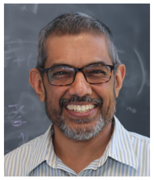
HTMDEC Kickoff
12-13 July 2022

DEVCOM ARMY RESEARCH LABORATORY

Caltech

HTMDEC

AI-enabled Rapid Direct Impact Test



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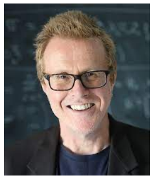

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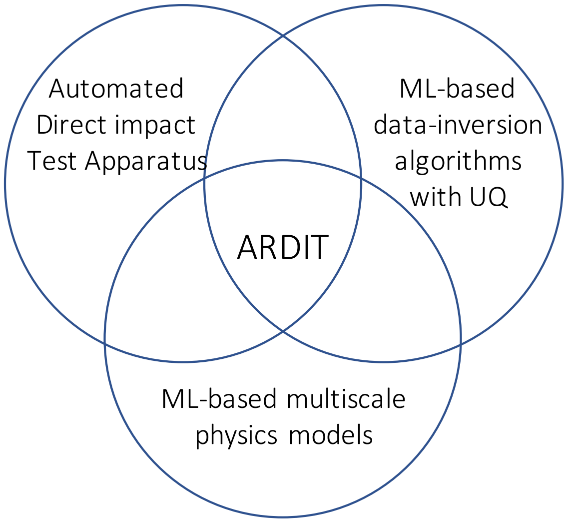
Overview

Goals

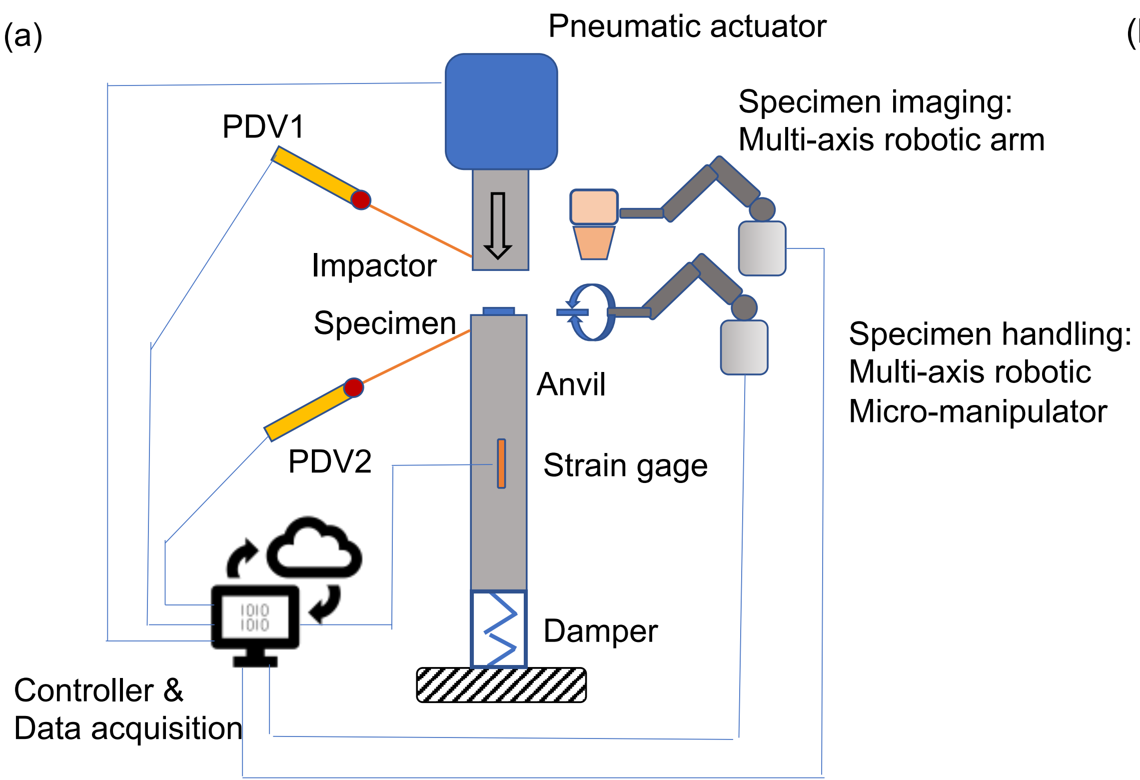
- Rapid characterization of mechanical properties under dynamic loads
    - 100s of test a day
    - Amenable to both materials screening and constitutive modeling
- Link macroscopic properties to microscopic materials

