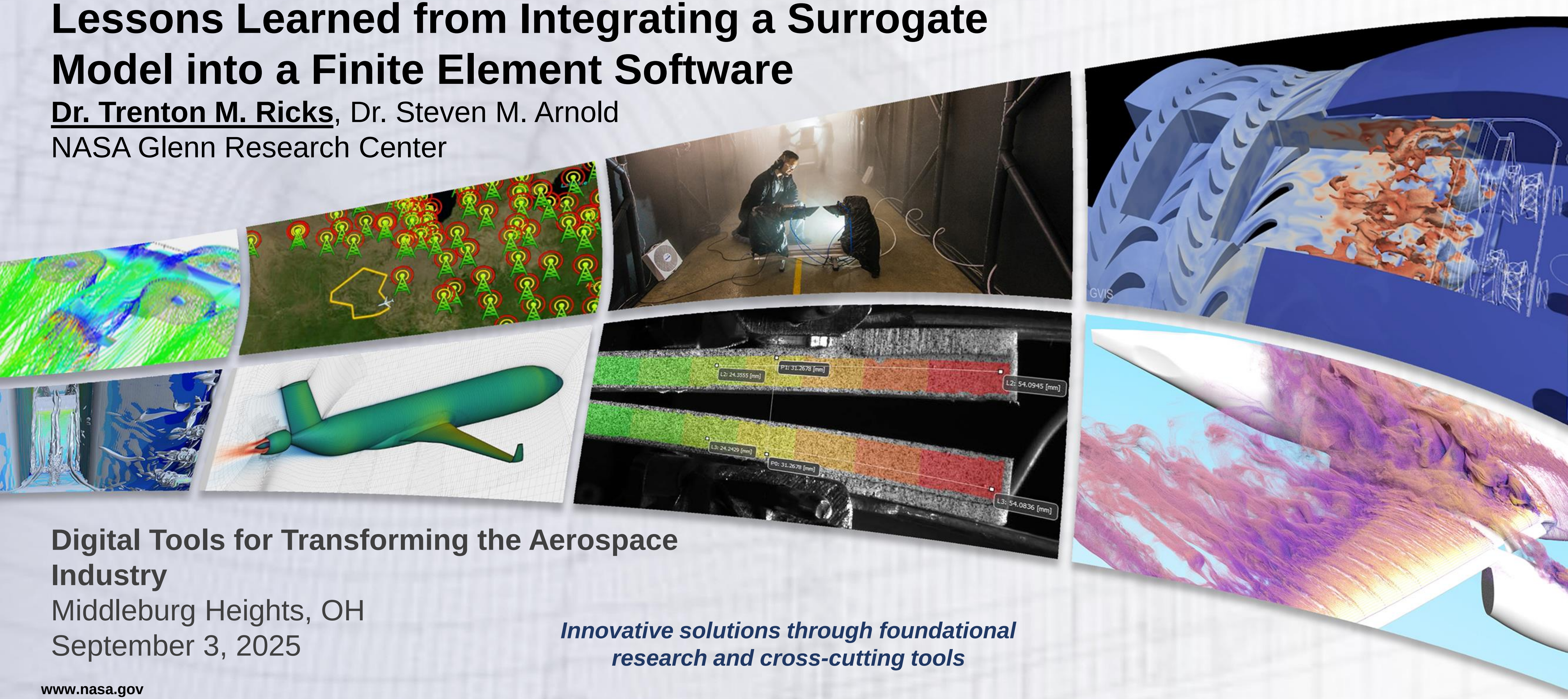
National Aeronautics and Space Administration

Transformational Tools and Technologies (T^3) Project

Lessons Learned from Integrating a Surrogate Model into a Finite Element Software

Dr. Trenton M. Ricks, Dr. Steven M. Arnold
NASA Glenn Research Center

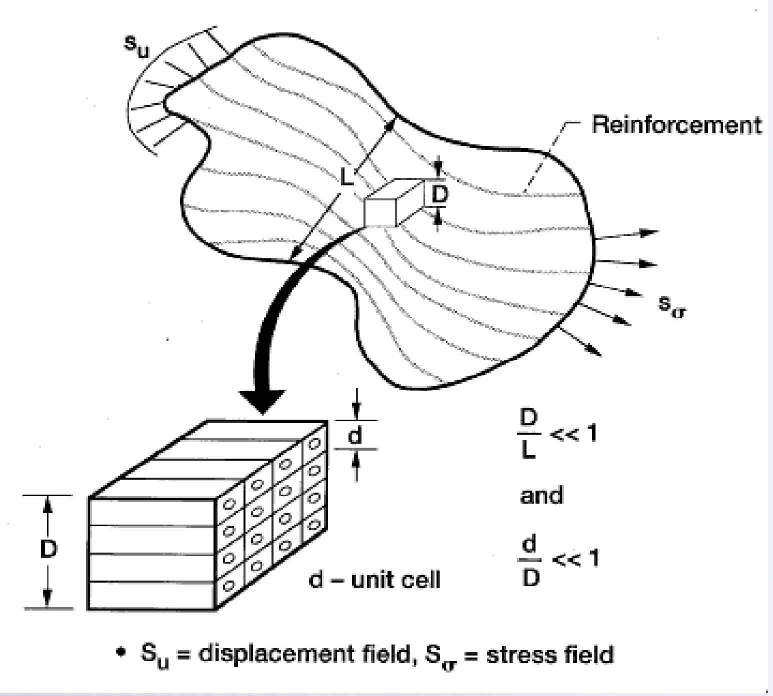


Digital Tools for Transforming the Aerospace Industry
Middleburg Heights, OH
September 3, 2025

Innovative solutions through foundational research and cross-cutting tools

Macromechanical Approach

Composite viewed as an anisotropic homogenous material in its own right – with its own experimentally measurable properties

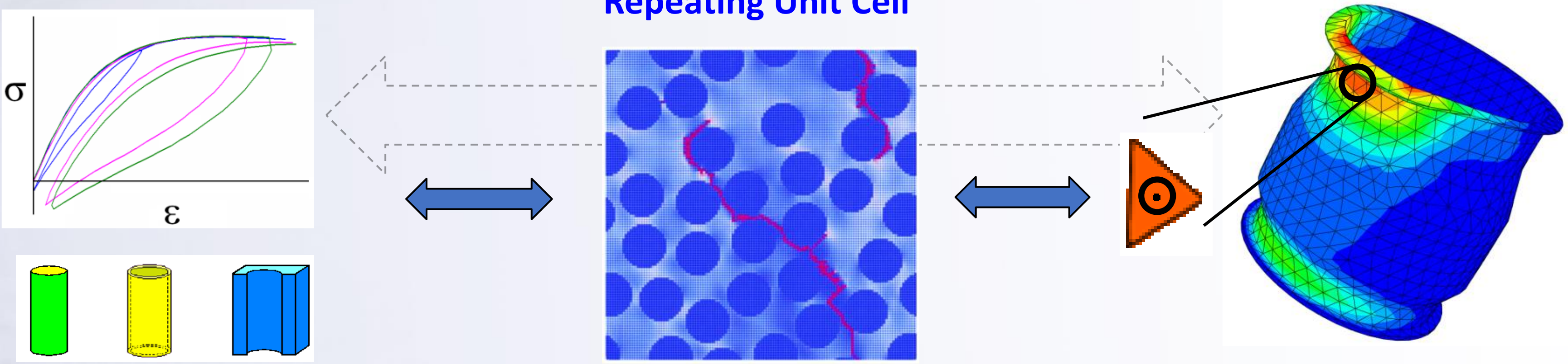


Representative Volume Element (RVE) Size Affects the Validity of Macromechanics Approach

- **Advantages**
  - Material itself performs the homogenization procedure from the micro to the macro scale.
  - Lends itself to explicit experimental characterization
  - Alleviates any assumptions inherent to micromechanical approach, i.e., in-situ constituent response, interface characterization, etc.
- **Disadvantages**
  - Significant experimentation to resolve material parameters (dependent upon fiber volume fraction, architecture, orientation) as each variation is like new material
  - Limited to isothermal behavior
- **Applicability dependent upon**:
  - *Size of the internal texture of the material*
  - Characteristic structural dimensions
  - Severity of gradients (stress, temperature, etc.)

