

MECHANICS OF STRUCTURE GENOME:

FILL THE GAP BETWEEN MATERIALS
GENOME AND STRUCTURAL ANALYSIS

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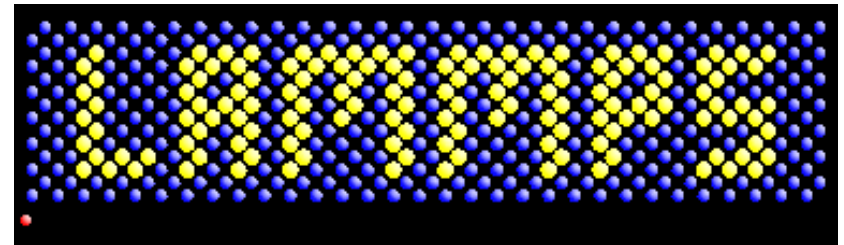
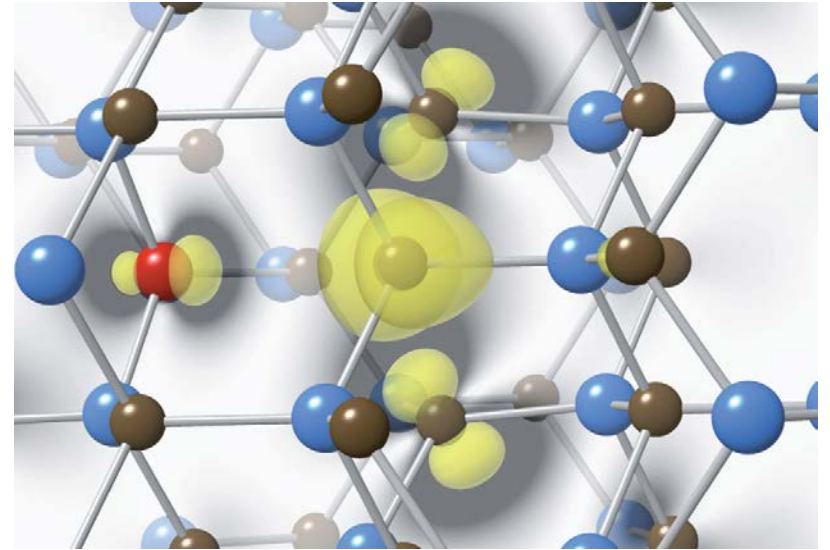
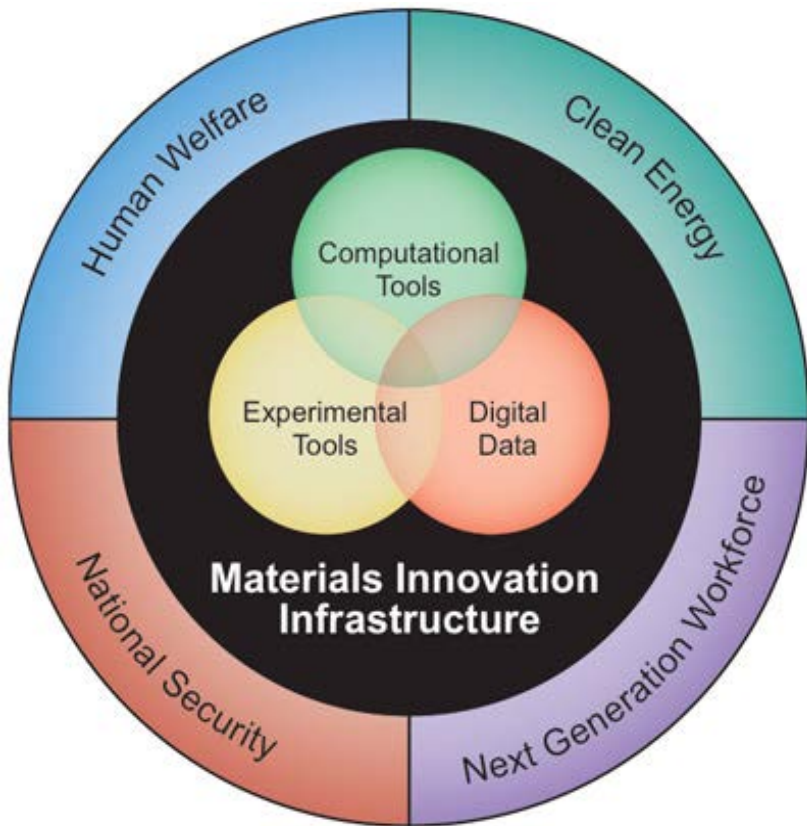


