

DuraMAT capability area:  
**Multi-scale, Multi-physics Modeling  
for PV Reliability**



PRESENTED BY

**James Hartley**, Sandia National Laboratories

DuraMAT Webinar, October 14, 2019

**SLAC** NATIONAL  
ACCELERATOR  
LABORATORY

**NREL**  
NATIONAL RENEWABLE ENERGY LABORATORY

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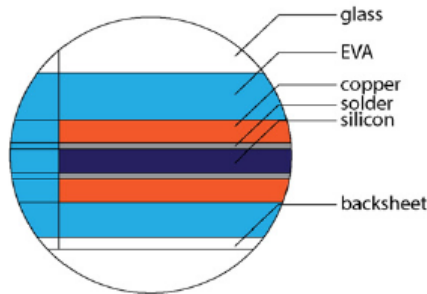


- Capability area introduction and goals
- How does modeling work: A start-to-finish analysis example
- Example applications and capabilities in development
- Summary

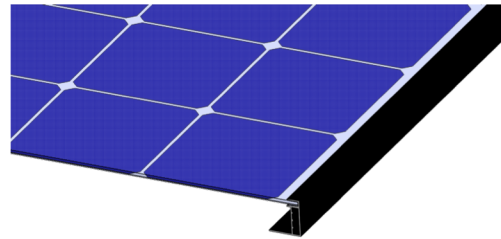
# Multi-scale, Multi-physics Modeling for PV Reliability



- **Goal:** A modeling capability to accurately predict module stressors
  - Applicable to multiple PV **scales**: From materials to interconnects to full modules
  - Incorporating multiple **physics**: Mechanical stress, thermal stress, materials effects, and more
- Applications for ranking stressors, identifying coupling, predicting lifetime, and more



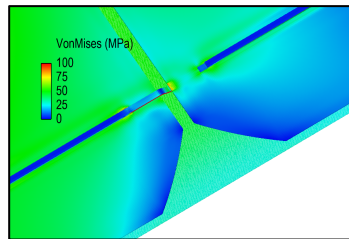
**Interconnect damage**  
[Bosco, NREL]



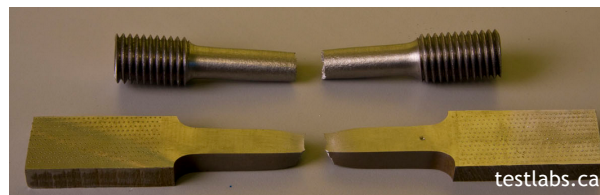
**Full Modules**



**Mini-Modules**  
[Hacke, Owen-Bellini; NREL]



**Thermal stress**



## Material responses:

- Encapsulant viscoelasticity [Maes, SNL]
- Electrically Conductive Adhesive damage mechanisms [Bosco, NREL]
- Backsheet aging [Owen-Bellini, NREL; Moffit, SLAC]



**Mechanical stress**

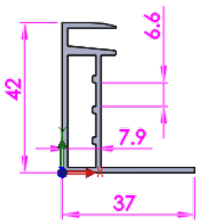


- Capability area introduction and goals
- **How does modeling work: A start-to-finish analysis example**
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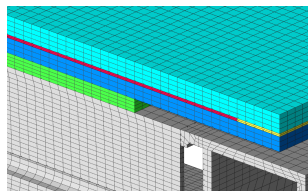
# How does modeling actually work? A step-by-step example



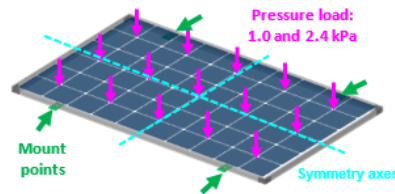
- **Computational finite element modeling** is a method for solving governing physical equations on complicated geometries, applied to problems of engineering interest
- **An example:** Full modules are subjected to 1.0 kPa and 2.4 kPa pressure loadings. What are the cell stresses that arise at these loadings?
  - Potential applications: How to replicate this stress in a minimodule test? Do encapsulant material properties affect the resulting cell stresses?
- **Notionally, the steps are as shown below**
  - Issues and complexities for each step to be discussed



Obtain geometric description



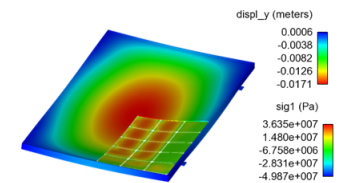
Generate a mesh of the geometry



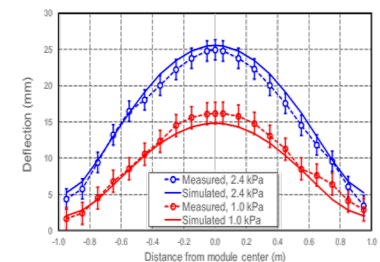
Apply materials and boundary conditions



Run the simulation



Answer the question!