Micromechanical Approach

Links the behavior of a composite material/structure to the behavior of the constituents (e.g., nonlinear response of the resin and fiber failure)



Constituent Response

Composite Micromechanics Repeating Unit Cell

Structural Model

Fiber **Interface** **Matrix**

Micromechanics Provides the Link Between Structures and Materials

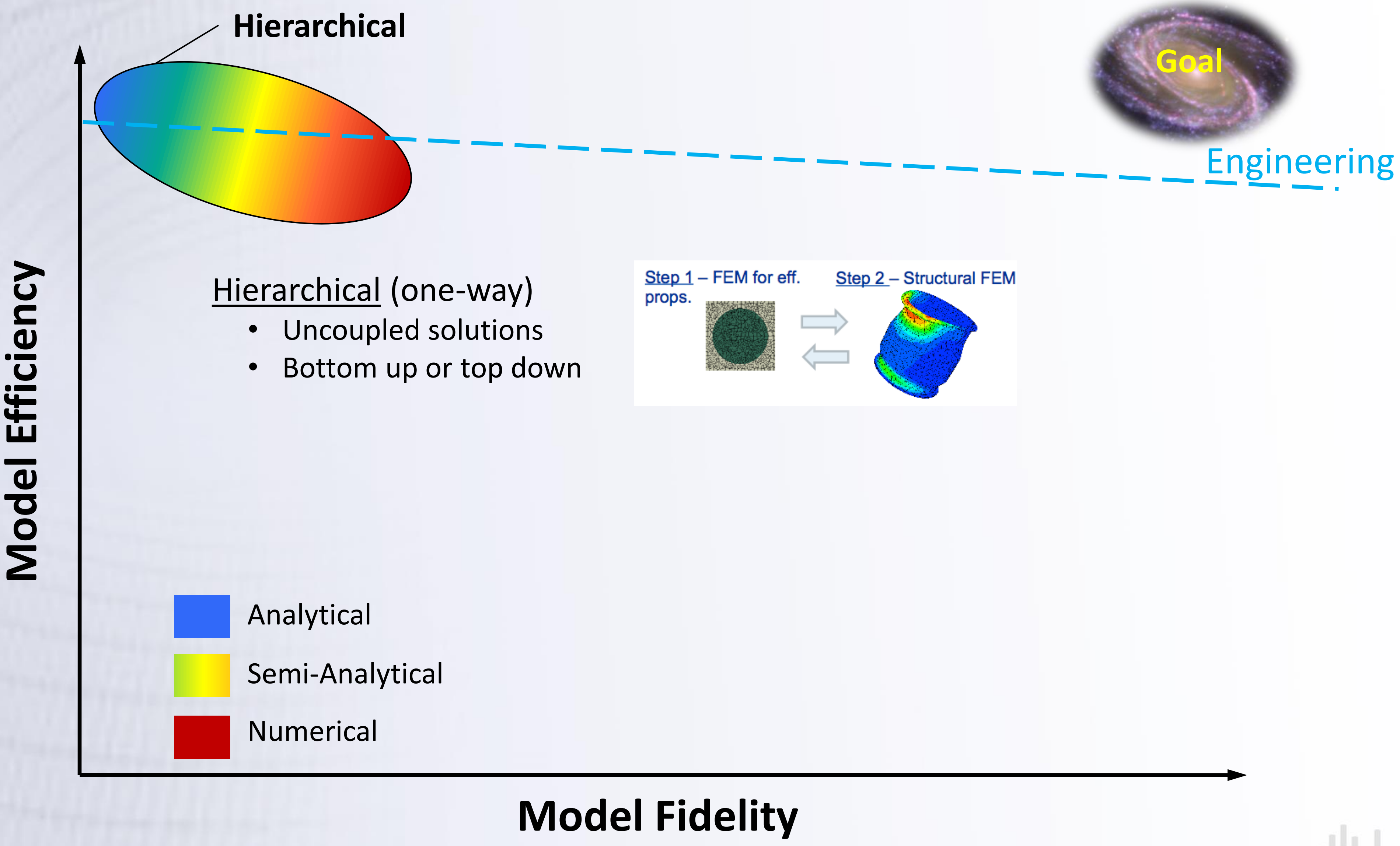
- The key link between the scales is micromechanics, which provides the composite response based on the constituent behavior and microstructure

Aboudi, J., Arnold, S.M., and Bednarcyk, B.A. (2013) *Micromechanics of Composite Materials: A Generalized Multiscale Analysis Approach*, Elsevier, Oxford, UK., pp 1-984.

Why Go Lower than the Ply?

	Advantages	Disadvantages
Macromechanical	1. Computational Efficiency 2. Experimental Testing incorporates all in-situ effects (interface, damage, etc) 3. Aligned with standard ply level design procedures 4. Tends to work well for • Fiber dominated situations • **Linear, isothermal regime**  =	1. **Anisotropic Constitutive Theory** 2. Requires additional complexities to handle • Tension/compression, Tertiary creep – damage • Multiaxiality/Hydrostatic interaction 3. Needs recalibrated (retesting) for changes in • Architecture/layup, Volume fraction, Processing history (residual stresses) 4. Phenomenologically based: accounts for physics of all nonlinearity on the wrong scale 5. Form of the constitutive law usually based on monolithic materials so applicability questionable 6. Adversely impacted by non-isothermal loading
Micromechanical	1. Predicts properties/behavior of any composite material 2. Enables capturing the physics of deformation and damage at more fundamental scale 3. Captures varying in-situ non-proportional, multiaxial stress and strain states (iso/nonisothermal) 4. Can employ simpler isotropic constituent constitutive models 5. Can employ simpler, more fundamental failure criteria 6. Microstructural effects explicitly captured 7. Can perform what-if scenarios for design of materials	1. **Increased computational expense** 2. Need for constituent material constitutive response (fiber/matrix) as well as composite testing for validation 3. Possible need to calibrate for in-situ effects 4. Interfacial behavior is a constant unknown 5. Lower Technology Readiness Level (TRL)

Practical Multiscale Models Must Balance Efficiency vs. Fidelity



Hierarchical (one-way)

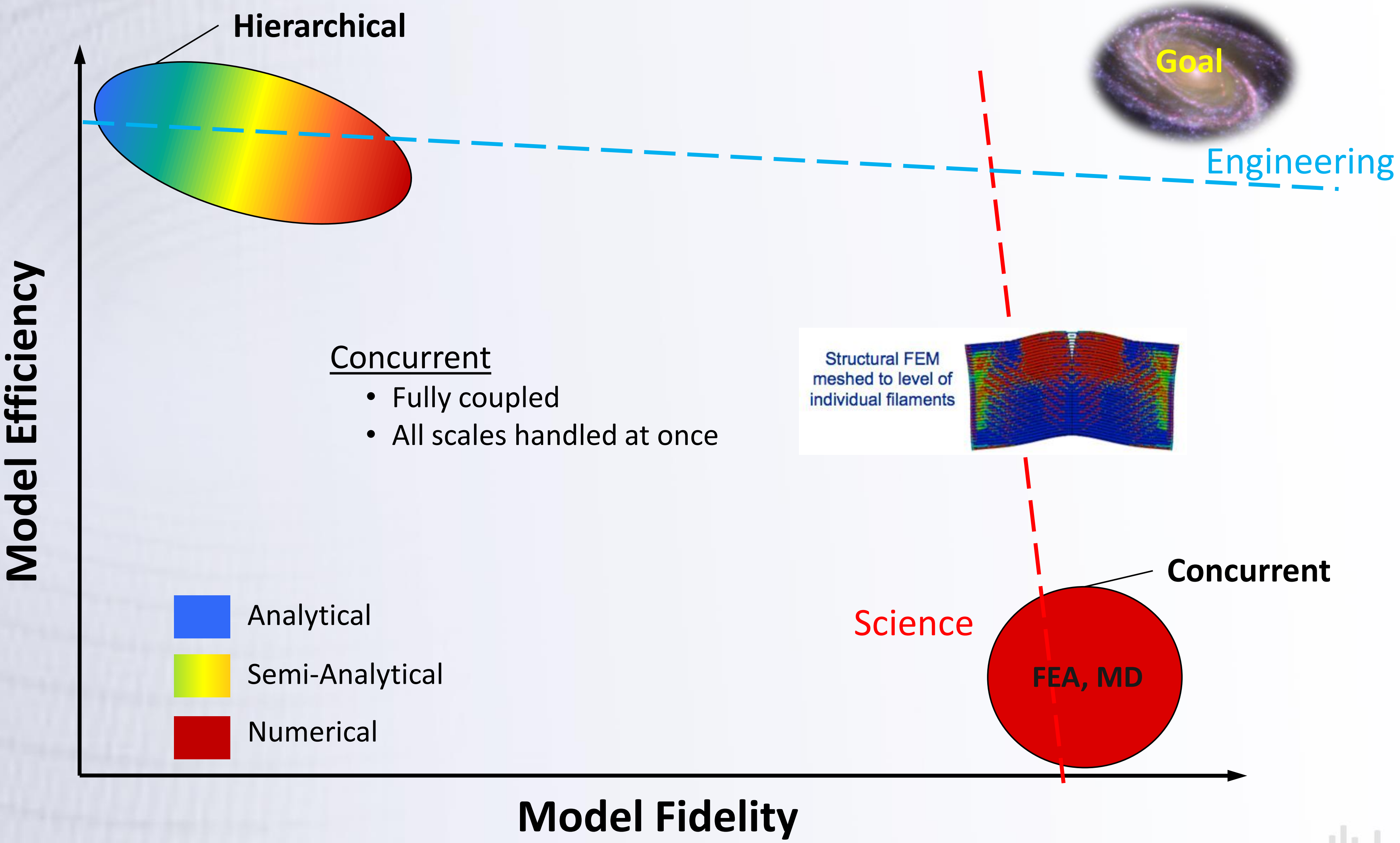
- Uncoupled solutions
- Bottom up or top down

