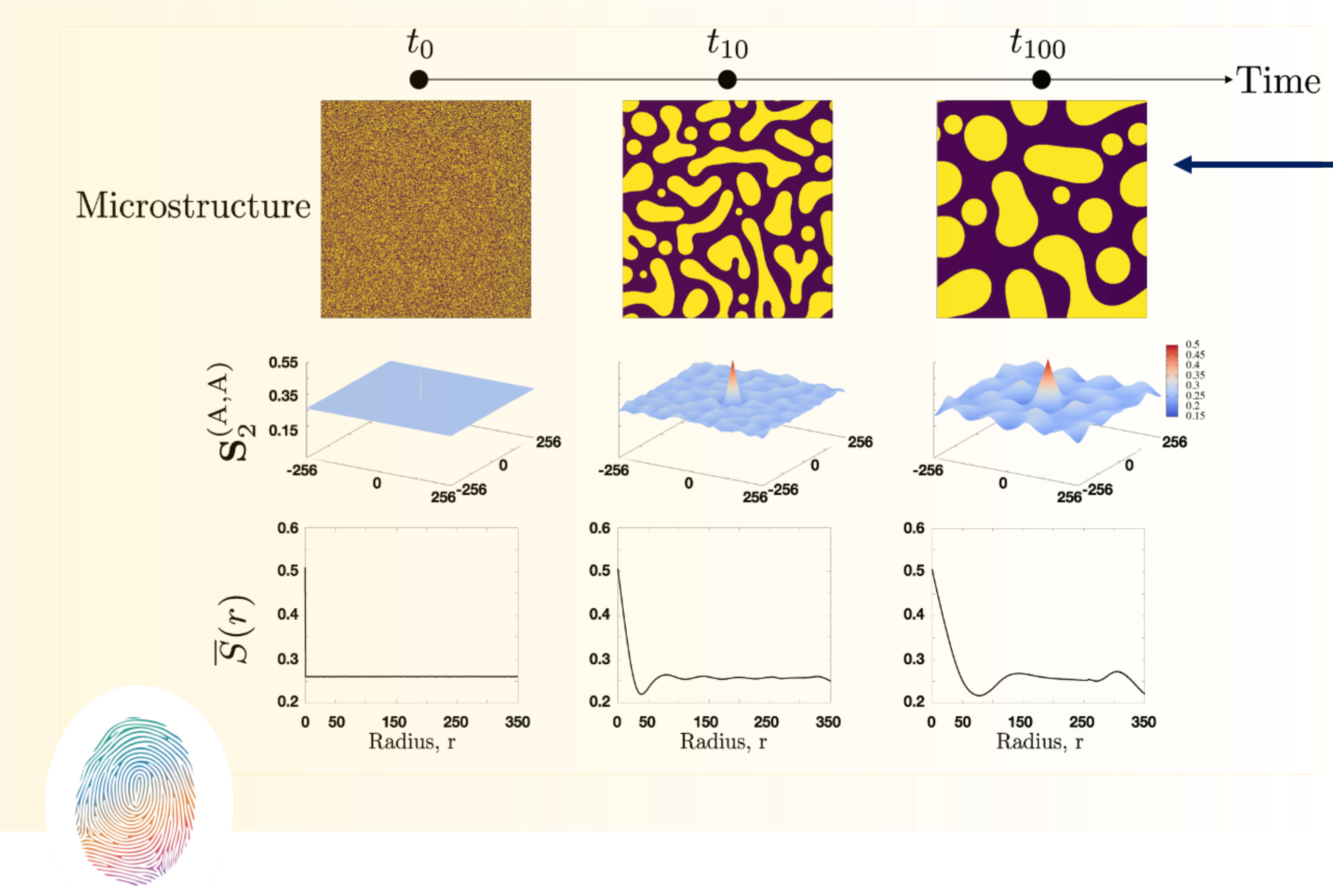
- Computational modelling of evolution requires to solve numerically complex and non-linear PDEs
- Require High-Performance Computing Environment
- Time-consuming.

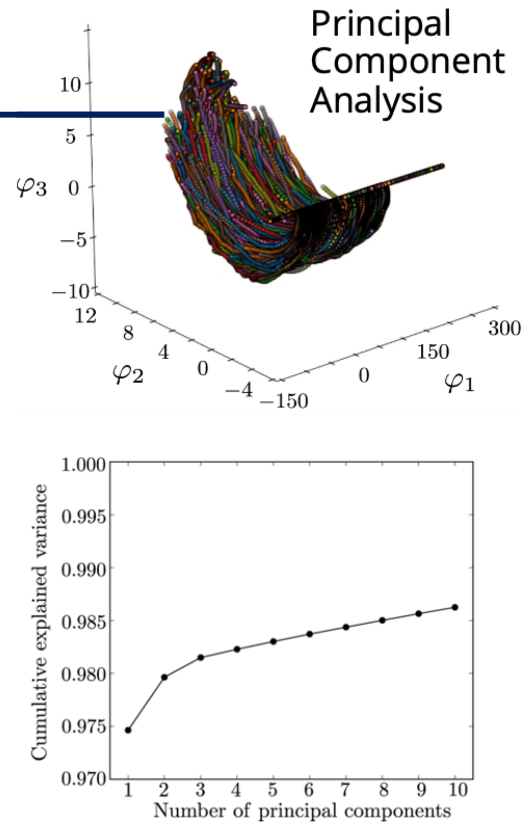
Experimental Exploration and Characterization:

- Capital Intensive
- Laboratory Required
- Physically build every possible combination