Vision/Mission/Values

- **Vision:** Design, manufacture, and certify advanced structures and materials by analysis.
- **Mission:** To advance predictive capabilities for advanced structures and materials and to train students with analysis fundamentals and job-ready skills.
- **Professional Values**
 - We pursue **truth** because truth can set us free.
 - We seek **unity** to systematically handle diversities.
 - We strike for **balance** between practicality and rigor.
 - We embrace **humble boldness** to learn from others and remain true to scholarship.

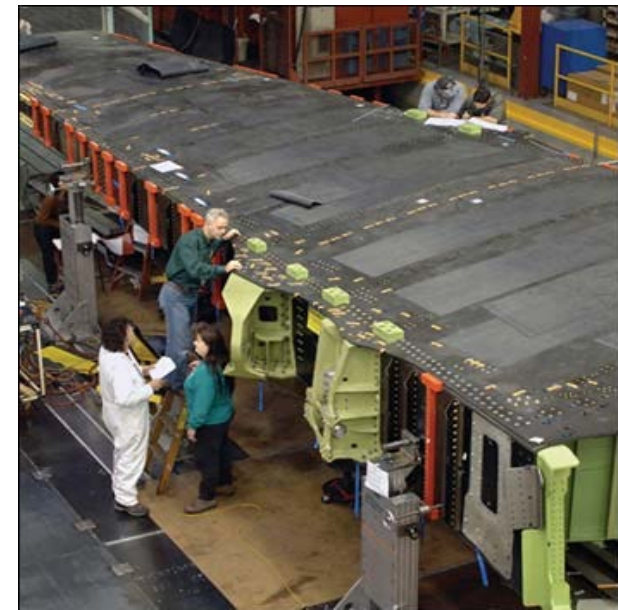
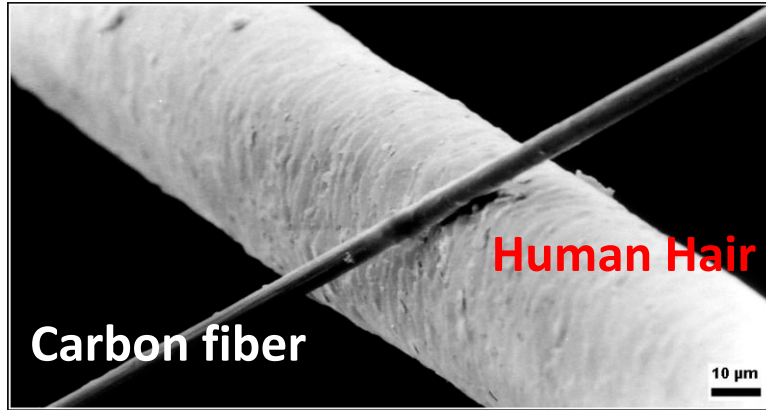


Materials Genome Initiative



MGI deliverables: properties, allowables, failure criteria for constituents (fiber, matrix), interfaces