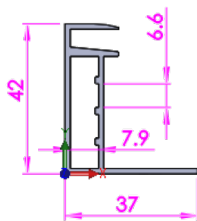


Analyze and Validate results

## Step I: Obtain a geometric description of the problem

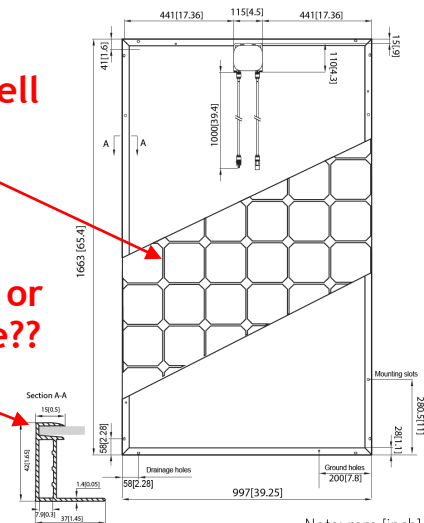


- **Physical definition of the geometry:** ‘Blueprints’ or a Computer Animated Design (CAD) of shapes and dimensions
  - Managed by common software packages: SolidWorks, Creo (Pro/Engineer), AutoCAD, etc...
  - Any engineered product should have this information, formats are generally interchangeable
- **In the current example:** Dimensions and assembly details for a test module
  - Obtained from datasheet and physical frame samples cut from an actual module
- **Issues and complexities:**
  - Details often incomplete (cell spacings; caulk dimensions)
  - How much detail is good enough?



What's the cell spacing??

Is there edge tape or silicone caulk here??



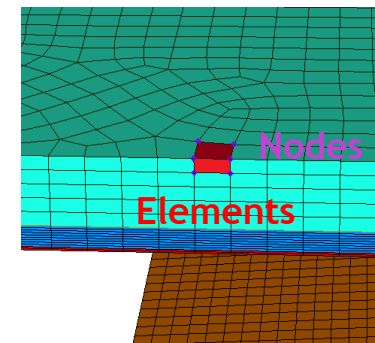
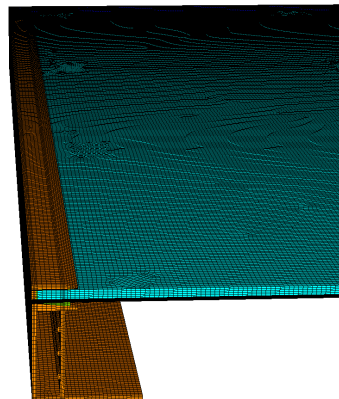
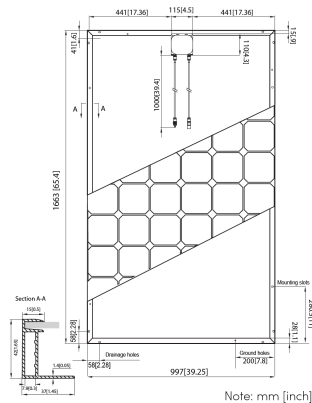
Note: mm [inch]

Actual module datasheet used to produce a CAD definition

## Step 2: Generate a mesh of the geometry



- Numerical methods for solving complicated partial differential equations (e.g. finite element methods) start by writing equations in discretized form in time and space
  - Meshing is the spatial discretization
- Software based process to translate CAD model volumes into:
  - Nodes:** Coordinates in space
  - Elements:** Discrete volumes formed by node connectivity
    - Hexahedral, tetrahedral, pyramid, mixed
  - Common meshing packages: CUBIT, ANSYS, COMSOL; theoretically interchangeable
- In the current example:** Module meshed with 5,621,162 elements and 6,859,032 nodes
  - Note: Elements carry size information but can scale arbitrarily



