Director’s Initiative

Developing a Foundation Model for Predicting Material Failure

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Early Career: Javier E. Santos, Aleksandra Pachalieva, Kai Gao
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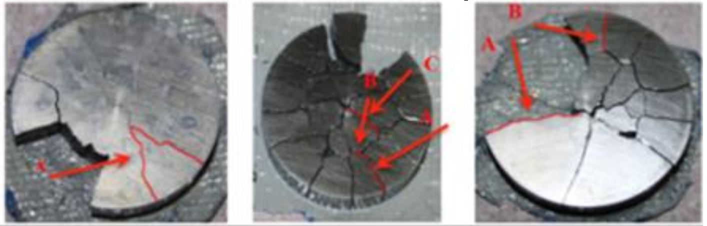
May 20, 2025

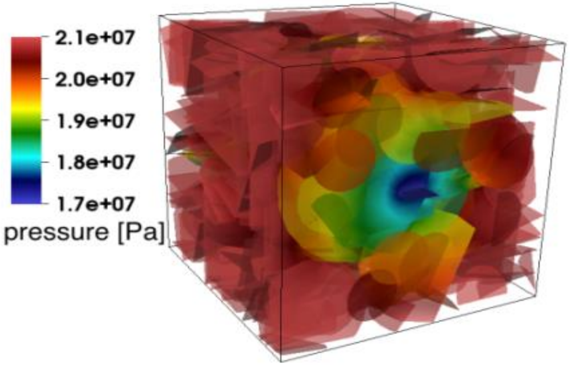
Why LANL: Fractures are critical to weapons & energy security

- **Weapons**: Understand dynamic fracture processes in metals and high explosives
- **Global Security:** Predict radionuclide seepage from underground nuclear explosions
- **Energy Security**: Control subsurface fractured systems to optimize enhanced geothermal, hydraulic fracturing, and hydrogen storage

LANL Brittle Fracture Experiments



LANL HPC Fracture Flow Simulations

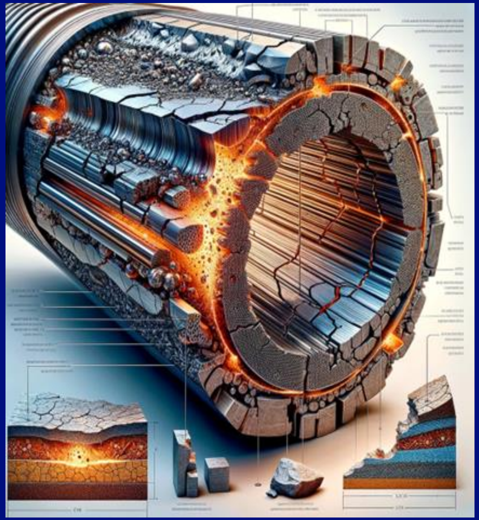


Current State of Knowledge

Problem: HPC fracture modeling is computationally expensive, and AI/ML surrogates are limited to single material systems

Need: Hard to predict time to failure, fracture pattern at failure, and other material properties

Innovation: We aim to break this cycle by developing a foundation model that can use few-shot learning to learn from just a few high-fidelity HPC simulations



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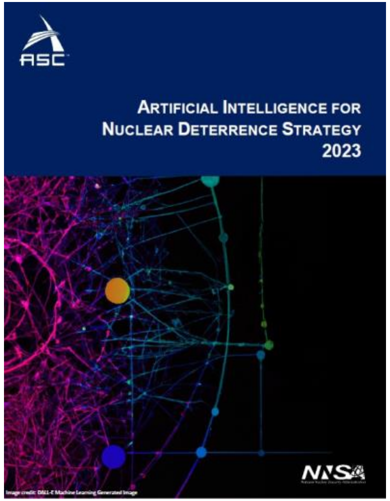
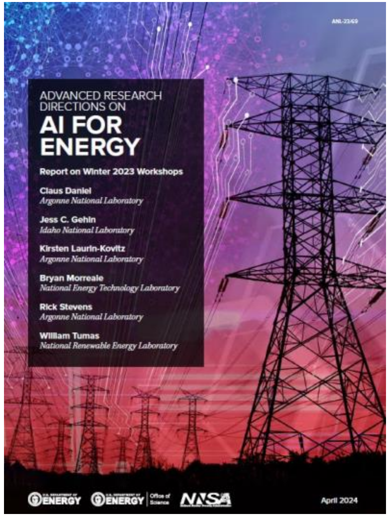
Lots of Activity Right Now in AI and Foundation Models


Lab Agenda
January 2024

Signature Institutional Commitment: Advancing Science and Security through Artificial Intelligence

LANL has successfully applied artificial intelligence (AI) technologies such as machine learning to multiple mission areas. Recognizing the accelerated breakthroughs in AI, especially in foundational models as demonstrated in natural language applications, LANL is making strategic investments to harness these potentially transformative approaches. For example, we have invested in Venado—a next generation computational platform optimized for AI.