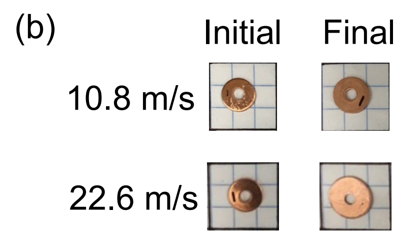


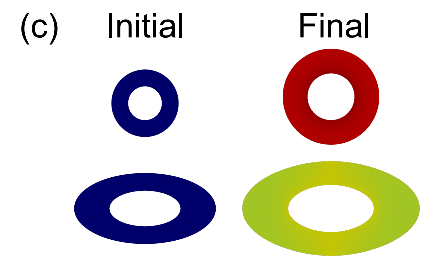
Concept: AI-enabled Rapid Direct Impact Test (ARDIT)

- Automated Direct Impact Test Apparatus (ADITA), which can be used to perform several hundreds of high-strain-rate tests per day without human intervention and supervision;
- ML algorithms for a Bayesian approach to inferring material properties from experimental observations with quantified uncertainties;
- ML-based multiscale physics models that link macroscopic experimental observations to microscopic mechanisms.

Automated Direct Impact Test Apparatus







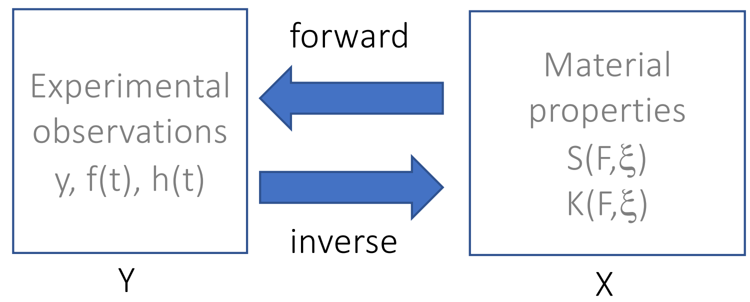
- 100s of test a day
- Strain rates of up to 10^5 s^{-1}
- Strains of up to 2
- Various strain paths
- Validate with copper and steel

Let's talk

- Broad range of materials

Inverse problem: Experimental observations to material properties

- Formulate as a Bayesian inverse problem: obtain material properties and uncertainties



- ML-enabled approach
  - Use numerical simulation of forward problem to generate data $\{X_i,Y_i\}$
  - Learning strategy A: learn the inverse map Y to X
  - Learning strategy B: learn the forward map X to Y and use it as a surrogate for the inverse map

- Materials screening and detailed characterization
  - Semi-inverse approach
  - Parameter fitting

  Inline data inversion for material screening

  - Constitutive discovery and identification of state variable

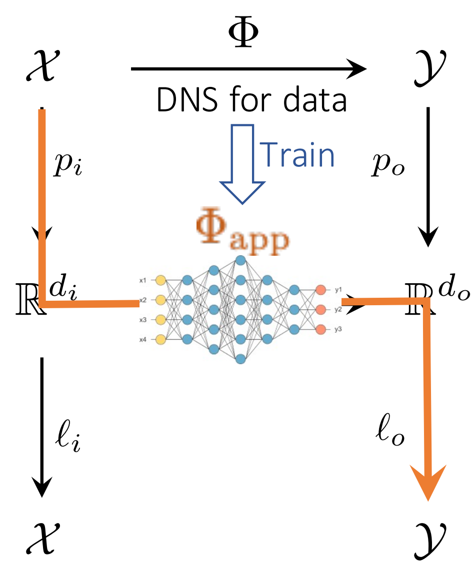
  Off-line data inversion for detailed characterization