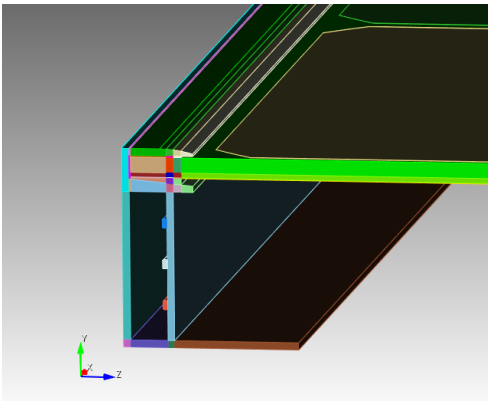
Mesh of the module shown previously

## Step 2: Generate a mesh of the geometry

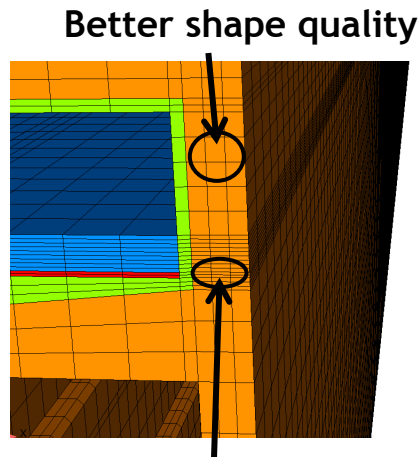


### Issues and complexities:

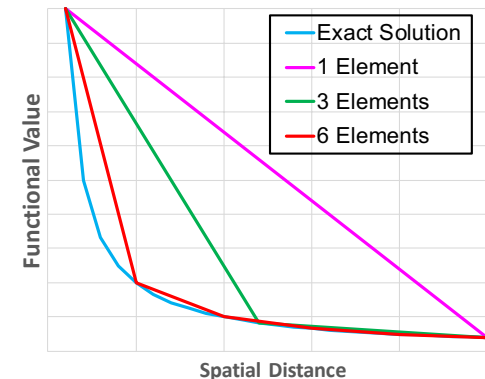
- Meshing algorithms are not robust to complicated geometries
  - Assignment requires strategic simplification and decomposition into primitive blocks (labor and analyst-intensive process)
- Resolution, quality, and accuracy vs. computational time
  - Not enough elements: Poor approximation of gradients
  - Poorly shaped elements: Numerical stability issues
  - Using more elements helps both but increases computational cost



Decomposition into primitive blocks for meshing



Poor shape quality  
Element quality considerations  
(ideal aspect ratio = 1)



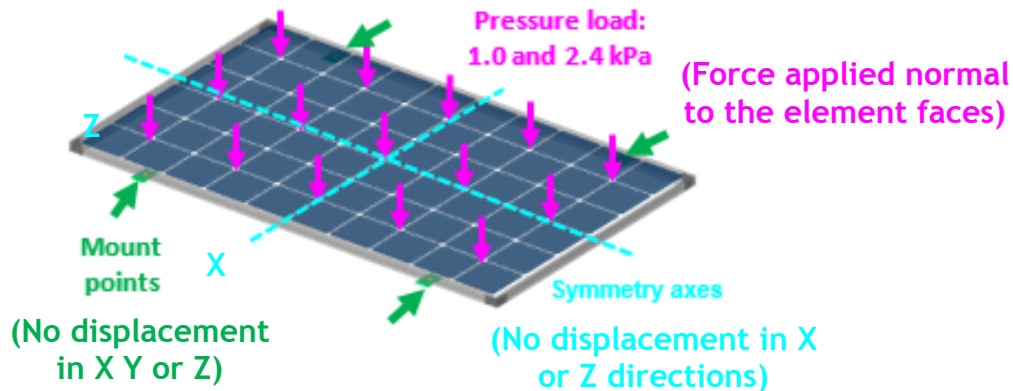
Mesh resolution vs. achievable accuracy



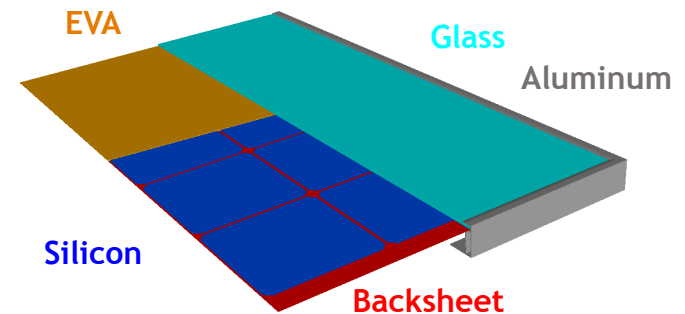
## Step 3: Apply materials and boundary conditions



- This step sets up the problem to be solved on the discretized geometry
- Associates conditions to specific parts of the mesh based on the problem to solve
  - Materials:** Describes how element volumes should respond to forcing
  - Boundary conditions:** Constraints or forces on element faces (surfaces), specific nodes, or volumes
  - Usually done graphically in the meshing software package; all mesh entities are accessible
- In the current example:**
  - Materials assigned as elastic (deformation proportional to forces sustained)
  - Pressure load to glass face (force per unit area normal to element faces)
  - Mount points fixed (nodes cannot move)