🟦 Analytical

🟨 Semi-Analytical

🟥 Numerical

Practical Multiscale Models Must Balance Efficiency vs. Fidelity



Hierarchical

Goal

Engineering

Concurrent

- Fully coupled
- All scales handled at once

Structural FEM meshed to level of individual filaments

Concurrent

Science

FEA, MD

🟦 Analytical

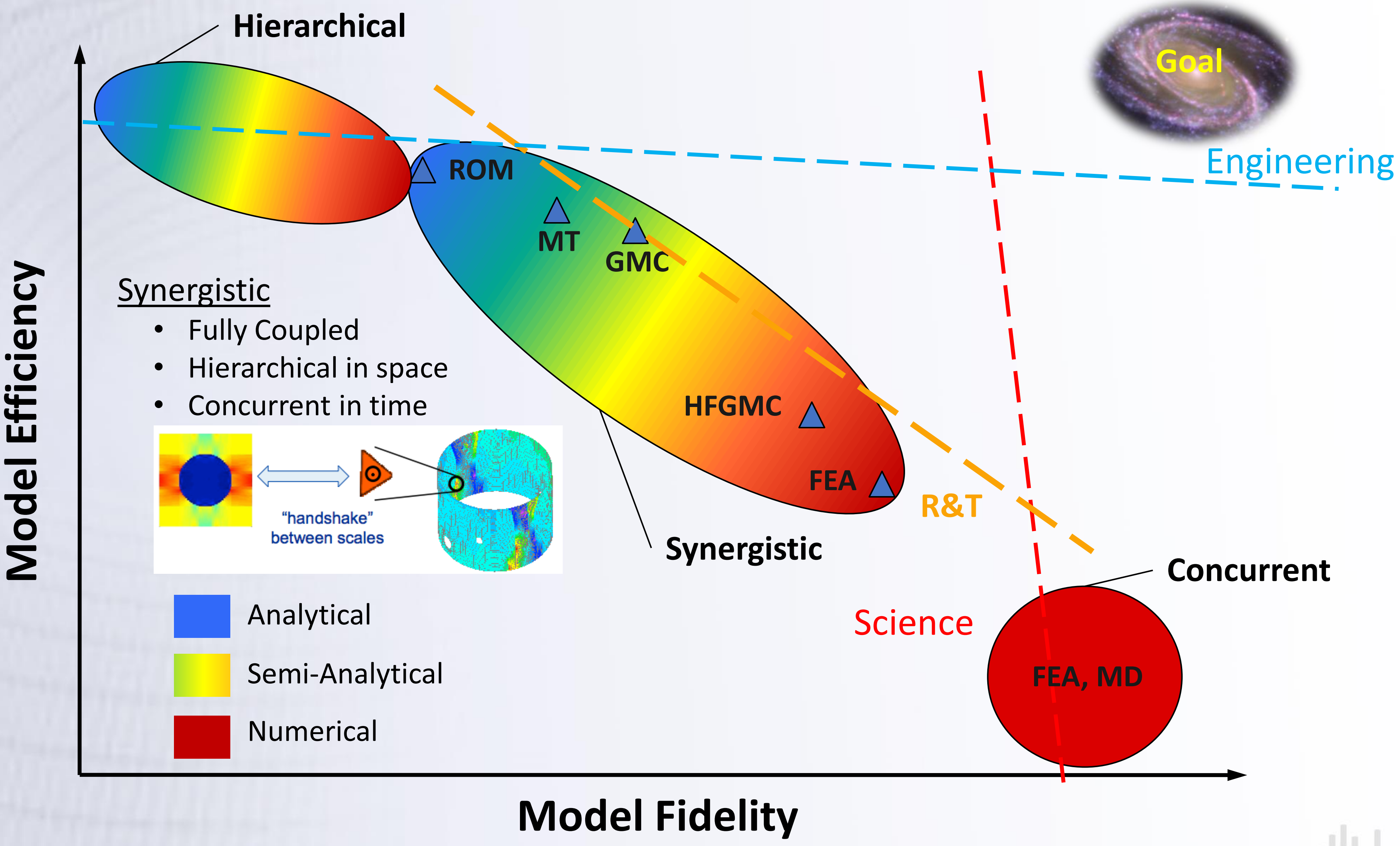
🟨 Semi-Analytical

🟥 Numerical

Model Efficiency

Model Fidelity

Practical Multiscale Models Must Balance Efficiency vs. Fidelity



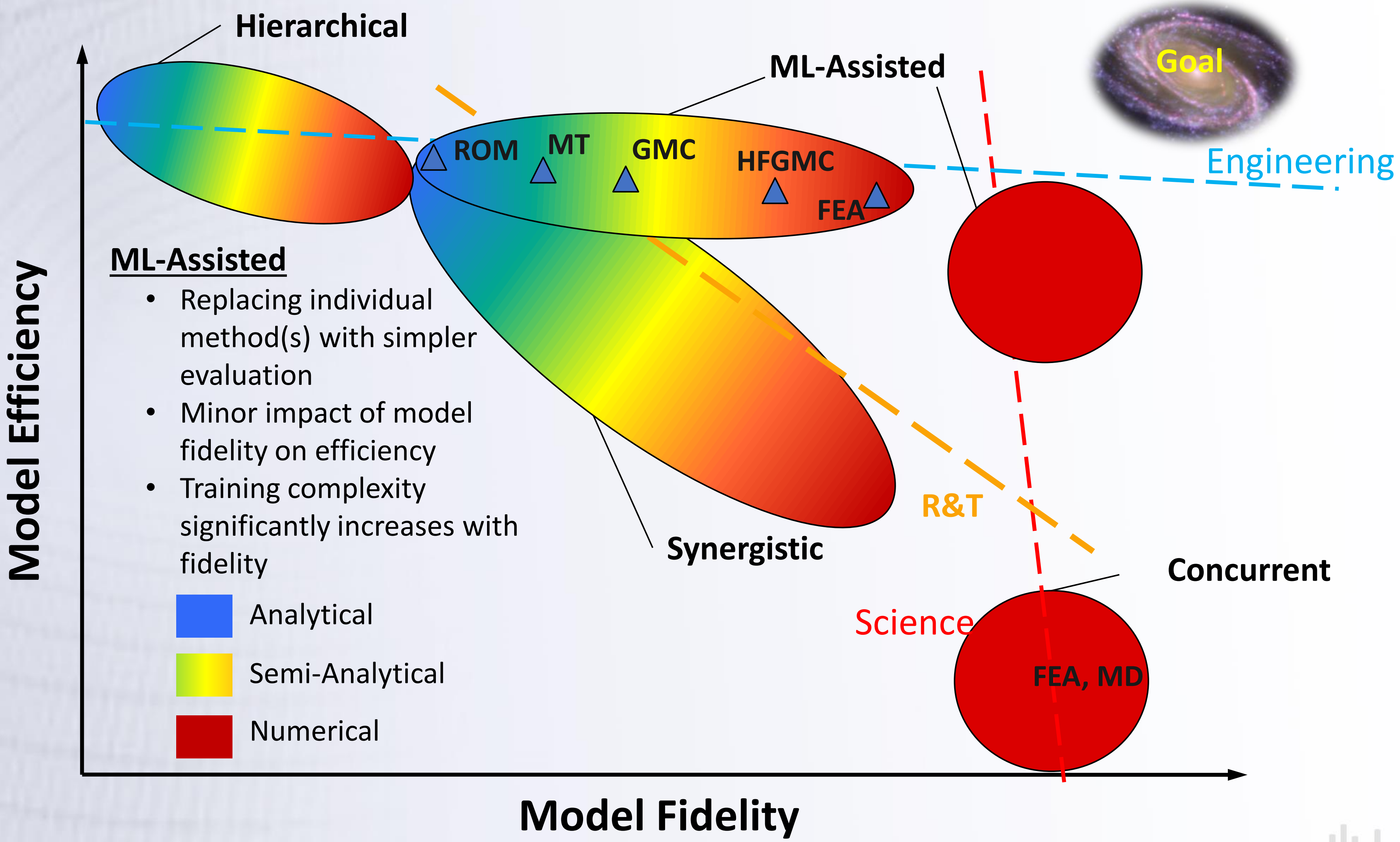
Synergistic
- Fully Coupled
- Hierarchical in space
- Concurrent in time