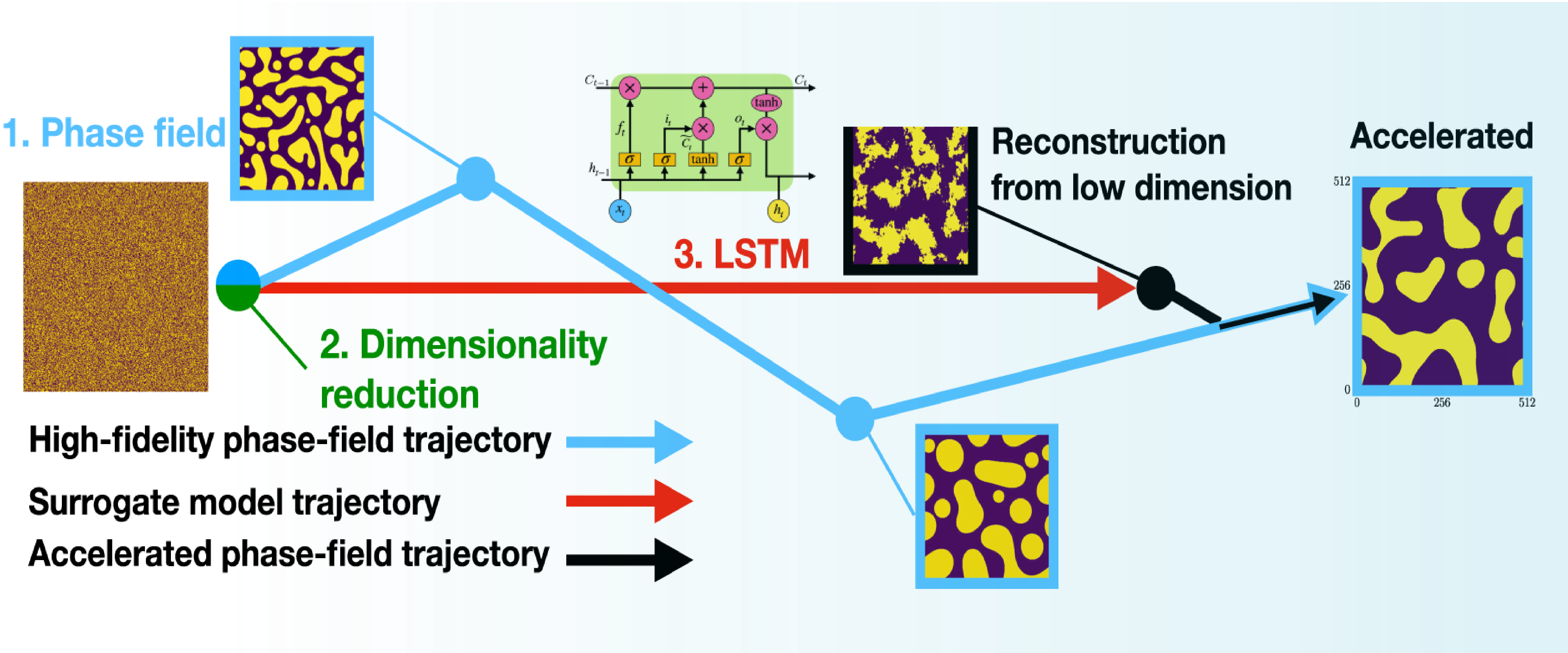
Are not able to perform an efficient exploration of the space and cannot provide a rapid prediction the effect of one of these parameters will have on the resultant structure.

Innovation in Materials: Thinking outside the Box





Innovation in Materials: Accelerated Simulation Framework



Innovation in Materials: Jumping forward in Time

40,000x faster
leaps through time

50,000 Simulations

9 years with
Phase-field

50 min with LSTM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ARTICLE OPEN

Accelerating phase-field-based microstructure evolution predictions via surrogate models trained by machine learning methods

David Montes de Oca Zapiain[1], James A. Stewart[2] and Rémi Dingreville[1]

The phase-field method is a ... associated properties for a w... models are inherently comp... integration schemes to achie... driven surrogate model that ... dependent machine-learning ... microstructure, obtained dir... autoregressive algorithm or ... performance and accurately ... in seconds, without the need for ... from our machine-learned surrogate model can be fed directly as an input into a classical high-fidelity ... accelerate the high-fidelity phase-field simulations by leaping in time. Such machine-learned phase-field framework opens a promising path forward to use accelerated phase-field simulations for discovering, understanding, and predicting processing–microstructure–performance relationships.

npj Computational Materials (2021)7:3 ; https://doi.org/10.1038/s41524-020-00471-8

INTRODUCTION

The phase-field method is a popular mesoscale computational method used to study the spatio-temporal evolution of a microstructure and its physical properties. It has been extensively used to describe a variety of important evolutionary mesoscale phenomena, including grain growth and coarsening[1–3], solidification[4–6], thin-film deposition[7,8], dislocation dynamics[9–11], vesicles formation in biological membranes[12,13], and crack propagation[14,15]. Existing high-fidelity phase-field models are inherently computationally expensive because they solve a system of coupled partial differential equations for a set of continuous field variables that describe these processes. At present, the efforts to minimize computational costs have focused primarily on leveraging high-performance computing architectures[16–21] and advanced numerical schemes[22–24], or on integrating machine-learning algorithms with microstructure-based simulations[25–31]. For example, leading studies have constructed surrogate models capable of rapidly predicting microstructure evolution from phase-field simulations using a variety of methods, including Green's function solution[25], Bayesian optimization[26,28], or a combination of dimensionality reduction and autoregressive Gaussian processes[29]. Yet, even for these successful solutions, the key challenge has been to balance the accuracy with computational efficiency. For instance, the computationally efficient Green's function solution cannot guarantee accurate solutions for complex, multi-variable phase-field models. In contrast, Bayesian optimization techniques can solve complex, coupled phase-field equations, but at a higher computational cost

(although the number of simulations to be performed is kept to a minimum, since each subsequent simulation's parameter set is informed by the Bayesian optimization protocol). Autoregressive models are only capable of predicting microstructural evolution for the values for which they were trained, limiting the ability of this class of models to predict future values beyond the training set. For all three classes of models, computational cost-effectiveness decreases as the complexity of the microstructure evolution process increases.