Boundary condition assignment



Material assignment

## Step 3: Apply materials and boundary conditions



### Issues and complexities:

- Material properties may not be known
- Material model may not exist
  - Or exists but is not a perfect match (is it good enough?)
  - Failure criteria are often considered material models
- What interactions and boundary conditions to include isn't straightforward
  - Interaction models may not exist either

Properties needed:

Young's modulus    Poisson's ratio

$$\varepsilon_{ij} = \frac{1}{E} \left[ \sigma_{ij} (1 + \nu) - \nu \delta_{ij} \sum_k \sigma_{kk} \right]$$

Linear elastic material model

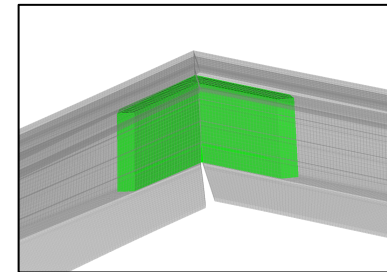
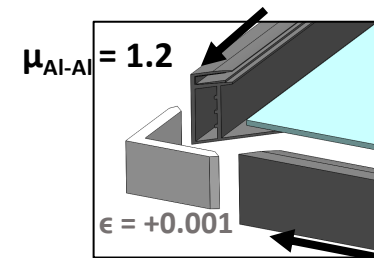
$$\sigma = E\varepsilon \quad \text{Elasticity}$$

$$\sigma = \eta \frac{d\varepsilon}{dt} \quad \text{Viscous term}$$

Generic viscoelasticity:  
Create a model in series  
or parallel?

Backsheet degradation vs. time,  
UV, moisture exposure...  
EVA modulus vs. crystal  
fraction, temperature, curing  
parameters...

Non-existent material models



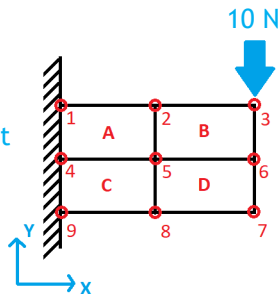
Frictional contact boundary condition at corner (is this important vs. contiguous block?)

# 11 Step 4: Run the simulation



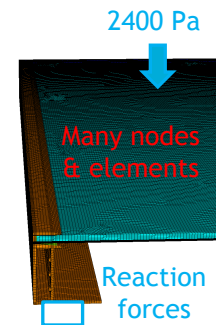
- Pick the equation to solve, as formulated by selected boundary conditions and materials (i.e. a system of equations) on the mesh
  - The simulation code applies iterative numerical methods to obtain a solution
  - Minor implementation differences across packages (SIERRA, COMSOL, ANSYS, ...)
- **In the current example:** We are solving  $\text{force} = \text{mass} * \text{acceleration} = 0$ 
  - Force provided by the pressure load on the module glass
  - Reaction forces supplied by the mount point constraints
  - Forces propagated through the materials in a linear elastic sense
    - Each element strains (deforms) proportional to stress (force/area)
  - Finding the material strain state which balances forces to 0 solves the problem
- **Issues and complexities:**
  - Poorly formulated problems can fail or require intermediate steps to solve
  - Finite computational power available

What are the displacements at each node?



- Nodes 1, 4, and 9 supply reaction forces
- Displacements at elements A and B are the same at nodes 2 and 5
- Node 3 has a force of 10N in the -y direction
- ... Assembles a system of equations!

Notional finite element problem...

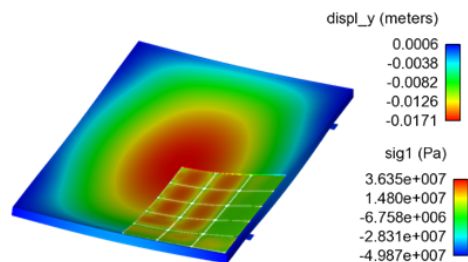


...Actual model application case

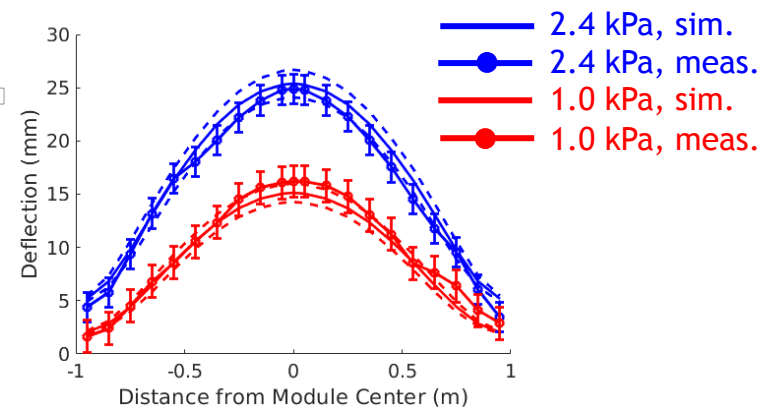
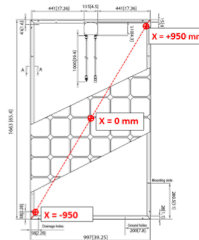
## Step 5: Verify and validate results