Lab Agenda: fine-tuning generic foundation models using high-quality domain-specific data and high-performance computing resources

AINDS: materials discovery, design, optimization

AISES: AI based surrogates for HPC, Foundational AI

AI for Energy: Develop foundation models from disparate multi-model data

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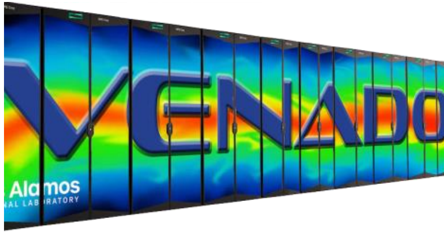
Materials Fracture Project Evolution

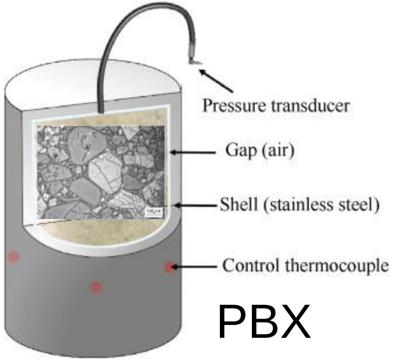
- Foundation model for generalization across multiple materials using large parameter models with Venado
- Leverage industry frontier large language models (LLMs) for context to help ML engine
- Future Work: Moving towards agents to automate workflow to develop an AI Scientist since we have access to frontier LLMs



Develop the first foundation model for predicting material failure across diverse conditions

- Make a paradigm shift from million parameter models for specific systems to generalized foundation models with billions of parameters
- Generalize predictions across different materials and boundary conditions.
- Handle diverse input formats (structured/unstructured grids) and multiple prediction tasks.
- Current Quantities of Interest: fracture pattern at failure, time to failure

Steel



PBX

Copper

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Our innovations

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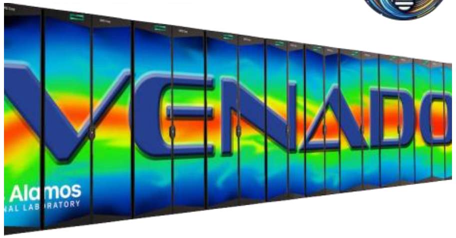
Development of the Senseiver for efficient field reconstruction from sparse observations

Javier E. Santos, Zachary R. Fox, Arvind Mohan, Daniel O'Malley, Hari Viswanathan & Nicholas Lubbers

Our transformer architecture enables unstructured meshes, different domain sizes and multimodal data (e.g., crack location and stress field)

LLM embeddings to help the our transformer zero-in on specific problem



Scaling to big models via on-the-fly data generation and utilizing many Venado nodes and curriculum learning

To achieve few-shot learning, we have a curriculum learning approach for our fracture foundation model