The Challenge: Multiple Scales



1 mm³ material block
~ **20 Million** DOFs



Bottom-up Multiscale Modeling

Structure

10^1 m



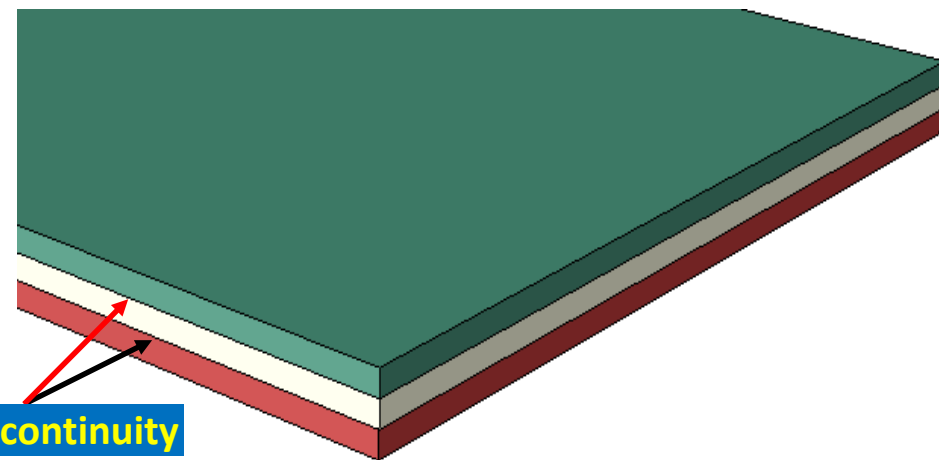
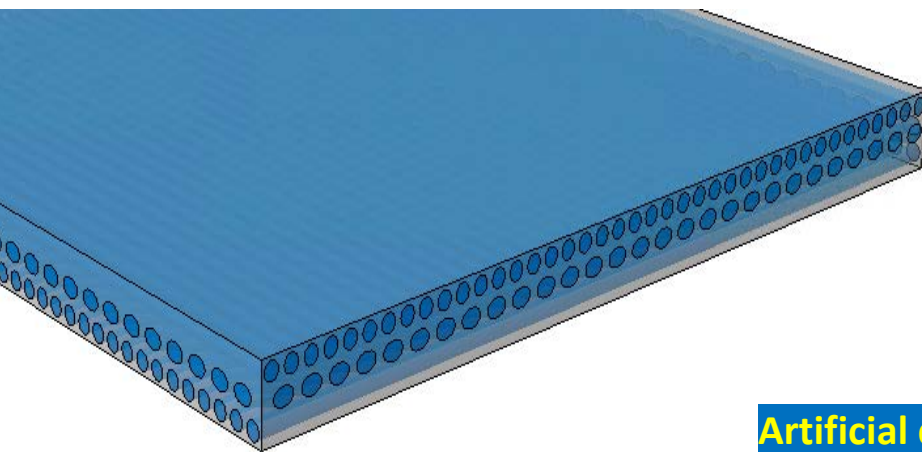
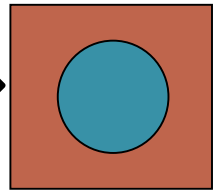
Meso