Let's talk
- Applicable to broad range of experimental methods
- Expands the universe of experimental design

- Uncertainty quantification

Key challenges

- Dimensionality
  - Mathematically, the experimental observation and properties are functions
  - Practically, observations and properties available at variable resolution/fidelity and must be transferable
  - We formulate these as neural operators maps between function spaces
    Examples: PCA-Net, Fourier Neural Operator, Recurrent Neural Operator
    (Joint work with Anima Anandkumar and others)



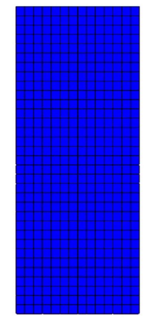
- History dependance and identification of state variables
- Well-posedness of the inverse problem
- Experiment design

Let's talk
- Versatile architectures for approximating operators

Link macroscopic properties to microscopic mechanisms

- Repeated solution of the fine scale
- Need to generate representative fine-scale structure
- Use a tiny portion of the information at the coarser scale

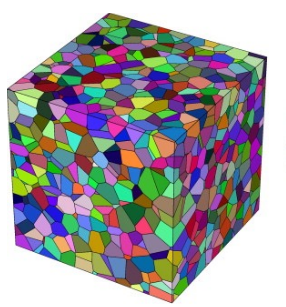
$$\{F(\tau) : \tau \in (0,t)\}$$



$$\begin{aligned}
&\nabla \cdot \bar{S} = \bar{\rho} u_{tt} && \text{on } \Omega \\
&u(x,0) = u_0(x), \quad u_t(x,0) = v_0(x) && \text{on } \Omega \\
&u(x,t) = u^*(x,t) && \text{on } \partial_1\Omega \\
&\bar{S}(\nabla u) n(x) = s^*(x,t) && \text{on } \partial_2\Omega
\end{aligned}$$

We seek to

- Learn the solution operator of the fine scale model using data generated by repeated solution
- Discover hidden physics or closure relation



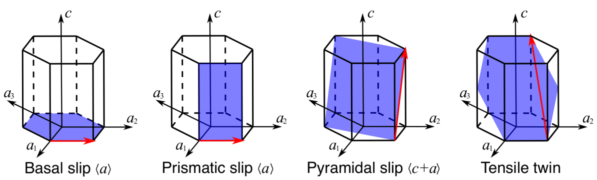
$$\begin{aligned}
&\nabla \cdot S(F + \nabla v, \xi, x, y) = 0 && \text{on } Y \\
&K(F + \nabla v, \xi, \xi_t, x, y) = 0 && \text{on } Y \\
&\xi(y,0) = \xi_0(y) && \text{on } Y \\
&v \text{ periodic}
\end{aligned}$$

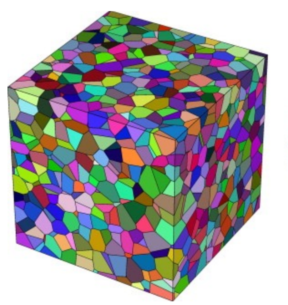
$$\bar{S}(t) = \langle S(F + \nabla v, \xi, x, y) \rangle_Y$$

We want to learn the actual operator, not postulate a law and learn parameters!