🟦 Analytical

🟨 Semi-Analytical

🟥 Numerical

Surrogates Enable More Complex Multiscale Analysis



ML-Assisted

- Replacing individual method(s) with simpler evaluation
- Minor impact of model fidelity on efficiency
- Training complexity significantly increases with fidelity

🟦 Analytical

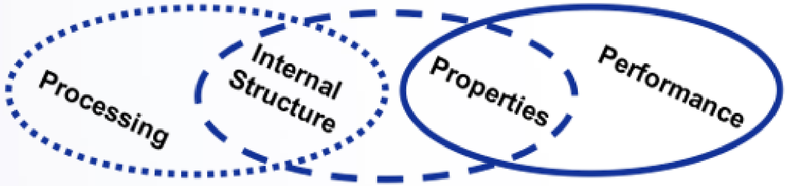
🟨 Semi-Analytical

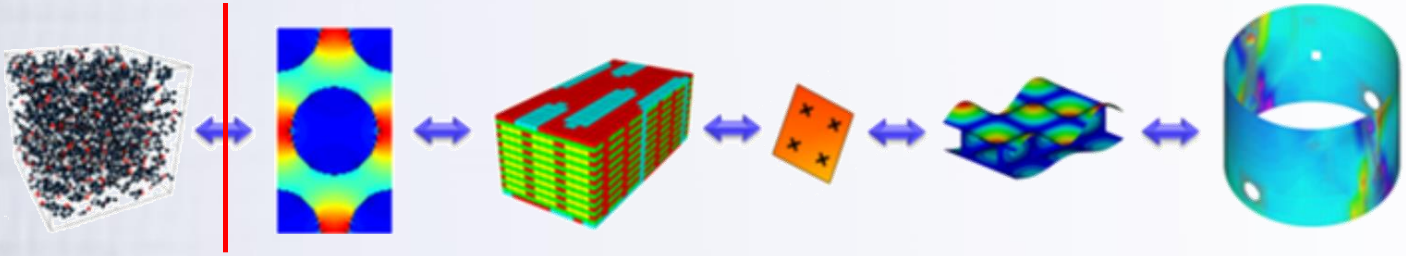
🟥 Numerical

NASA Multiscale Analysis Tool (NASMAT)

- Successor to MAC/GMC and FEAMAC toolsets
- Clean-sheet redesign of 25+ years of software tools
- Framework designed to support massively multiscale modeling suitable for both design and analysis problems
  - Solves industrial-sized, nonlinear, thermo-mechanical and multiphysics problems
- Ability to tailor analyses to balance accuracy and efficiency
- Library of constitutive laws, damage models, and micromechanics theories
- Flexible modular design to support “plug-and-play” capabilities
- Developed for enhanced interoperability with 3rd party codes (e.g., FEA)
- Pre- and post-processing to support multiscale model development and visualization

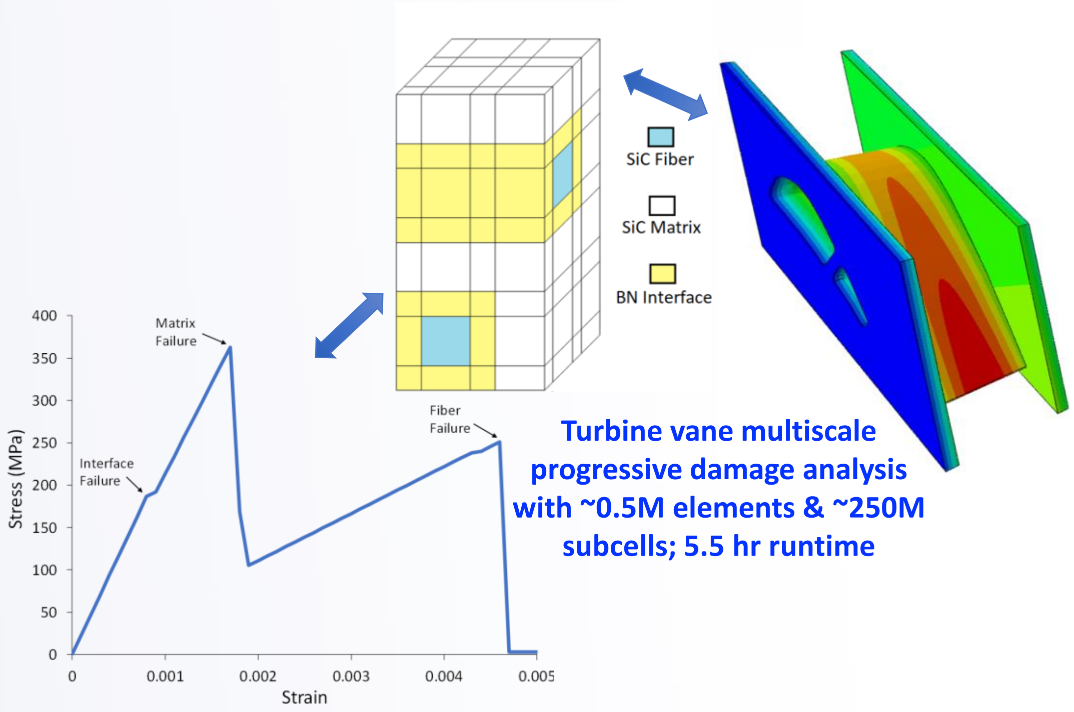
NASMAT
NASA Multiscale Analysis Tool





High-Fidelity Multiscale Modeling Unable to Simulate Large Structures (Practically)

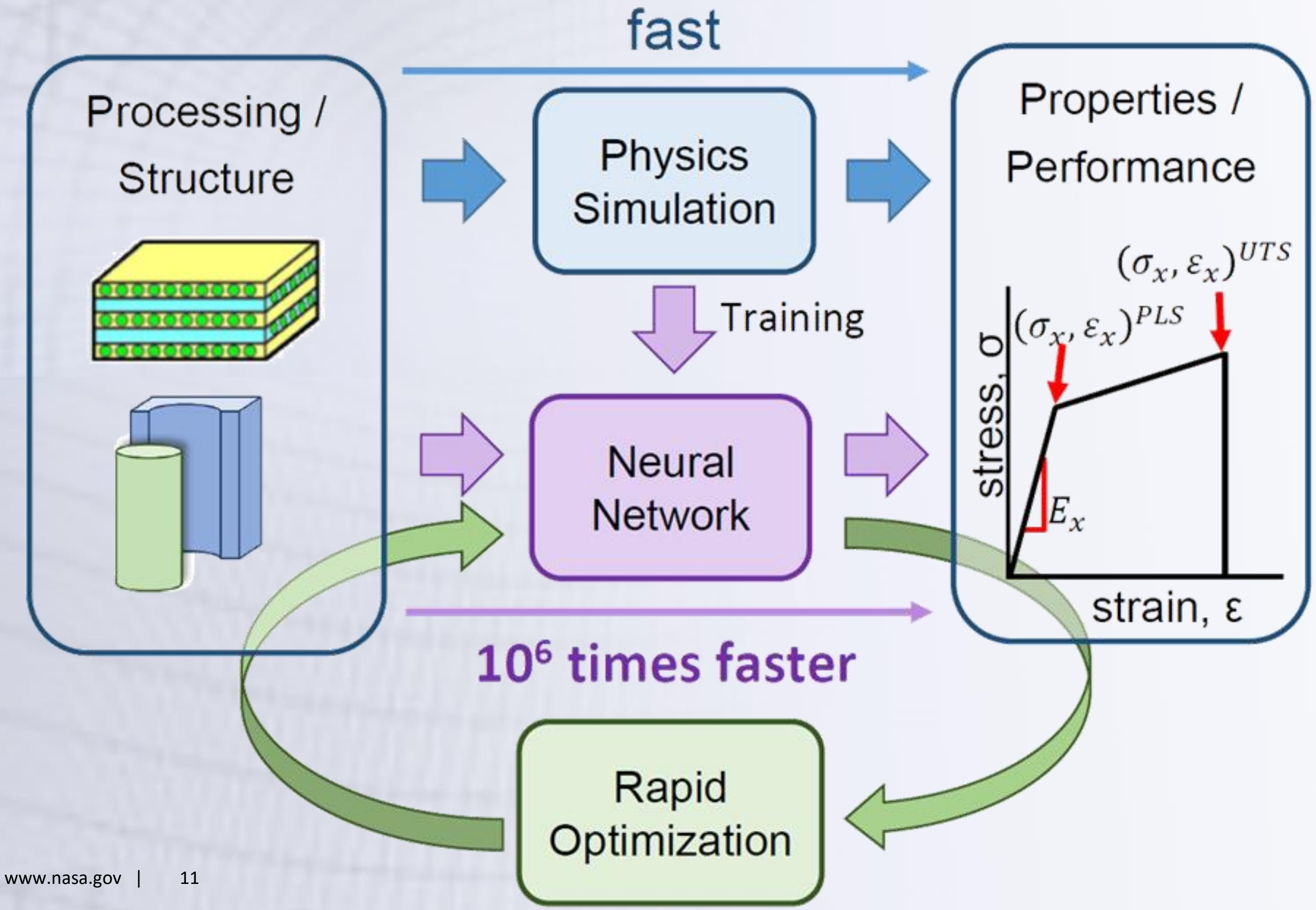
- Multiscale analysis of a turbine vane previously demonstrated (VERY large analysis over typical)
  - But…
    - Single vane
    - Single physics
    - Single NASMAT RUC
    - Simplified unit cell and micromechanics method
    - Linear elastic constitutive model
    - Simple failure model
- Extending approach to simulate larger structures virtually impossible (for typical computing capabilities)
  - Runtime and memory
- Challenges increase as number of scales/features increase
- **Replacing high-fidelity methods with surrogate models could circumvent these shortcomings**