PRE-TRAINING PHASE → **FINE TUNING**

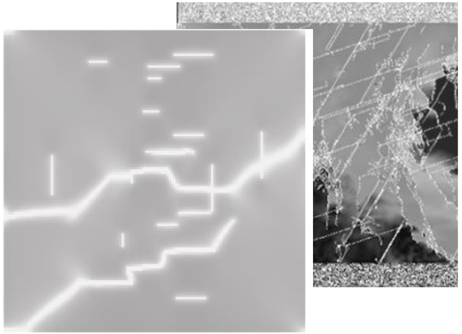
Simplified dataset

T growth

Simplified dataset

X growth

Physics-based dataset



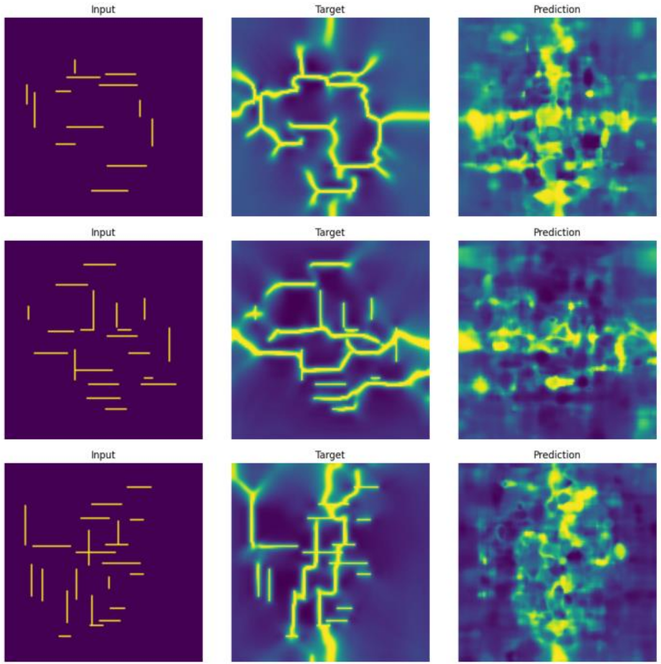
- Huge dataset produced on-the-fly during the training
- Initial training phase

- Huge dataset produced on-the-fly during the training
- Less training is needed to learn a new growth model

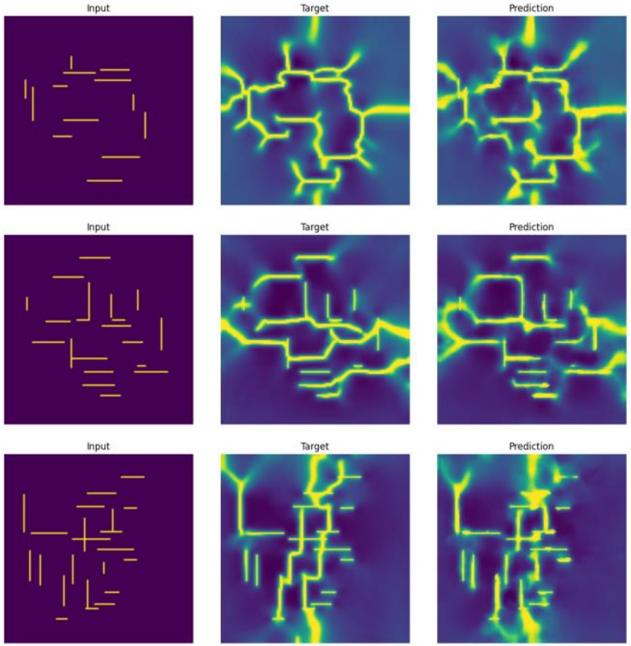
- Limited dataset due to the simulation cost
- We again show a less training is needed to learn more physics

Curriculum Learning Works!

Training from scratch on phase field



Pretrained on rule-based



500 samples per material + BC

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The goal of LLM embeddings is to enable updating problem specification without retraining from scratch

Ingest input decks

Original boundary conditions

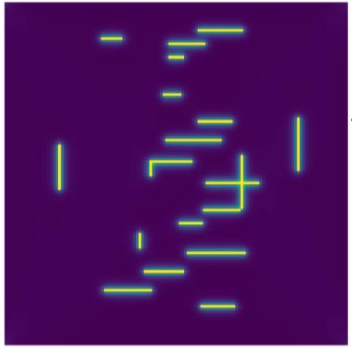
Material:	• Steel • Copper • PBX
Simulator:	• Rule-based • Phase-field • HOSS