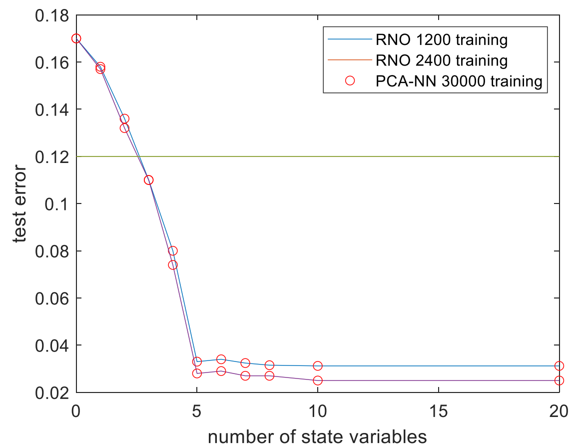
Link macroscopic properties to microscopic mechanisms

Generate data with from simulation



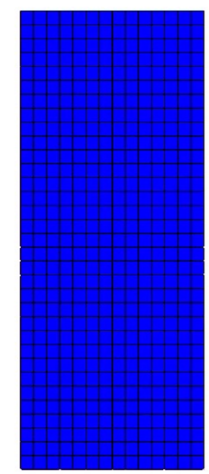


Use data to train an RNO



- Identifying state variables is part of the learning
- State variables provides insight into operating mechanisms

Use in macroscopic simulation

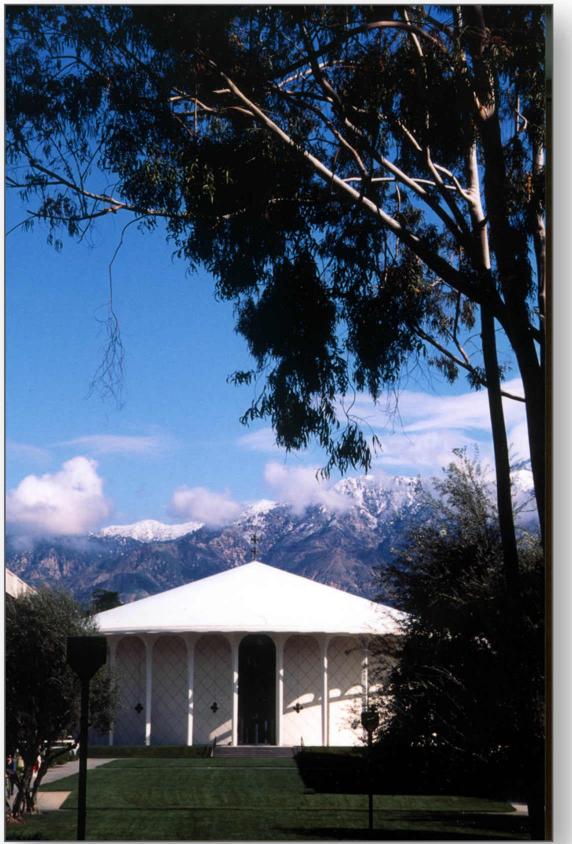


Let’s talk

- An approach to learn hidden physics
- Incorporate microscopic mechanisms in device design

Collaboration

- Monthly virtual seminars
- Close interaction with the data seedlings
- Visit ARL and other sites
- Host visitors at Caltech
- Workshop in January



Timeline

	Q1	Q2	Q3	Q4
ADITA and experimental campaign				
Fabrication of ADITA				
Preliminary data (Copper and TRIP steel)				
High throughput datasets				
ML-based data inversion and uncertainty quantification				
General UQ framework				
Data inversion with steps 1 and 2; strategy A				
UQ characterization for steps 1 and 2				
Data inversion with step 3; strategy B				
ML-based multiscale Physics models				
Multiscale plasticity and hidden variables (step 3)				
Mechanism identification from data				
Plasticity and failure (step 4); parametric				
Collaboration strategy				
Coordination with ARL researchers				
Coordination with other seedlings				
Caltech workshop				
Center building				

Goals for April 2023

- Build ADITA and validate using copper and steel
- Data inversion algorithm and first implementation
- Methodology to identify active mechanisms from data
- Collaboration with ARL and other seedlings
  - Learn from your methods
  - Transfer our methods
  - Integrate approach into a rapid material design loop

Some references

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