- Upon simulation completion, the mesh is populated with all solution variables, associated to nodes (displacement, temperature) and elements (stress, strain, energy)
  - Verification: Solved the correct problem, correctly (user/code error, numerics)
  - Validation: Simulation actually represents reality
- **In the current example:**
  - We were looking for: cell stress state in a full module at 1.0 and 2.4 kPa loads
    - Verification: Error check, mesh refinement, solver tolerance check
    - Validation: Compare model-predicted deflection against experiments
- **Issues and complexities:**
  - Numerical error assessment requires multiple runs with parameter perturbations:
    - Sometimes simulation is already at limits (mesh resolution, residuals, etc.)
  - Clean validation data difficult to obtain; is it representative enough? What to do when results don't match?



Simulation results: full field displacement, stress, etc.

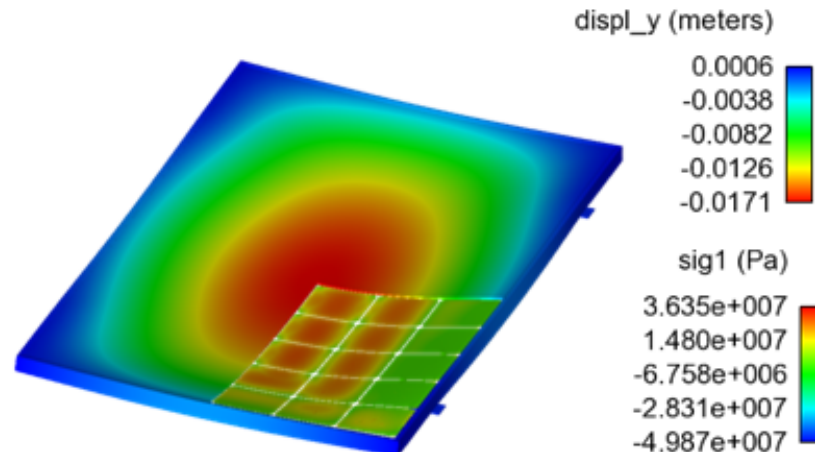


Validation against deflection vs. load test data

## Step 6: Answer the question!



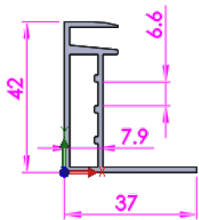
- Interpret results to answer the original reason for why we created the model
- **In the current example:**
  - We were looking for cell stress states in a full module 1.0 and 2.4 kPa- Done!
    - Can visualize or output as text at specific points, process max/min, etc.
    - Recall: Solution information has the same resolution as the mesh
  - Believable because validated against deflection
- **Issues and complexities:**
  - Interpretation and follow on questions: Is cell principle stress the correct quantity to assess? Effect of interconnects? Effect of EVA properties?
    - Analysis may reveal subtleties that create more questions!



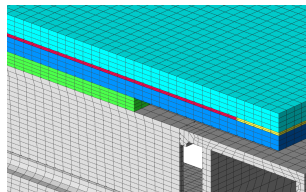
Visualization of deflection and 1<sup>st</sup> principle stress in full module model @2.4 kPa



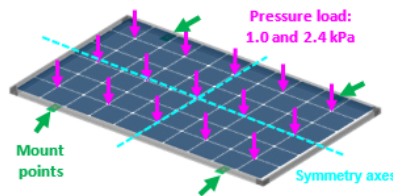
- **Computational finite element modeling** is a method for solving governing physical equations on complicated geometries, applied to problems of engineering interest
- The key needs for a modeling analysis are:
  - **A detailed geometric description**
    - Dimensions; needed to create a mesh
  - **Information about materials and boundary conditions**
    - Material assignments, properties, assembly processes and methods
  - **Knowledge of the physics relevant to the problem**
    - Governing equations: Solid mechanics, thermal transport, etc.
  - **Baseline validation data (Highly recommended)**



Obtain geometric description



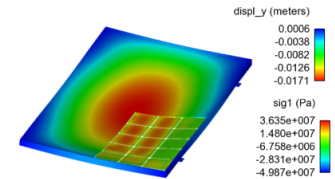
Generate a mesh of the geometry



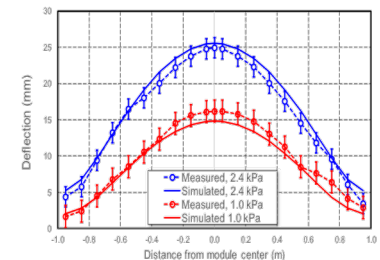
Apply materials and boundary conditions



Run the simulation



Answer the question!