Turbine vane multiscale progressive damage analysis with ~0.5M elements & ~250M subcells; 5.5 hr runtime

Multiscale Surrogate Able to Rapidly Predict Macroscale Performance Metrics

- Inputs: 13 possible composite layups, constituent properties
- Outputs: macroscale performance metrics



fast

Processing / Structure

Physics Simulation

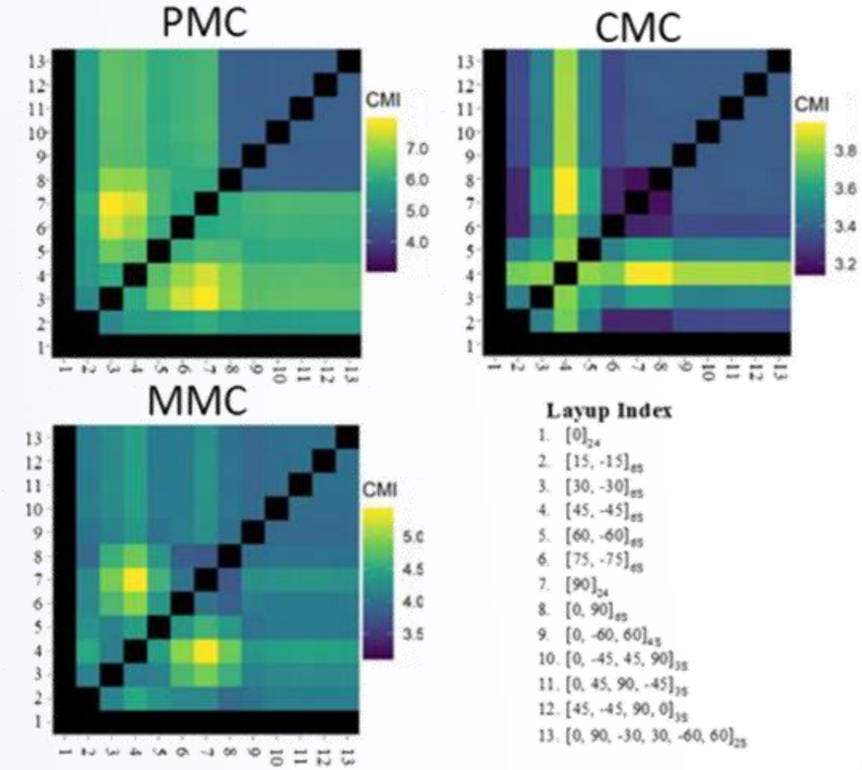
Training

Neural Network

Properties / Performance

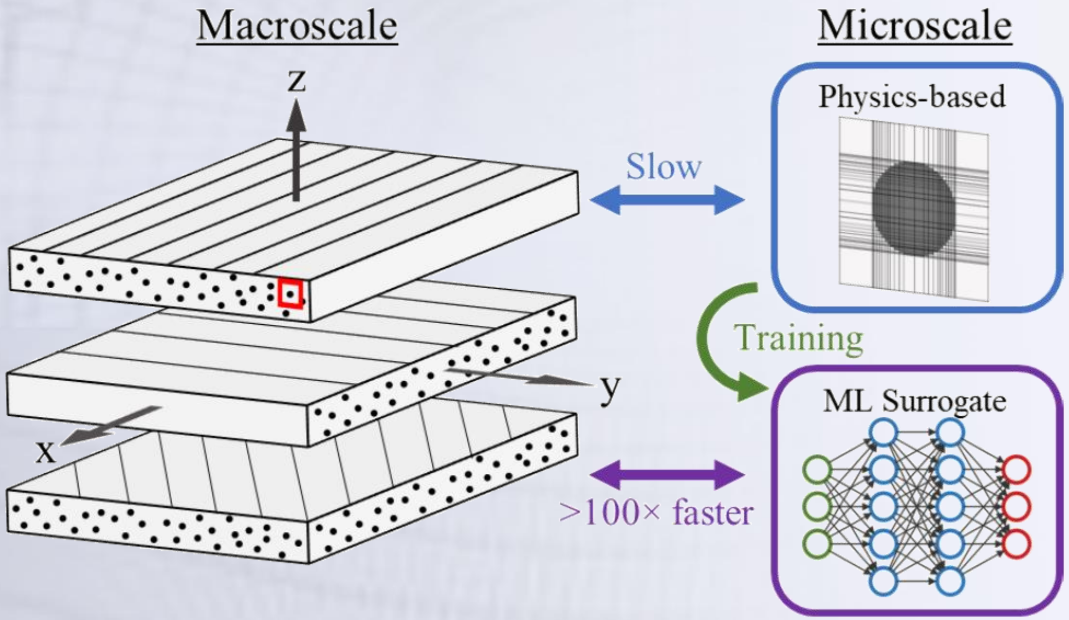
10^6 times faster

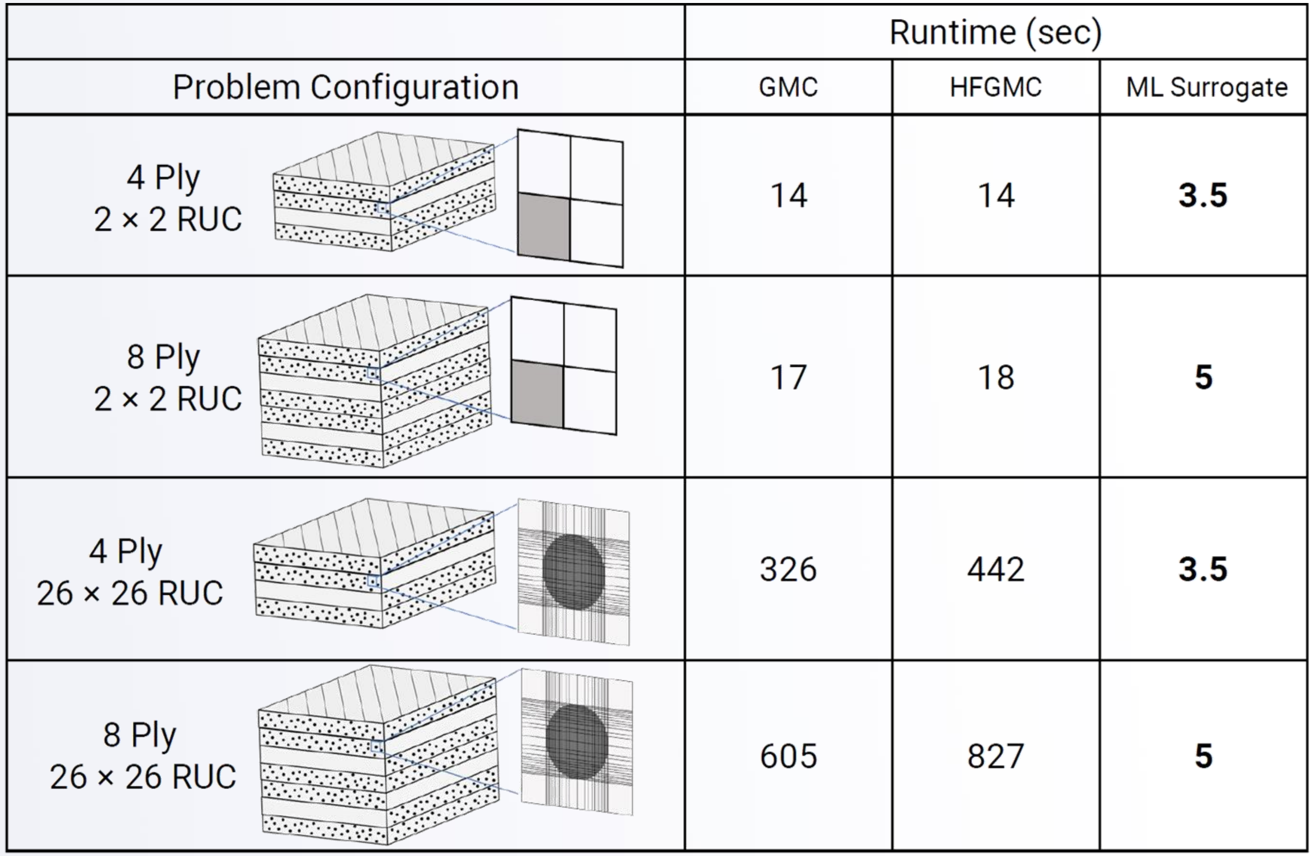
Rapid Optimization