New boundary conditions

Boundary conditions:	• Horizontal pulling • Vertical pulling • Combined pulling

LLM embeddings to provide

Our team: Santos et al., *Nature Machine Intelligence* 2023

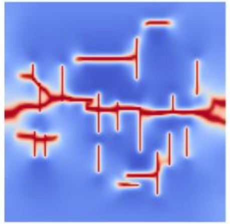


Initial configuration

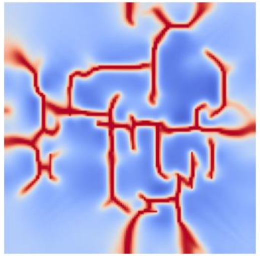
Fracture Foundation model

Predicted output

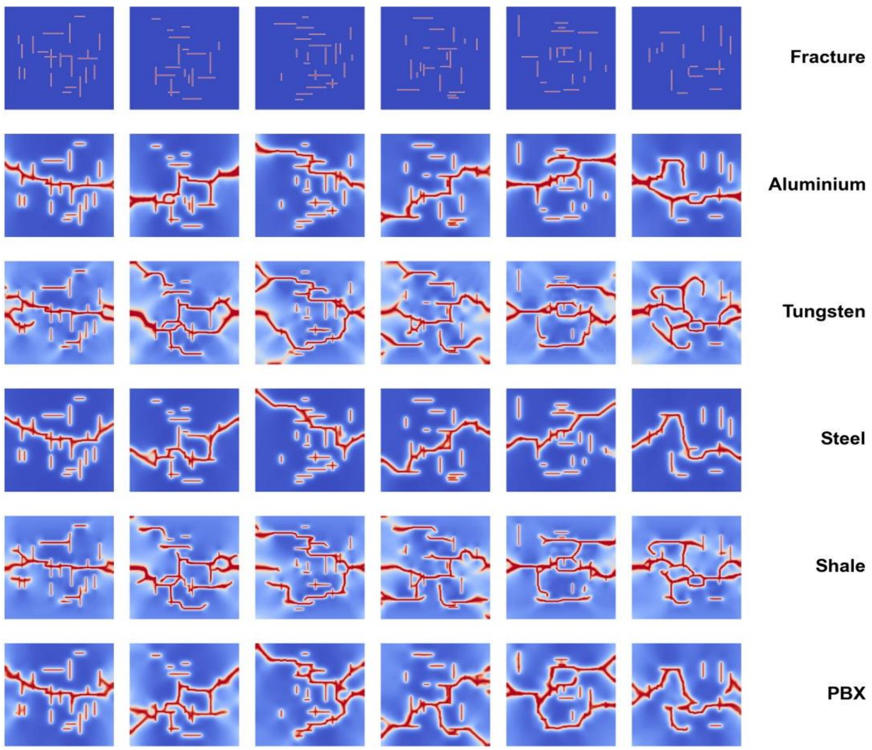
New boundary conditions



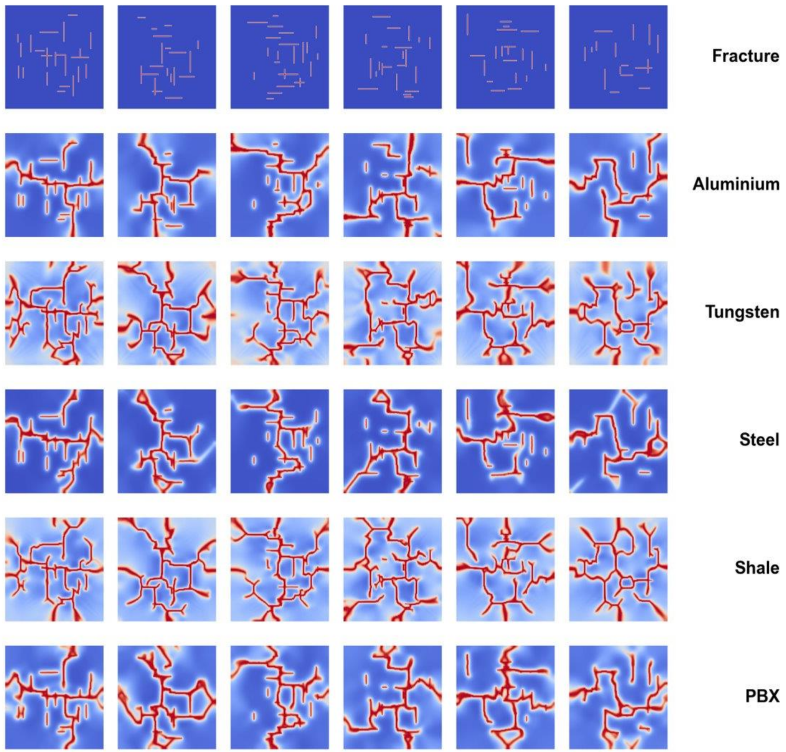
New boundary conditions



Our foundation model accurately predicts failure time and pattern for five materials