Analyze and Validate results

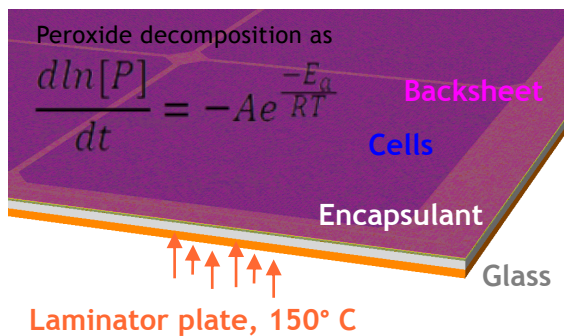


- Capability area introduction and goals
- How does modeling work: A start-to-finish analysis example
- **Example applications and capabilities in development**
  - A thermal-chemical analysis of lamination
  - A high-fidelity viscoelastic encapsulant material model
  - Correlation of mini-module behavior to full modules
  - A coupled, multi-physics mini-module simulation with failure prediction
- Summary

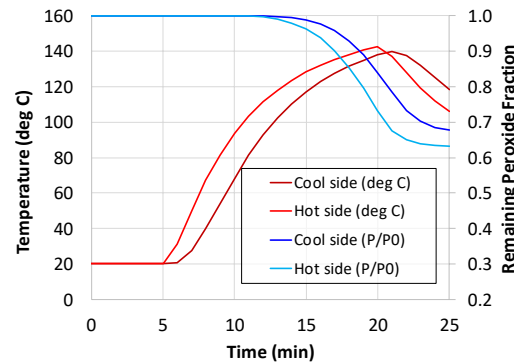
# Thermal-chemical analysis of lamination



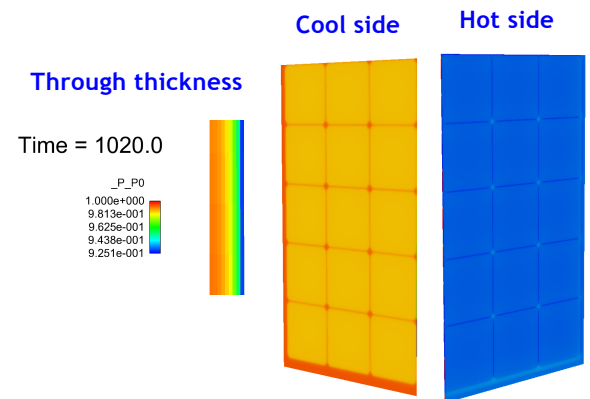
- **Problem statement:** Raw encapsulant sheets contain peroxides which decompose to initiate crosslinking during lamination. However, the reaction is highly temperature dependent, so if lamination temperatures are not perfectly uniform, the reaction could proceed nonuniformly and result in spatially nonuniform mechanical properties. How significant can this effect be and where in the module can this occur?
- **Geometry and mesh:** Full module laminate from previous, minus frame
- **Physics, materials, boundary conditions:** Thermal diffusion and chemical kinetics; heat capacities and thermal conductivities for materials, fixed temperature on laminator plate for ~15 minutes of lamination time, generic peroxide decomp. equation
- **Validation:** None so far; temperature may be confirmed with testing
- **Conclusions:** Cell gap areas front to back show the largest difference in peroxide yield. Investigate true temperature profiles more for accurate magnitudes.