10^{-3} m



Micro

10^{-6} m



Artificial discontinuity

Top-Down Multiscale Modeling

Structural Analysis

10^1 m

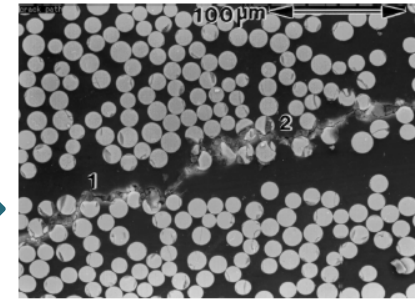
Microstructure

10^{-6} m



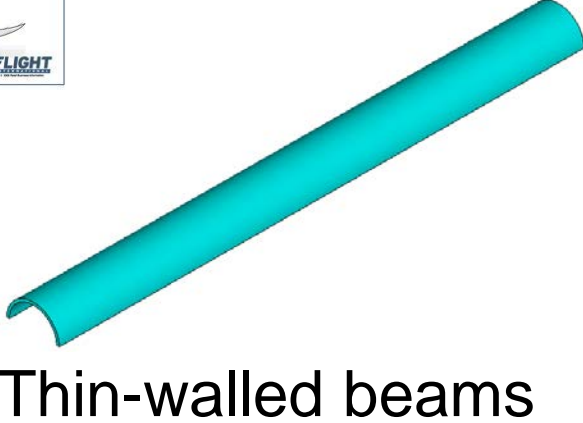
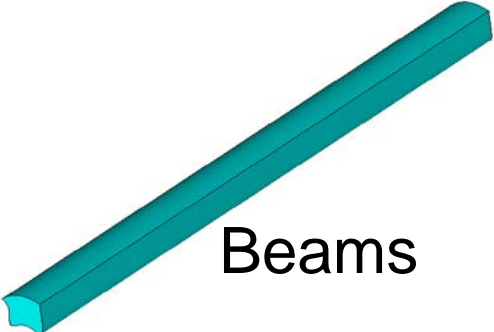
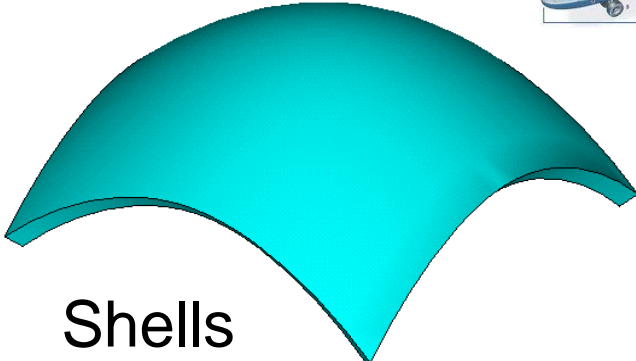
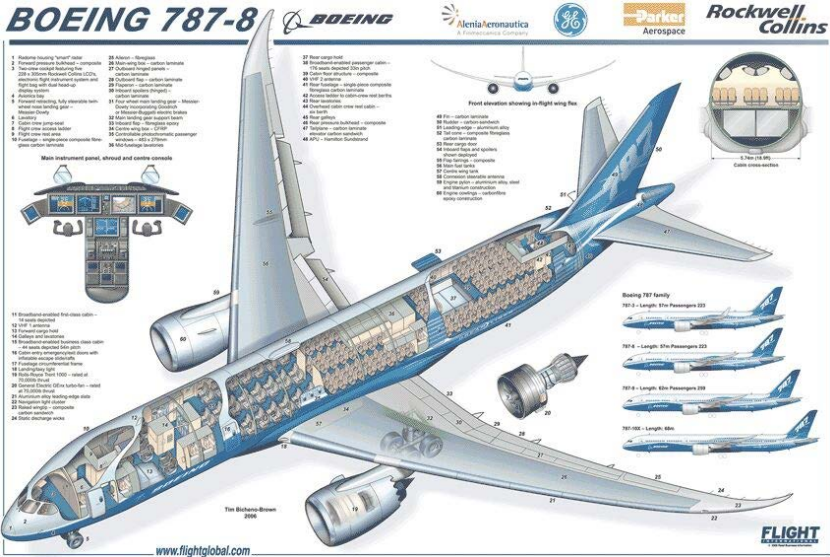
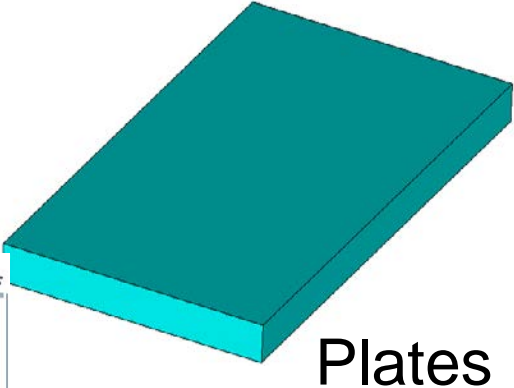
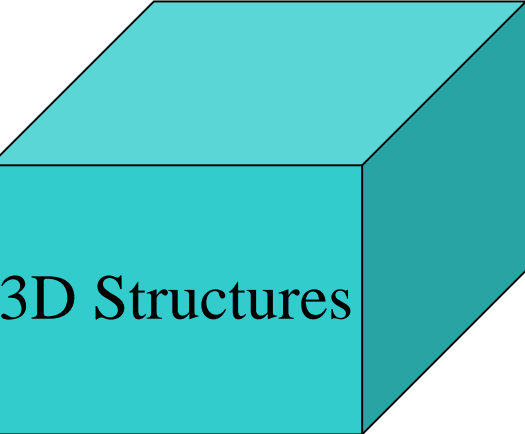
Mechanics of
Structure Genome