Ply Level Surrogate Gives Broader Generality, but at a Cost

- Replacing physics-based model for the ply with surrogate
- Still utilizing physics-based model to get macroscale behavior

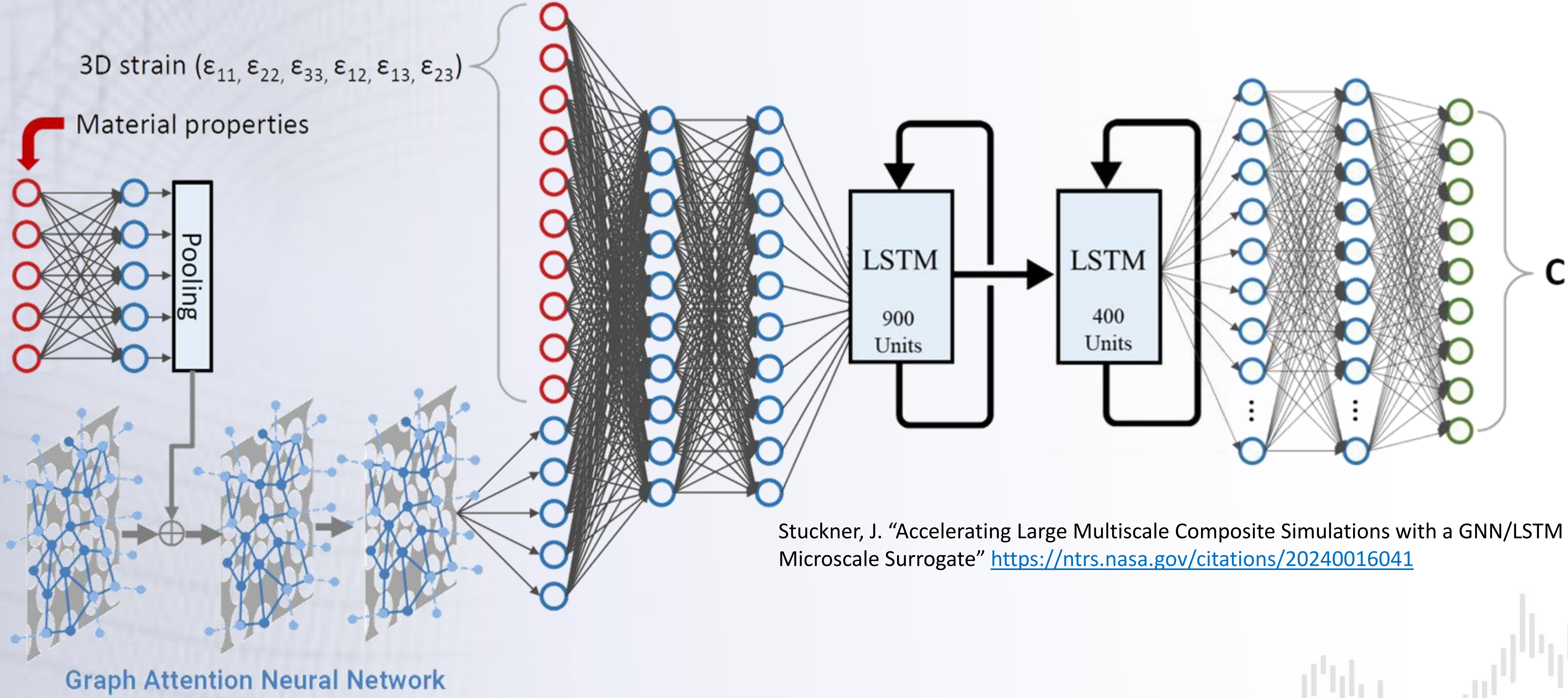




Problem Configuration	Runtime (sec)		
	GMC	HFGMC	ML Surrogate
4 Ply 2 × 2 RUC	14	14	**3.5**
8 Ply 2 × 2 RUC	17	18	**5**
4 Ply 26 × 26 RUC	326	442	**3.5**
8 Ply 26 × 26 RUC	605	827	**5**

A Surrogate Model to Replace NASMAT HFGMC2D

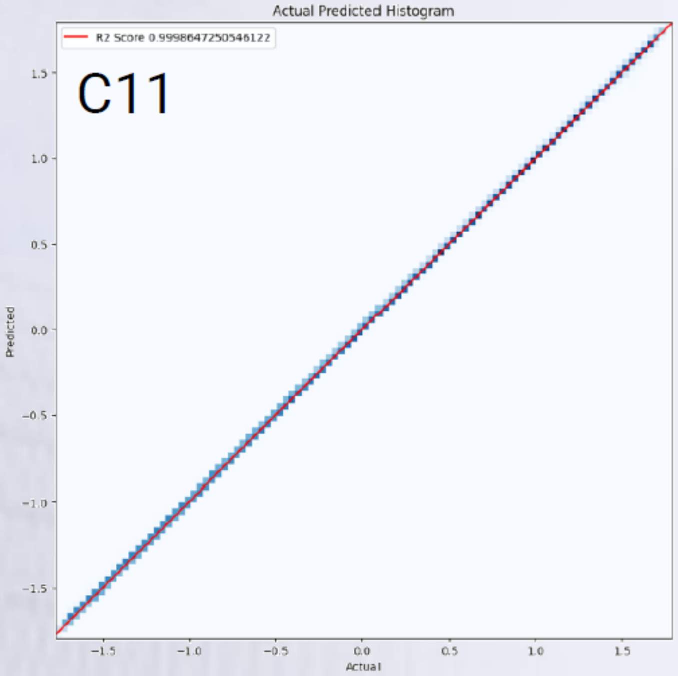
Including material property and geometric variability