Geometry with boundary conditions



Temperature and peroxide fraction vs. time, front and back



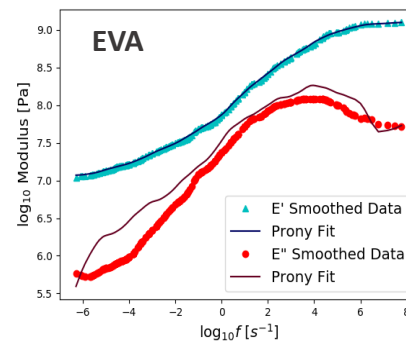
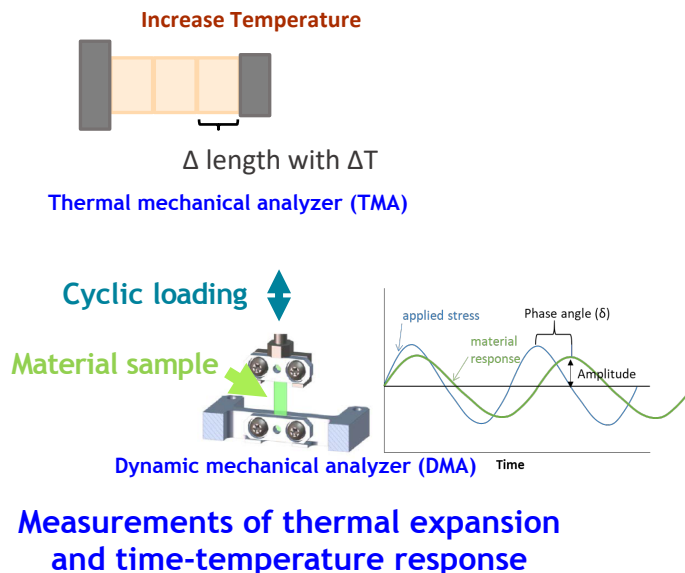
Qualitative concentration distributions



# A high-fidelity viscoelastic encapsulant material model

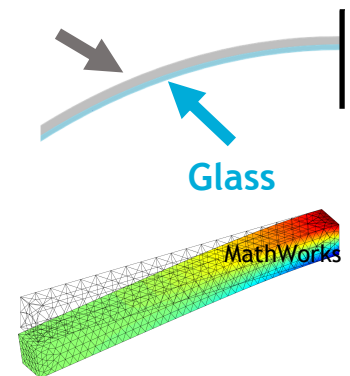


- **Problem statement:** Ethylene Vinyl Acetate (EVA) is a common encapsulant material and occurs in finite element models of PV-relevant geometries. What effect does its temperature- and rate-dependent properties have on simulation predictions?
- **Geometry and mesh:** Material models exist independently of geometry
- **Physics (to be derived):** Material strain vs. stress, temperature, and time
- **Validation:** Material model can be analytically validated. Computational implementation can be validated with simulations of the test geometries (strips under tension, beams) matching measurement output
- **Conclusions:** Validated material model can then be applied in a PV-relevant geometry
  - Adds temperature and time dependencies



Validation of mathematical model against measured data

Encapsulant

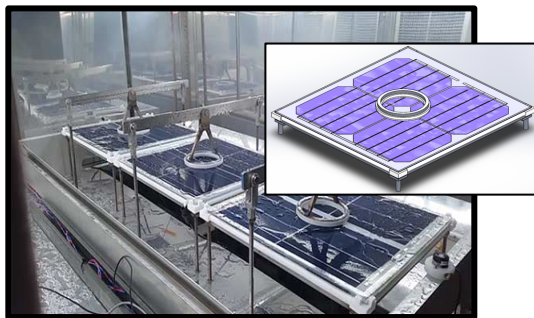


Validation of computational material model implementation

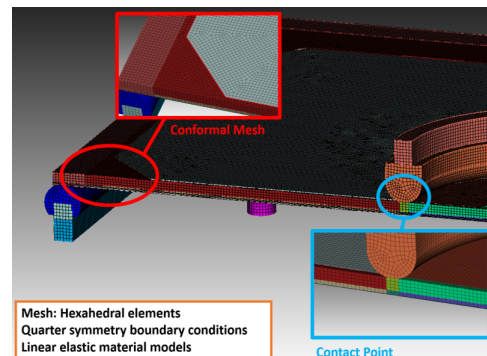
# Correlation of mini-module mechanical stress to full module behavior



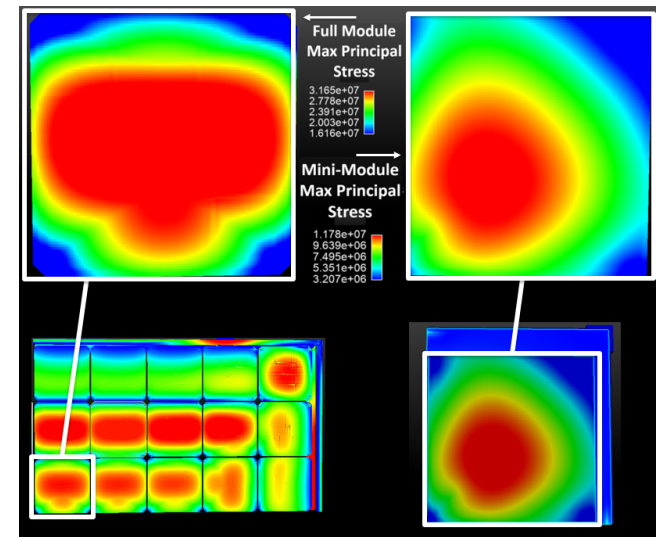
- **Problem statement:** Accelerated tests (C-AST) use mini-modules for size and cost advantages. But, are the mechanical loads applied to mini-modules actually representative of the 1.0 and 2.4 kPa loads applied to full modules?
- **Geometry:** Minimodule + support frame + loading donut
- **Mesh:** 190,000 hexahedral elements
- **Physics, materials, boundary conditions:** Mechanical physics, Linear elastic materials, contact friction between module, donut, and frame, fixed at mounting post
- **Validation:** Deflection vs. load comparisons at full module and minimodule level
- **Conclusions:** Some differences exist; model allows quantification and probing of where they occur and magnitude