In this work, we create a cost-minimal surrogate model capable of solving microstructural evolution problems in fractions of a second by combining a statistically representative, low-dimensional description of the microstructure evolution obtained directly from phase-field simulations with a history-dependent machine-learning approach (see Fig. 1). We illustrate this protocol by simulating the spinodal decomposition of a two-phase mixture. The results produced by our surrogate model were achieved in fractions of a second (lowering the computational cost by four orders in magnitude) and showed only a 5% loss in ... compared to the high-fidelity phase-field ... improvement, our surrogat... simulations as ... the microstruct... As illustrated ... framework ... simulatio... evolution... mobilities, M_A a... features of the microst...

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Published in partnership with the Shanghai Institute of Ceramics of the Chinese Academy of Sciences

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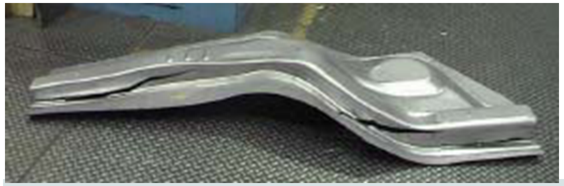
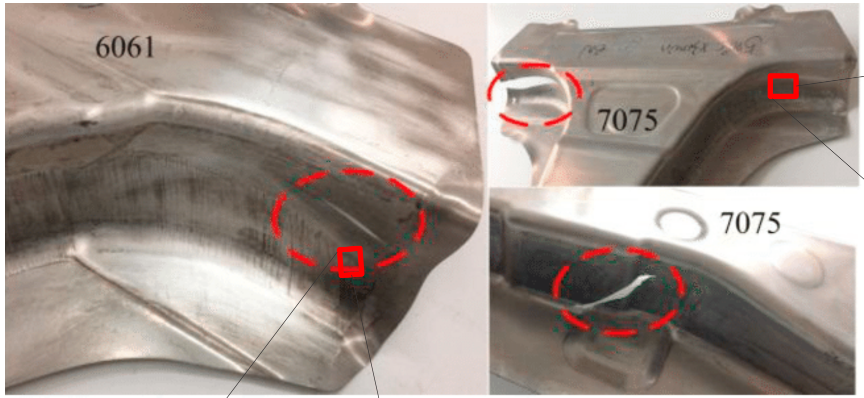
Innovation in Materials: Metal Stamping and Forming

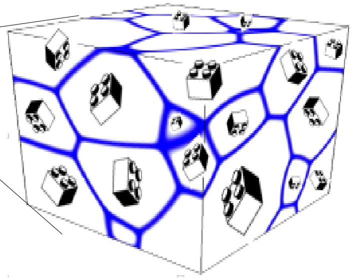
- Manufacturing processes that can shape new materials into desired shape.

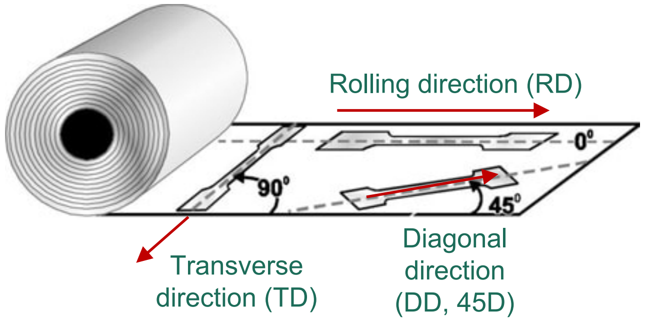
- Metal Stamping and Forming Processes deforms sheet metals into complex parts.
- Imposed deformation coupled can cause ruptures/ cracks.
- Manufacturing trials and die trials are needed to ensure material can be shaped into desired component.
  - These trials cost millions of dollars per year per plant.

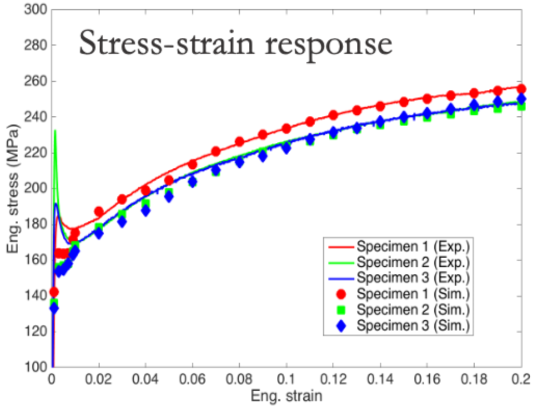


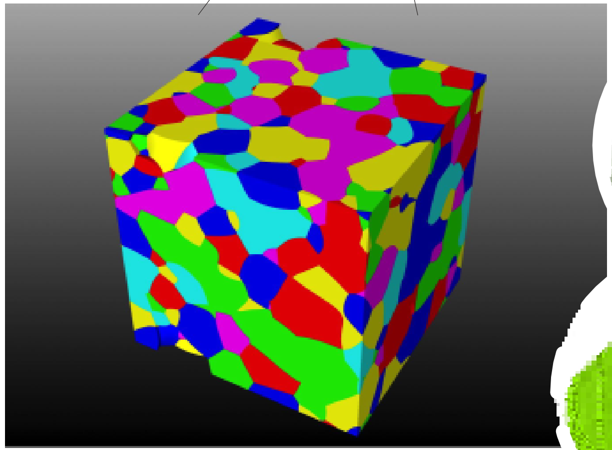
Innovation in Materials: Quantifying the Effect of the Internal Structure