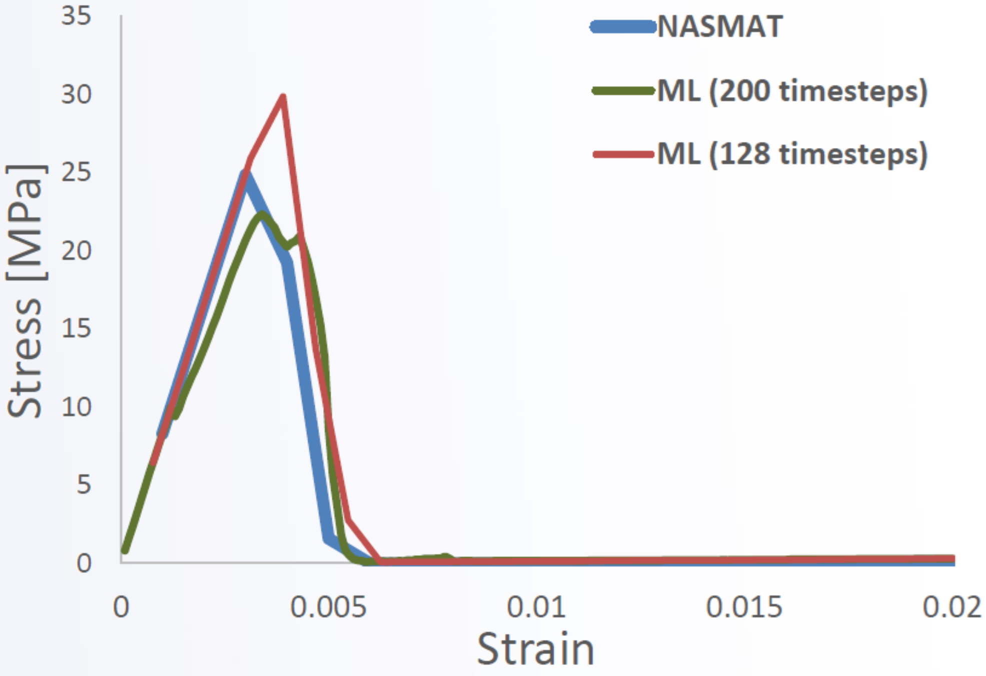


Stuckner, J. “Accelerating Large Multiscale Composite Simulations with a GNN/LSTM Microscale Surrogate” https://ntrs.nasa.gov/citations/20240016041

Surrogate Able to Accurately Capture Nonlinear Material Behavior at a Fraction of the Runtime

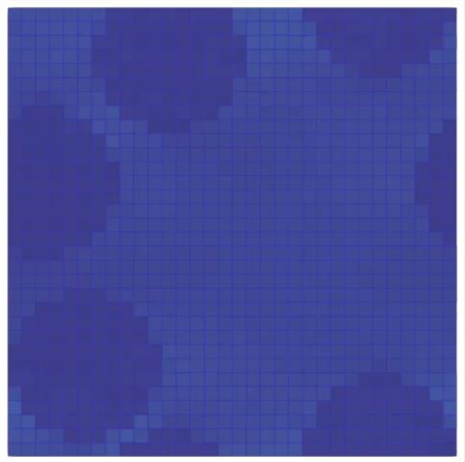
- r^2: 0.985-0.999 for each stiffness matrix component
- **Orders of magnitude less time to evaluate**

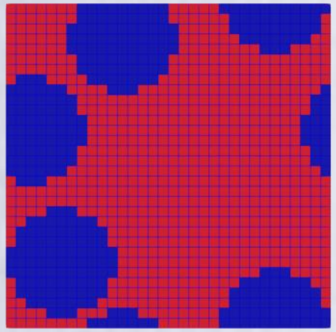




Performing Multiscale Analysis with Finite Element Software

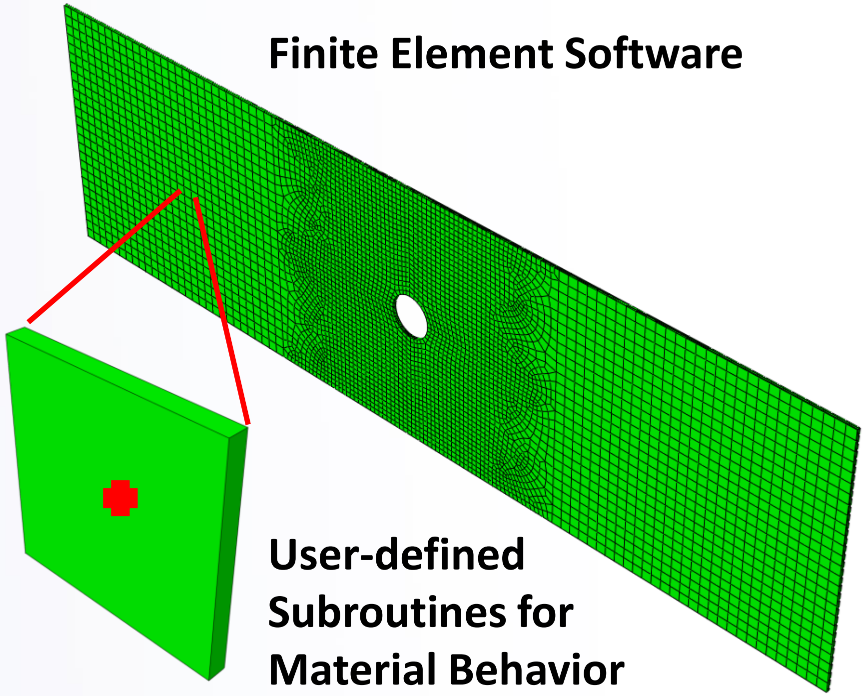
- Traditional approach common to multiple software packages (e.g., Abaqus, Ansys Mechanical, LS-DYNA, CalculiX)





NASMAT
NASA Multiscale Analysis Tool

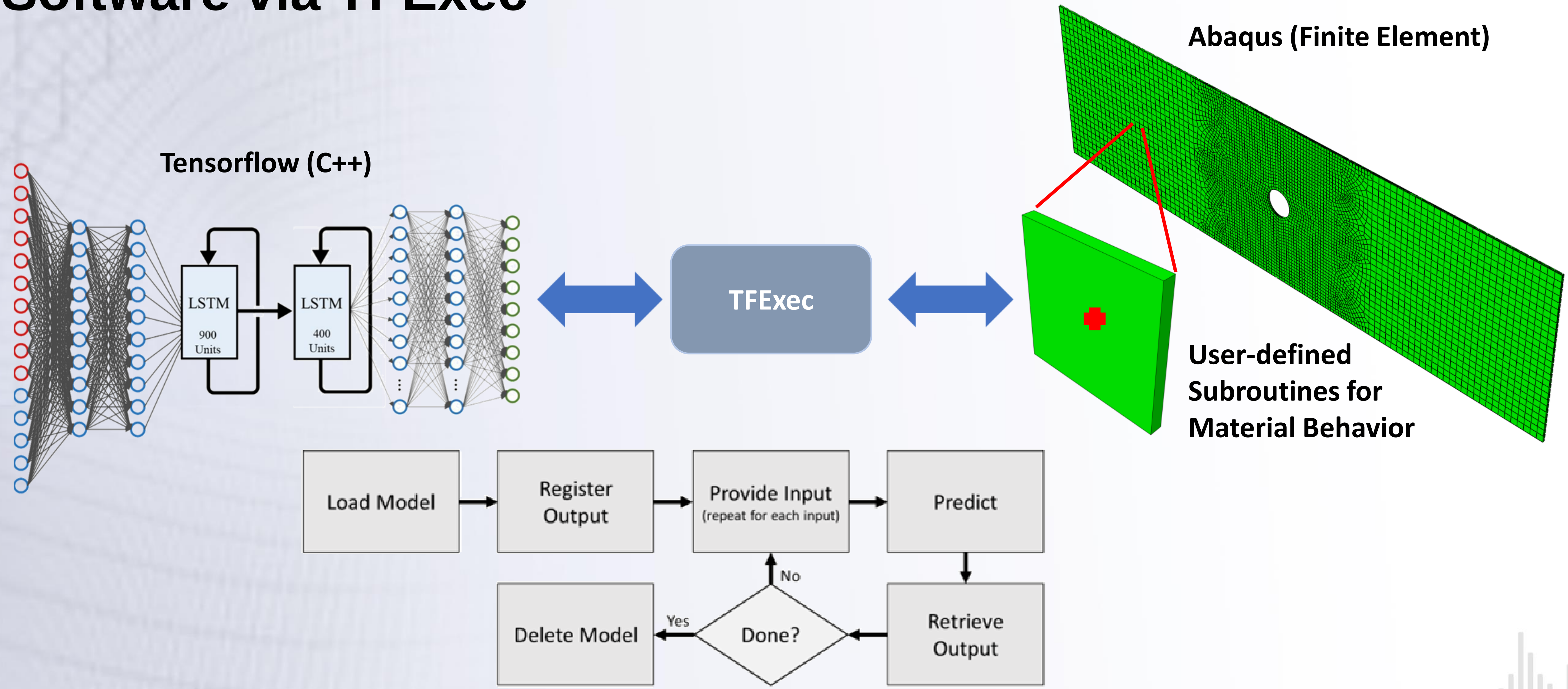
- Micromechanics Method
- RUC Geometry
- Constituent Model and Properties
- Failure Model



Finite Element Software

User-defined Subroutines for Material Behavior

Surrogate Model Coupled to Finite Element Software via TFExec



Tensorflow (C++)

TFExec

Abaqus (Finite Element)

User-defined Subroutines for Material Behavior

Load Model

Register Output

Provide Input
(repeat for each input)

Predict

Retrieve Output

Done?