Actual test setup  
photo & CAD model



Mesh with boundary  
conditions

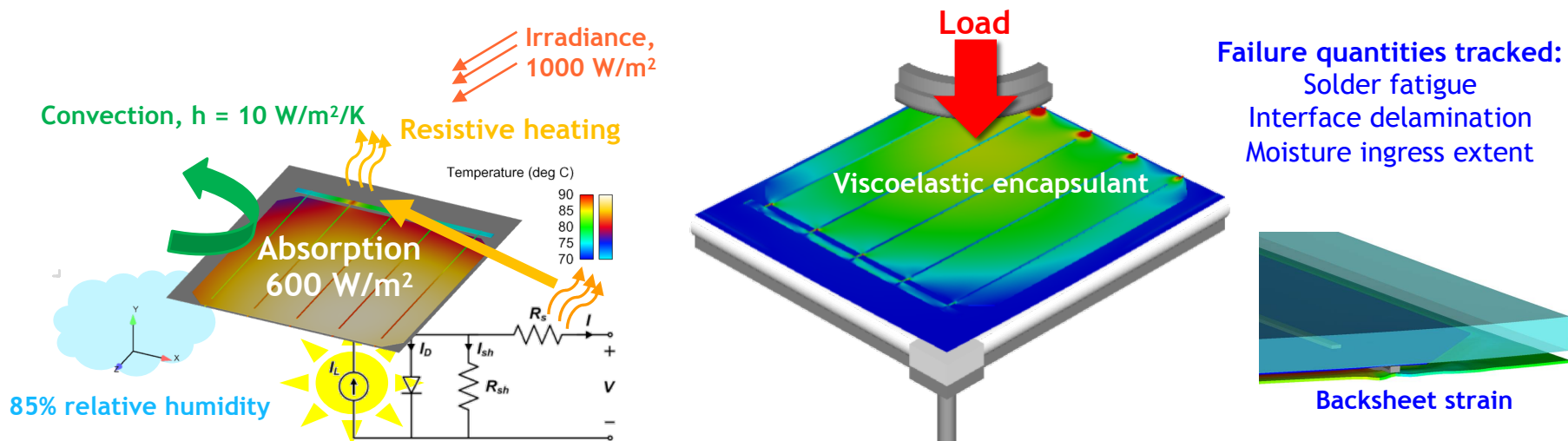


Simulated mimo cell stress  
vs. full module stresses

# A multi-physics mini-module modeling platform



- **Problem statement:** Mini-modules in accelerated testing experience failures- delamination, solder breakage, backsheet cracking- among others. What initiates these failures- the mechanical, thermal, UV, moisture, or electrical environment?
- **Geometry and mesh:** Minimodule + support frame + loading donut (as before)
- **Physics, materials, boundary conditions:** Mechanical physics and interactions as before; add viscoelasticity (thermal and time dependencies); add electrical coupling (additional heat source); add solder failure material models, add interface delamination failure models; add moisture diffusion model
- **Validation:** Comparisons to tested minimodules
- **Conclusions:** Helps to rank stressors or identify coupling



Ability to track multiple physical inputs and effect on failure-relevant quantities



- Capability area introduction and goals
- How does modeling work: A start-to-finish analysis example
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- **Summary**



- **Computational finite element modeling** is a method for solving governing physical equations on complicated geometries, applied to problems of engineering interest
- **This webinar ran through:**
  - The general process for creating a model
  - Several PV-relevant example applications and capabilities in development
    - At **scales** from full modules to minimodules to material behavior
    - Across **physics** ranging from mechanical stress and material behavior, thermal transport, electrical transport, and chemical kinetics
- **Takeaway point:** There are many more applications for modeling available in PV- all that's needed to get started is:
  - Information about the geometry of interest
  - Information about the governing physics of the problem
  - Relevant material properties and boundary conditions
  - Quantities of interest sought
- **Questions?**