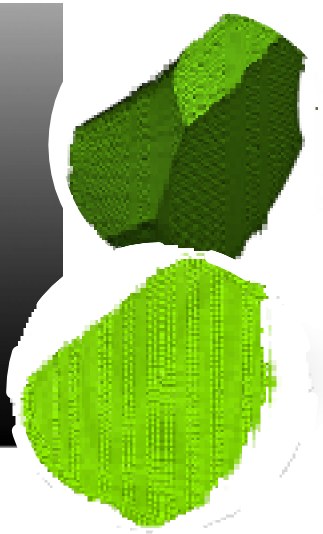






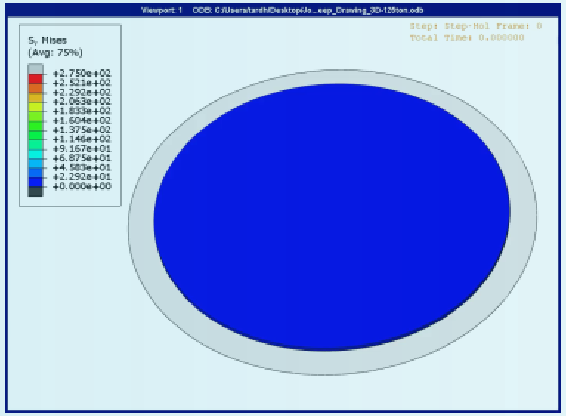


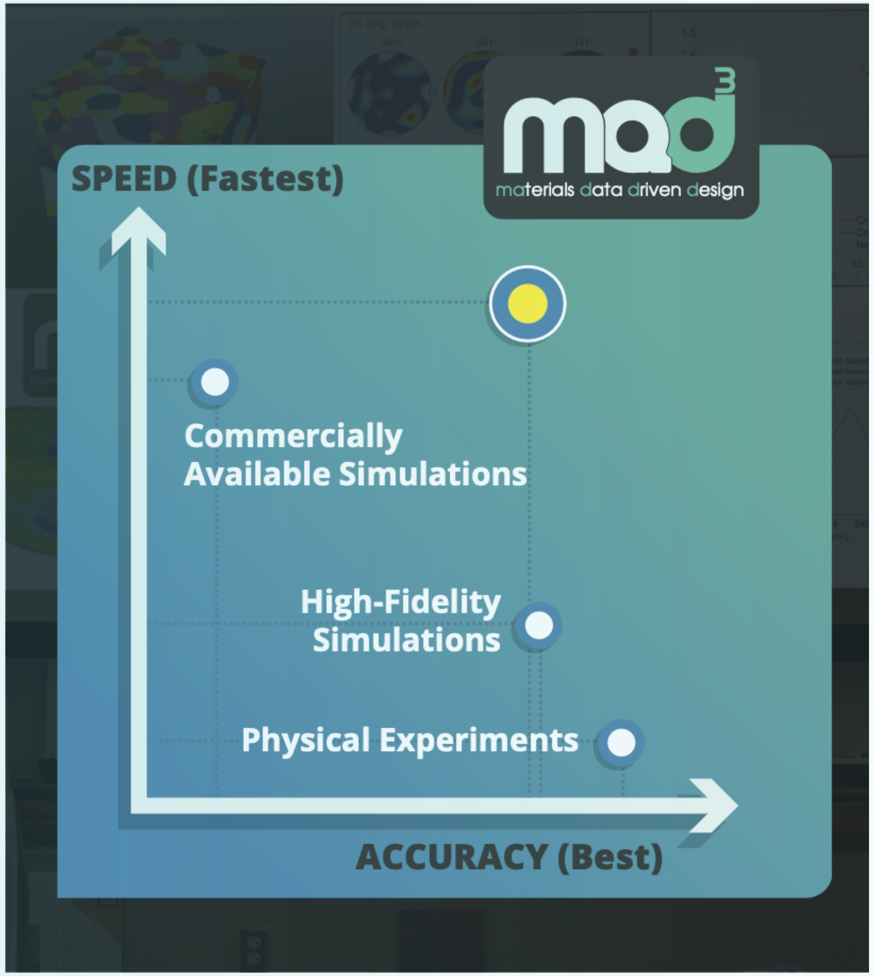


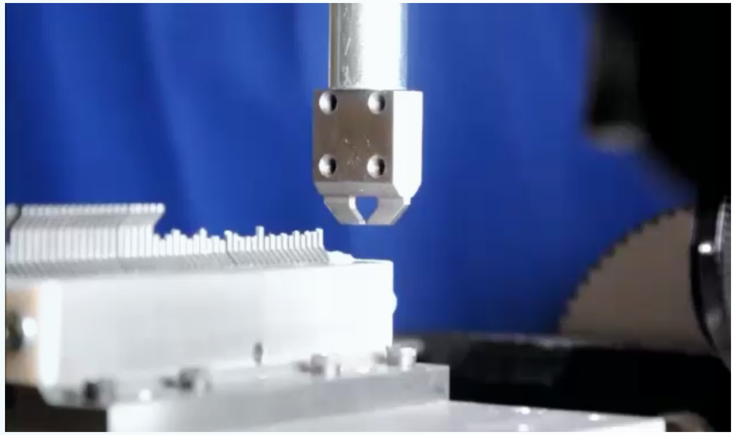


- The metal alloys show complex polycrystalline grain structure that heavily affects the deformation depending on the orientation of the grains or of the loading.
- An agile manufacturing process requires an efficient way to account for the effect these grain structures have on the deformation.