Minimize Information Loss

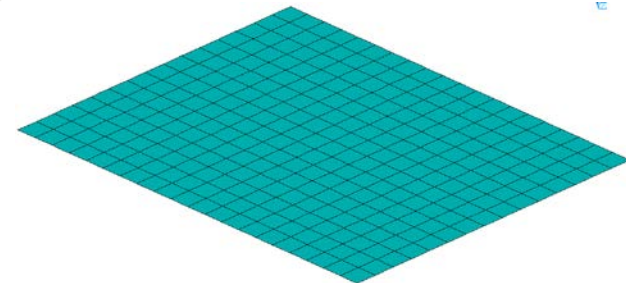
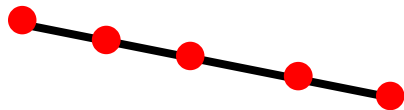
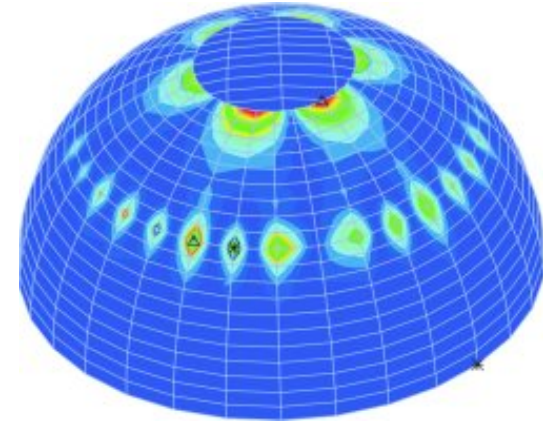
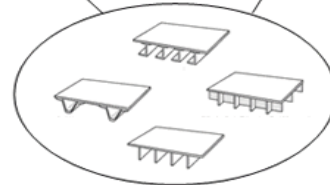
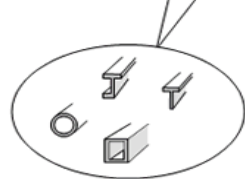
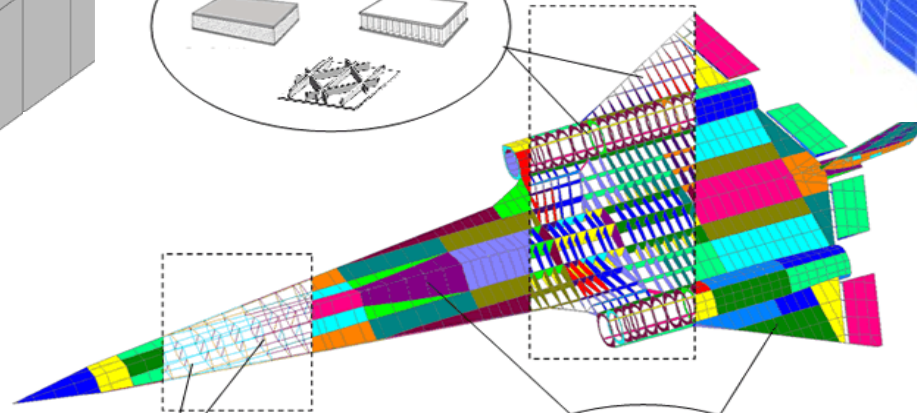
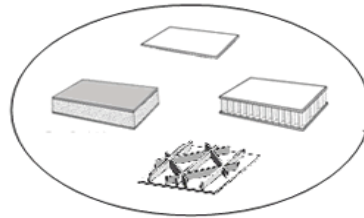
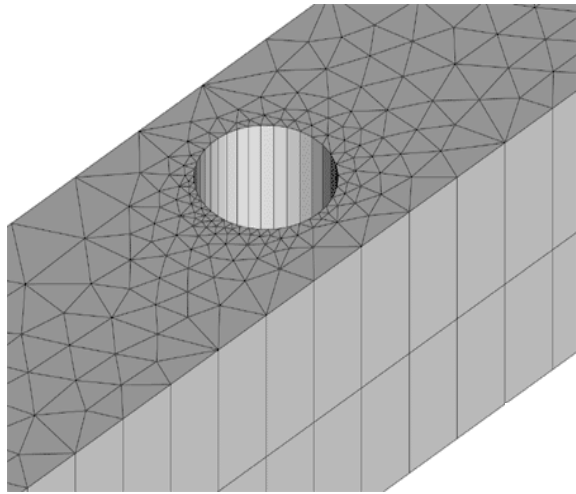