No

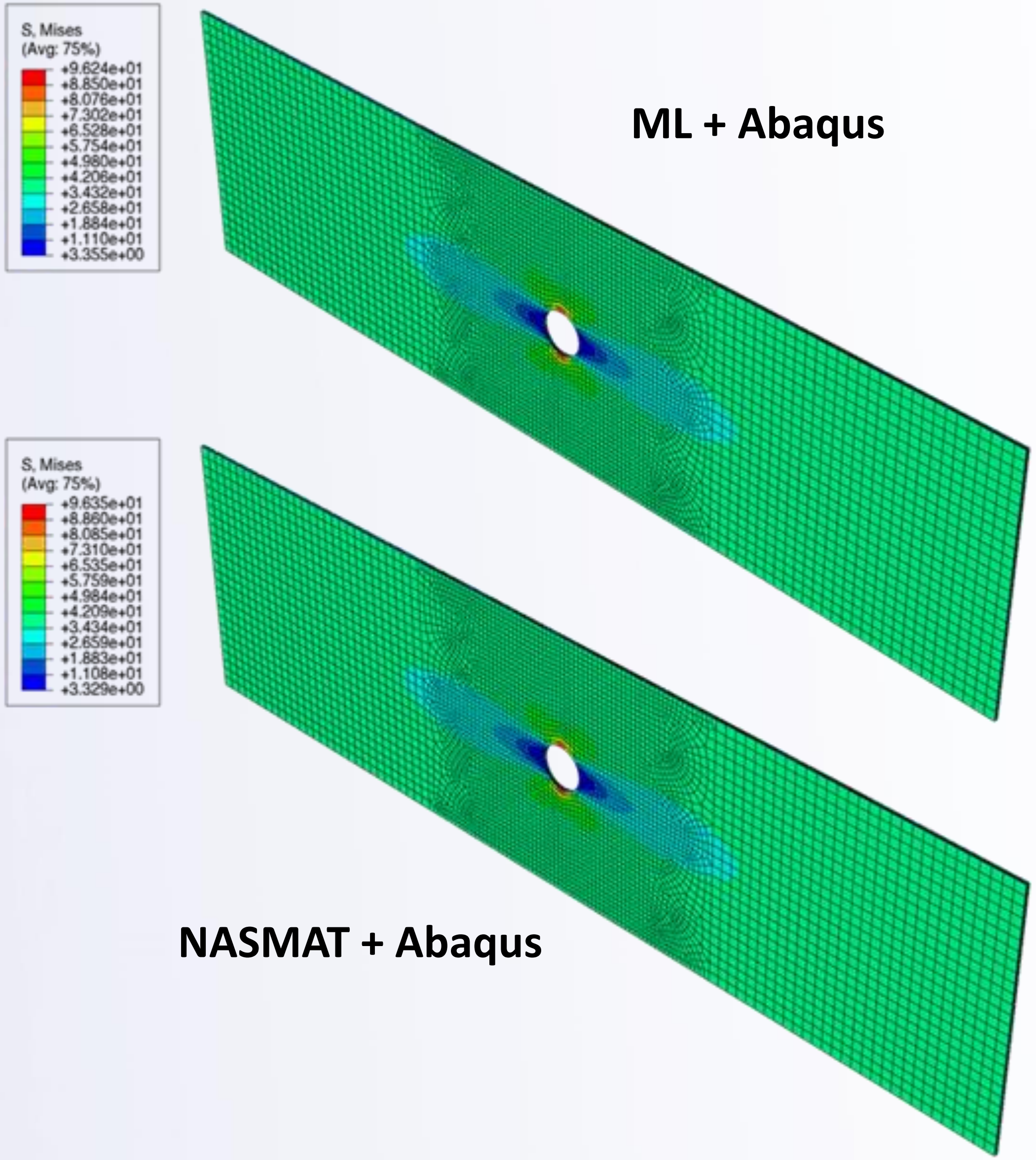
Yes

Delete Model

Howell, I. et al. “TFExec—A Fortran Bridge for TensorFlow Models” NASA/TM-20250005606. [GitHub - nasa/tfexec]

Surrogate Model Able to Replicate Physics-Based Model Results

- Same problem run with NASMAT and ML with Abaqus (12,348 elements)
- Consistent code architectures
  - E.g., limited NASMAT output
- Comparable stress fields obtained between ML and physics-based models



0.1% difference in max stress

Surrogate Model Performance Gives Mixed Results

	NASMAT	Surrogate (CPU)
Total Runtime (s)	5317	4315
---Preprocessing (s)	237	0.7
---User Material (s)	4995	4096
Memory (GB)	401	1

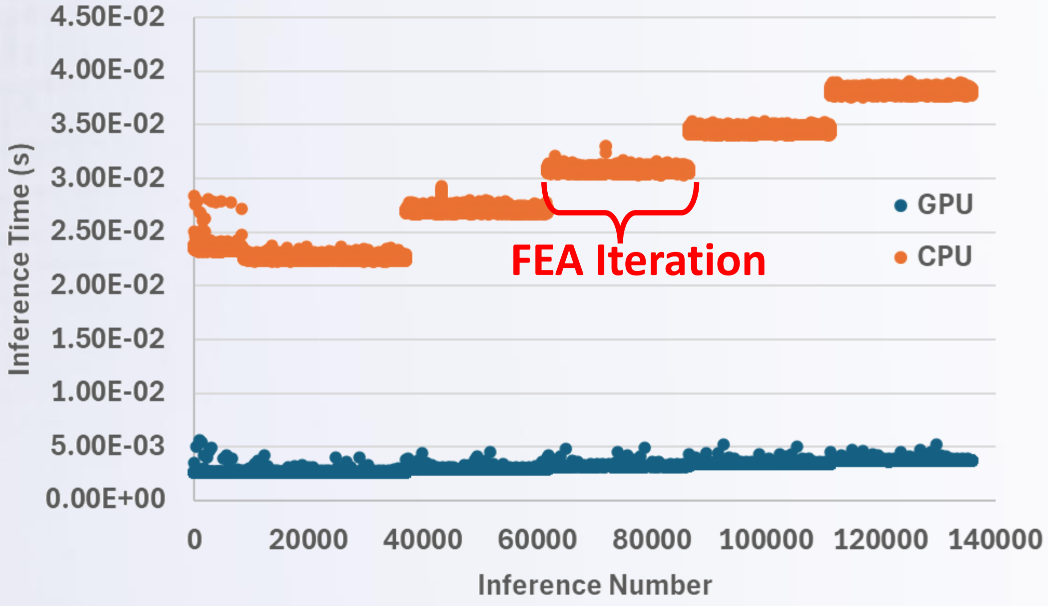
- Surrogate model runtime same order of magnitude as physics-based model
  - Reduced pre-processing time
- Required 400x less memory

Surrogate Model Performance Gives Mixed Results

	NASMAT	Surrogate (CPU)	Surrogate (GPU)
Total Runtime (s)	5317	4315	601
---Preprocessing (s)	237	0.7	2.2
---User Material (s)	4995	4096	445
Memory (GB)	401	1	4

- Significant difference when evaluating surrogate on GPU
  - 9x faster than physics-based model
  - 9x faster inference time
- More memory required for GPU, but 100x less than physics-based model

Surrogate Model Evaluation Choice Matters!



- Surrogate model input choice likely a key driver performance disparity
- Traditional finite code architectures set up to evaluate integration-point behavior
- Generally not able to leverage the power of GPUs to evaluate multiple points in parallel
  - Expecting further improvements in runtime should that capability be added

Lessons Learned and Observations

- Implementing a surrogate model within a traditional finite element-based multiscale analysis feasible
- Efficient high-fidelity multiscale analysis possible with surrogates
  - No significant efficiency gap between surrogates for different fidelity micromechanics
  - Training costs may become prohibitive as fidelity increases
- Potential memory savings for utilizing surrogate models significant
  - Can allow much larger finite element meshes to be considered
  - Possibly enabling multiscale analysis of large structures
- Surrogate model inference (CPU vs. GPU) appears to be a big driver of overall runtime
- Traditional finite element software packages require modification to efficiently leverage GPUs

Acknowledgments

- Work supported by the NASA Aeronautics Research Mission Directorate's Transformational Tools and Technologies Project
- Josh Stuckner with machine learning assistance


NASA