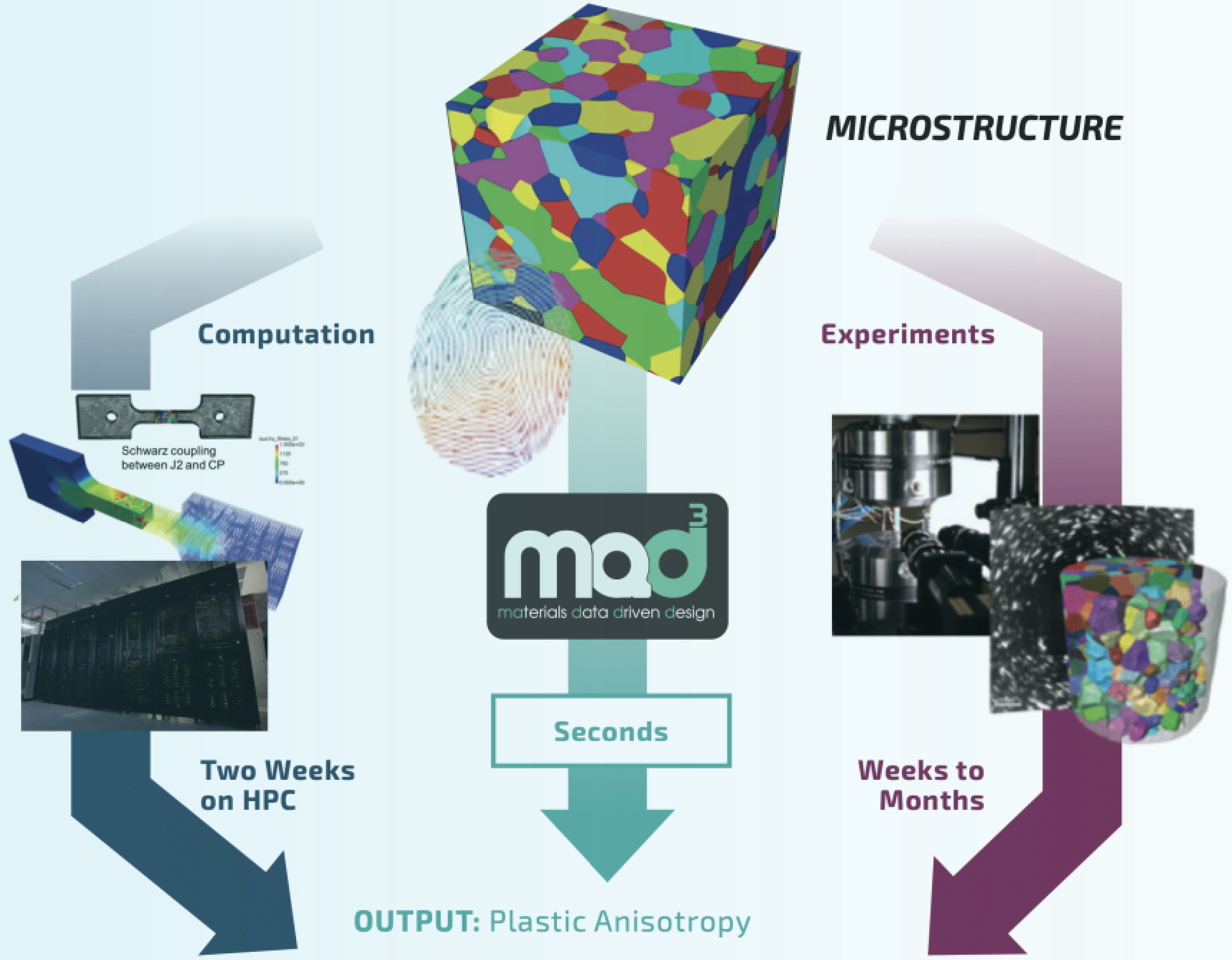
Innovation in Materials: Addressing the Engineering Dilemma





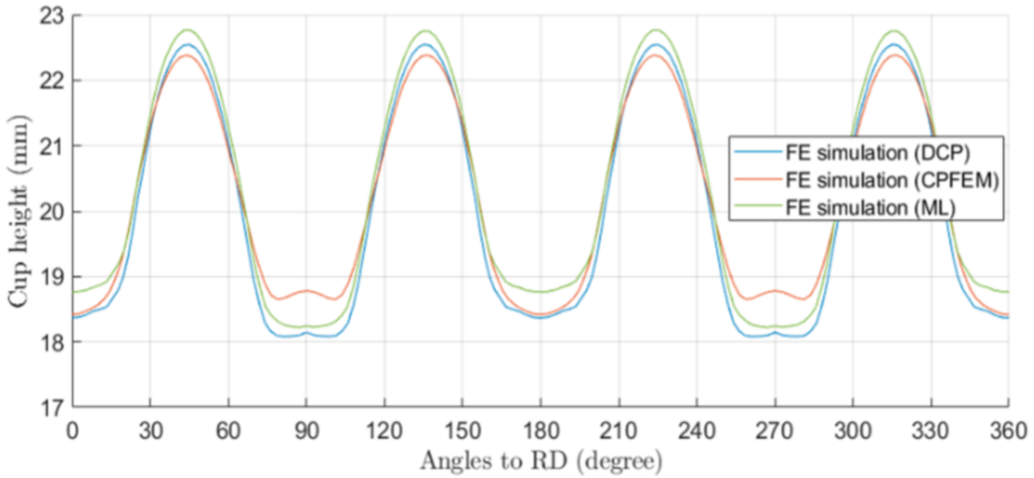


Innovation in Materials: Developing an Agile Characterization Framework using Machine Learning