Pulling Horizontally



Pulling Horizontally and Vertically

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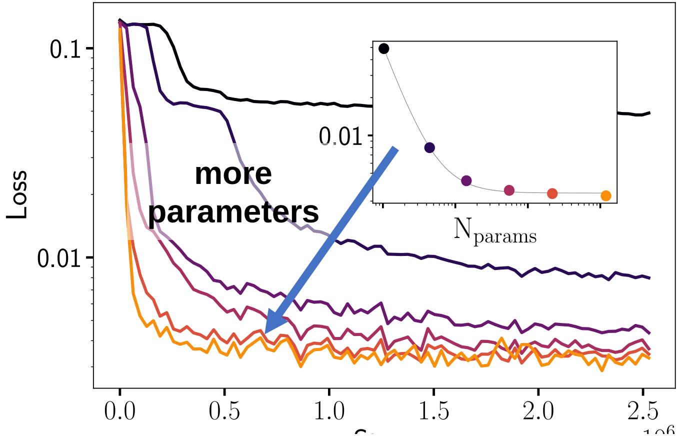
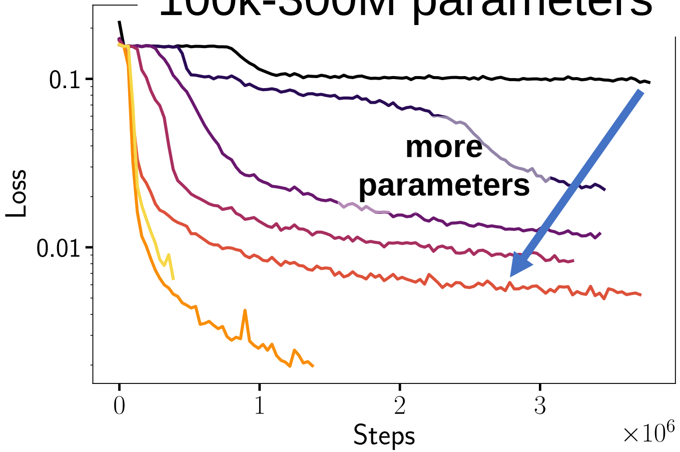
As physics complexity increases, more parameters are needed

- Scaling laws for fast rule-based fracture model
  - Very quickly the model performance saturates at ~5M parameters due to the relatively simple rule-based model
- Scaling laws for a quasistatic phase field model
  - Takes longer to saturate due to additional complexity (40M paramters)
  - Difficult to generate enough data leading to overfitting
- For fully dynamic model (HOSS), we anticipate even more parameters will be needed
  - How can we balance model complexity and speed to generate sufficient training sets?



100k-300M parameters



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Fracture Modeling Evolution

AI/ML

2014 — 2017 — 2019 — 2021 — 2023 — 2025

2014

Fracture DR
(20140002DR)
PI: Viswanathan
CNES

2017 (AI/ML)

Critical Stress
in Earth Crust
(20170004DR)
PI: Johnson
CNES

Advancing
Predictive
Capability for
Brittle Failure
using Dynamic
Graphs
(20170103DR)
PI: S
IS&T

2019

BES Core Funding
PI: Carey, P
Johnson,
Viswanathan,
C Johnson

U.S. DEPARTMENT OF ENERGY
Office of Science

Enabling Predictive Scale-
bridging Simulations Through
Active Learning
PI: Germann/Viswanathan
IS&T

2021

SMART ML FECM
PI: Viswanathan

SMART

Orphan Wells
PI: Viswanathan

CATALOG Consortium Advancing Technology for Assessment of Lost Oil & Gas Wells.

EFRC Carbon
Mineralization
PI: Viswanathan

U.S. DEPARTMENT OF ENERGY
Office of Science

2023

Director's Initiative
Foundation Models
PI: Viswanathan/O'Malley

Early Career Award
PI: O'Malley
ML and Quantum for
Fractured Systems

U.S. DEPARTMENT OF ENERGY
Office of Science

2025

FASST Initiative?

Project Snapshot

PROJECT EVOLUTION

- Where it started: Surrogate models for single material systems
- Progress so far: Models that generalize to multiple material types
- Next steps: Design high entropy alloy (HEA) materials with high fracture toughness using agentic AI

Artemis DI

IMPACTS

- Fracture prediction spans weapons & energy security
- Software: dfnWorks and HOSS are RD100 winners used to generate training data
- Tech deployment & implementation: in progress
- Publications & citations:
  Santos et al., Nature MI, 2023;
  Marcato et al., Neurips, 2025
- Comparisons to competitors: foundation model new to fracture modeling

Contributors & Collaborators

EES, CCS, T and XCP divisions

Collaborations with NAS/NAE members such as Bazant, Detournay, and Pyrak-Nolte

Numerous multi-laboratory national lab projects

Numerous projects that have involved industry (e.g. Chevron), academia and national labs.

Funding Sources

LDRD Directors Initiative on Artificial Intelligence with Office of Science, NA-22, Civilian Nuclear, and Applied Energy projects