Innovation in Materials: Using Extracted Knowledge

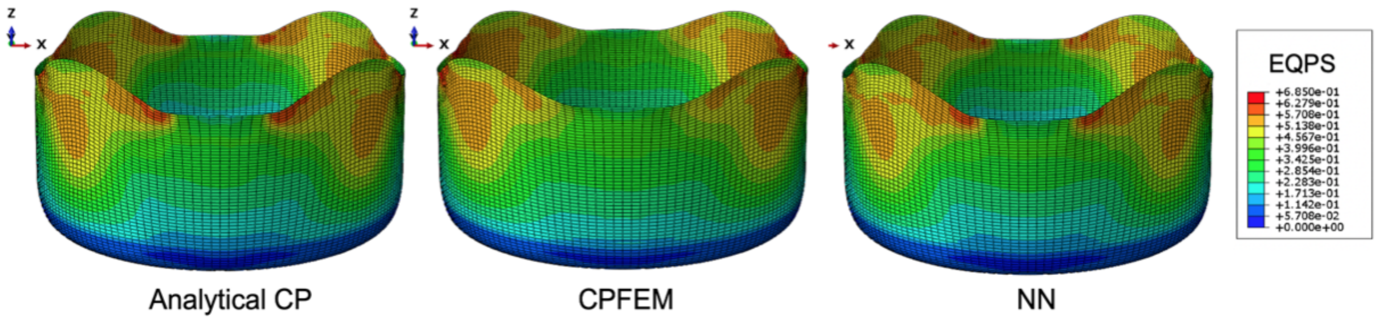
Earing profiles of Al5053



Parameterizing Hill's quadratic anisotropic yield model:

$$f = F(\sigma_{yy} - \sigma_{zz})^2 + G(\sigma_{zz} - \sigma_{xx})^2 + H(\sigma_{xx} - \sigma_{yy})^2 + 2(L\sigma_{yz}^2 + M\sigma_{zx}^2 + N\sigma_{xy}^2)$$

Al6061-T6	F	G	H	L	M	N	TIME
Experiments	0.6097	0.5495	0.4061	-	-	-	3-6 months
Crystal plasticity-FE	0.5268	0.5261	0.4739	1.5258	1.4788	1.7604	~10 h in HPC
Neural Network predictions	0.5298 ±0.0013	0.5369 ±0.0010	0.4631 ±0.0010	1.5735 ±0.0017	1.5296 ±0.0013	1.6548 ±0.0015	<1 sec.



Obtain Parameterized Constants 36000 times faster than Crystal Plasticity.

Sharing Innovation: Building a Product is not enough

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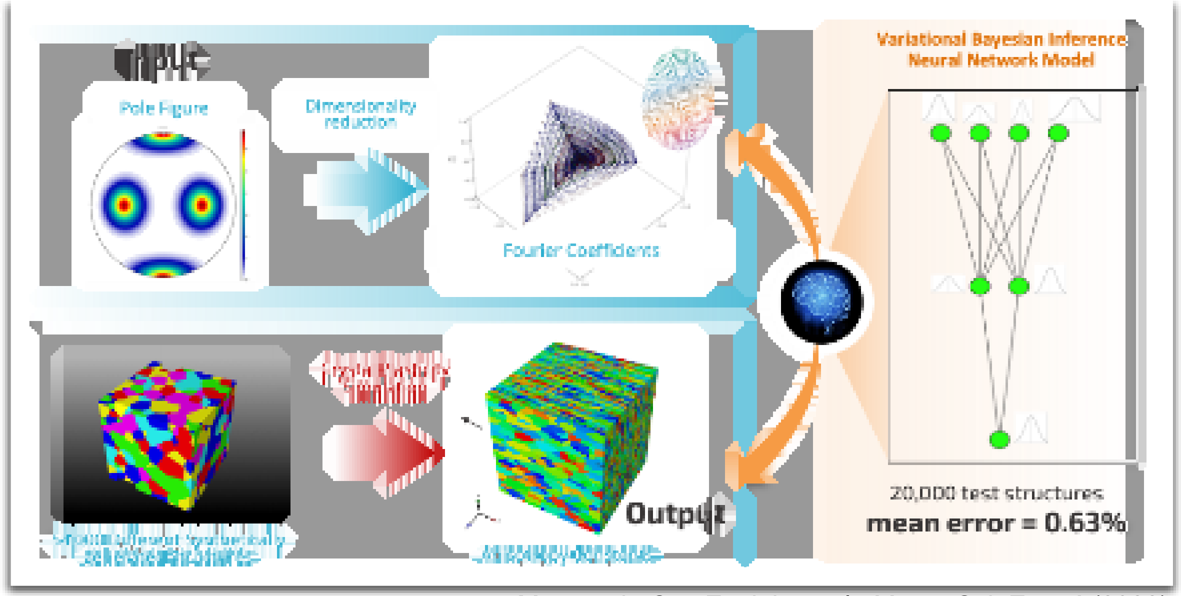
Sharing Innovation: Deploying a Usable Product

ip@sandia.gov

Actual GUI shown.

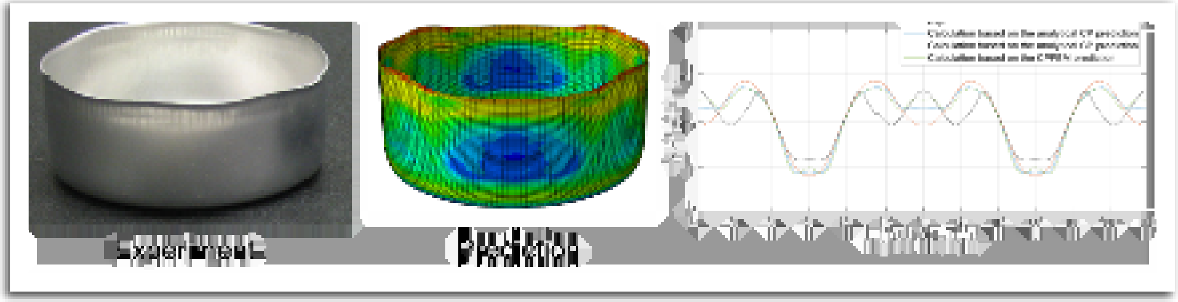
DOE Software Copyright Assertion (SCR#2683)

Theory: Machine Learning based anisotropy prediction

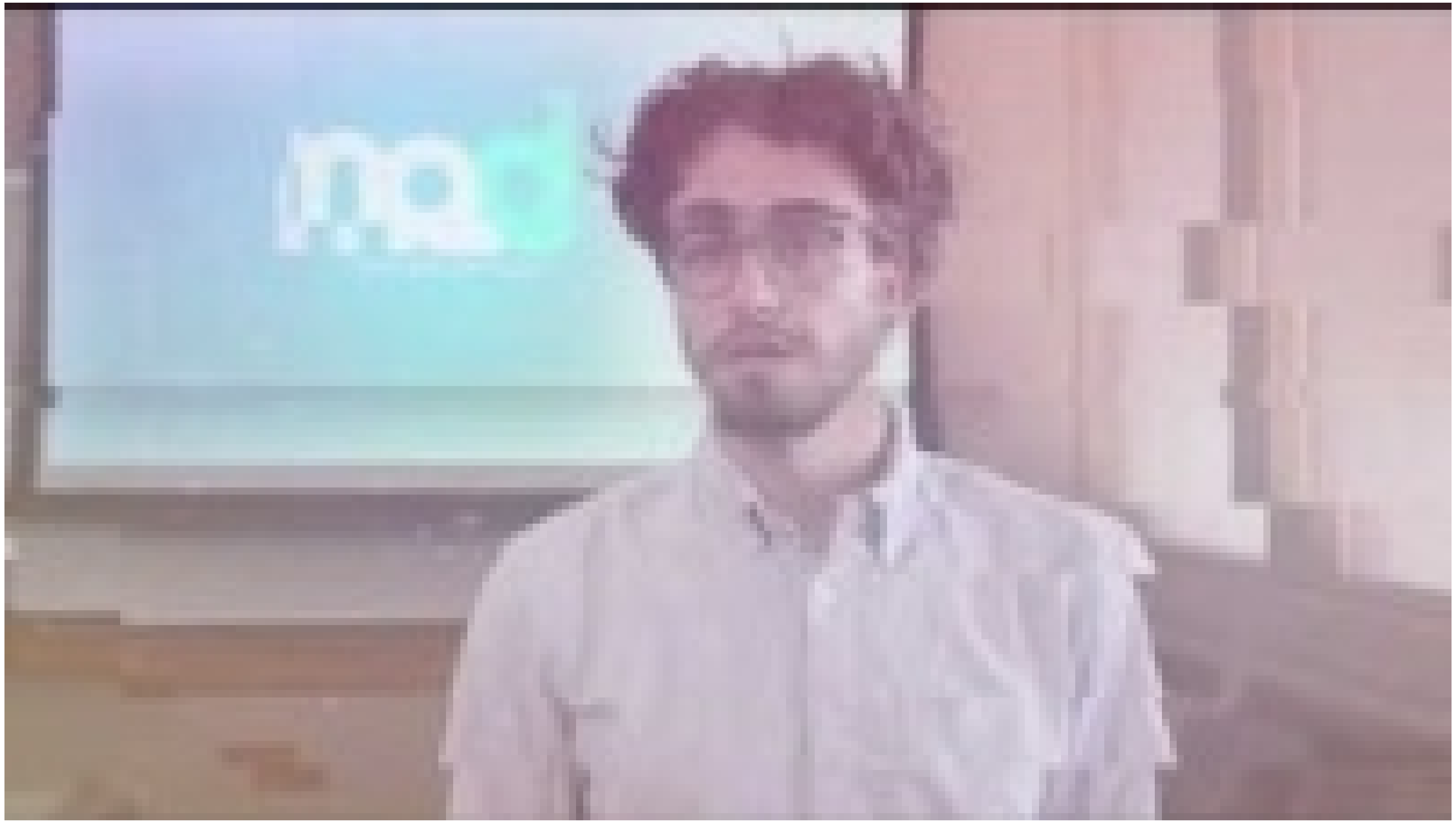


Montes de Oca Zapiain et al., *Mater. Sci. Eng. A* (2022)

Application (e.g., metal forming analysis)

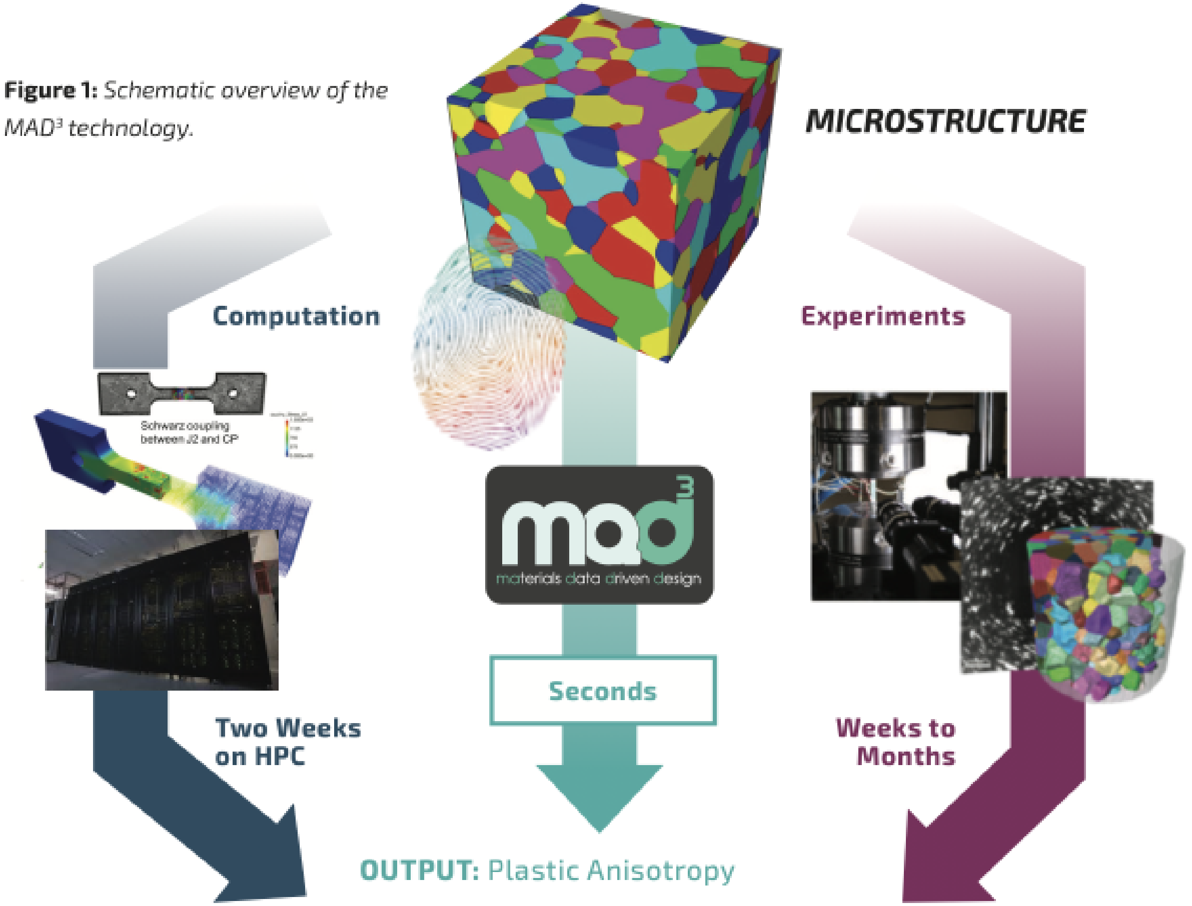


Sharing Innovation: Introducing Materials Data-Driven Design (MAD^3)



Sharing Innovation: Materials Data-Driven Design

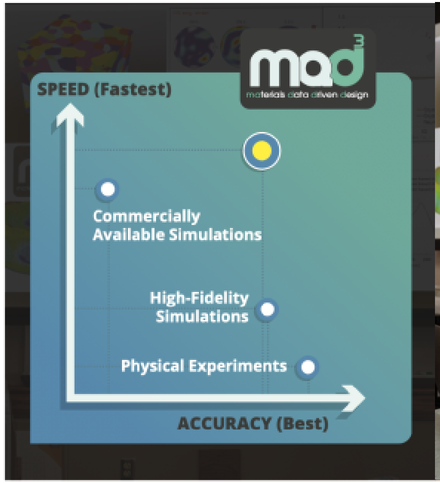
Figure 1: *Schematic overview of the MAD³ technology.*



OUTPUT: Plastic Anisotropy

54 anisotropy parameters: 18 normalized yield stresses and 36 lateral strain increments

MAD³ PROVIDES THE UNIQUE ABILITY TO INCORPORATE A MATERIAL'S MICROSTRUCTURAL INFORMATION INTO METAL-FORMING PROCESSES BY LEVERAGING THE POWER OF MACHINE LEARNING.



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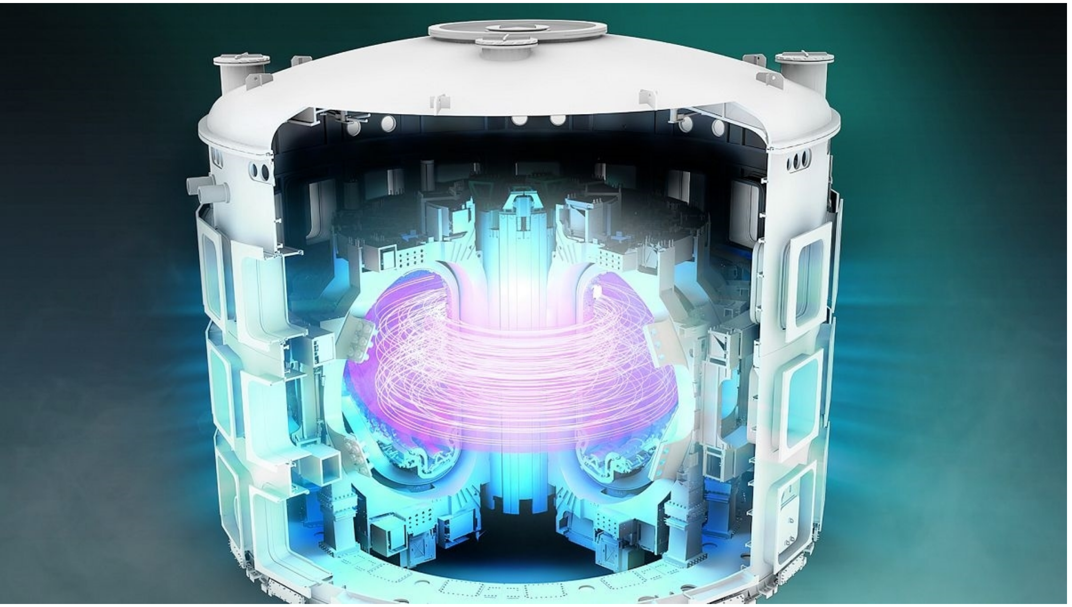
Innovation in Materials: Shoot for the Stars and Land on the Moon



Innovation in Materials and ME: Shaping the World

- ME provides you with unique skills for a diverse and rewarding career path:
  - Technical Expertise
  - Unique Insight
  - Outside-of-the-box thinking
- Bottom-line ME can take you as far as your dreams can go and this is just one example of how an ME can shape world!
- Please join the other seminar series to learn of all the different ways GT Alumni are making the future a reality.

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Materials Science & Engineering

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NNSA National Nuclear Security Administration

STM Sandia Technology Maturation Program

CINT Center for Integrated Nanotechnologies

Energy I-Corps U.S. Department Of Energy

Materials Margins Assurance

LDRD Laboratory Directed Research & Development

Questions?