For since the fabric of the universe is most perfect and the work of a most wise creator, nothing at all takes place in the universe in which some rule of the maximum or minimum does not appear.

Typical Structural Components



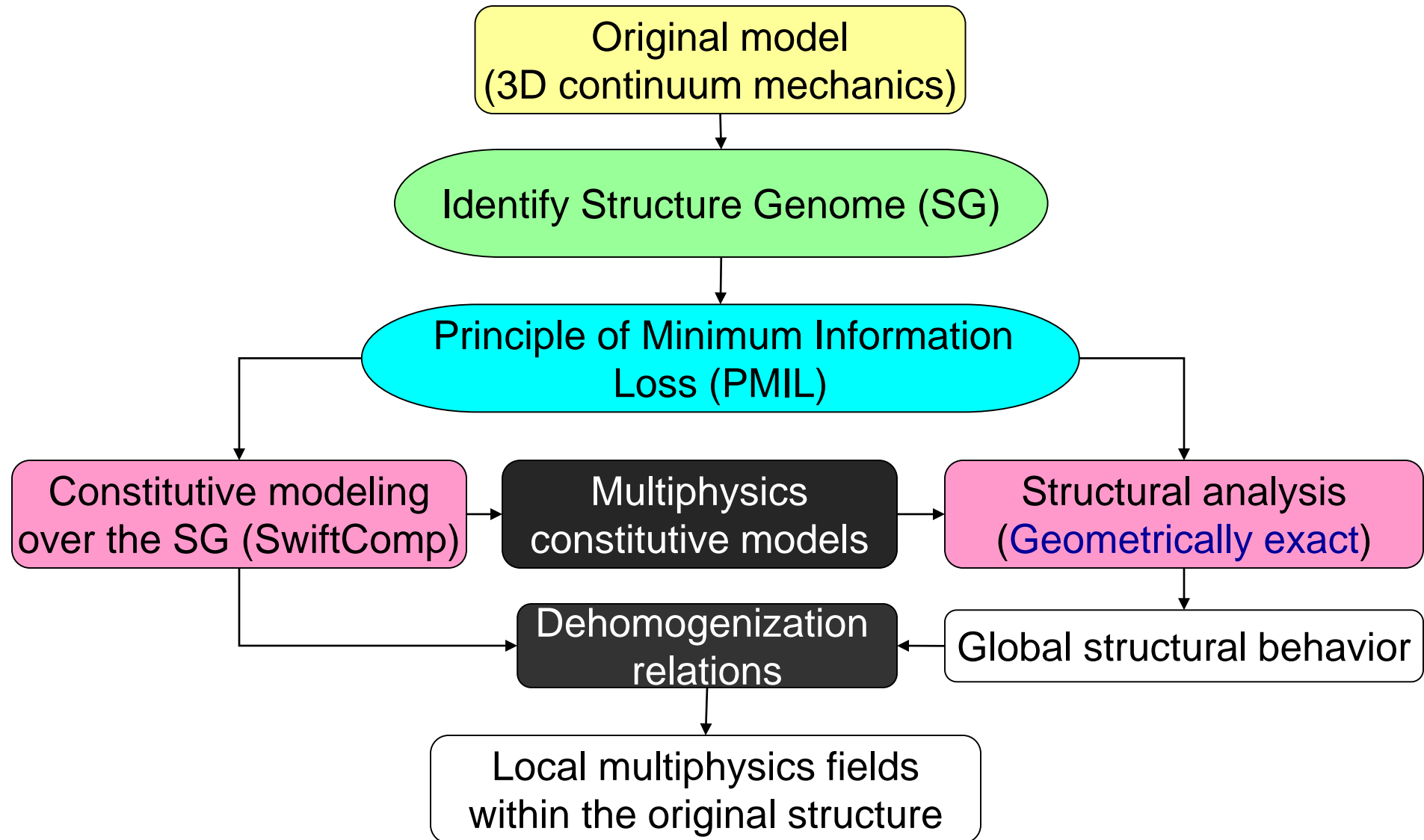
Structural Analyses



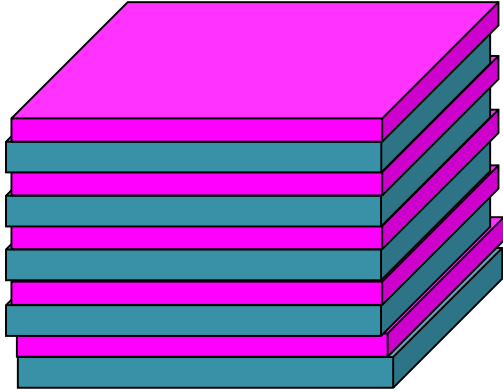
Structural Models

	Kinematics	Kinetics	Constitutive Relations
3D	$\epsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$	$\sigma_{ij,j} + f_i = 0$	$\begin{Bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{Bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ c_{12} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ c_{13} & c_{23} & c_{33} & c_{34} & c_{35} & c_{36} \\ c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} \\ c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} \\ c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66} \end{bmatrix} \begin{Bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ 2\epsilon_{23} \\ 2\epsilon_{13} \\ 2\epsilon_{12} \end{Bmatrix}$
2D (Plate/ shell)	$\epsilon_{\alpha\beta} = \frac{1}{2}(\bar{u}_{\alpha,\beta} + \bar{u}_{\beta,\alpha})$ $\kappa_{\alpha\beta} = -\bar{u}_{3,\alpha\beta}$	$N_{\alpha\beta,\beta} + p_\alpha = 0$ $(M_{\alpha\beta,\beta} + e_{\alpha\beta}q_\beta)_{,\alpha} + p_3 = 0$	$\begin{Bmatrix} N \\ M \end{Bmatrix} = \begin{bmatrix} A & B \\ B^T & D \end{bmatrix} \begin{Bmatrix} \epsilon \\ \kappa \end{Bmatrix}$
1D (beam)	$\gamma_{11} = \bar{u}'_1$ $\kappa_1 = \Phi'_1$ $\kappa_2 = -\bar{u}''_3$ $\kappa_3 = \bar{u}''_2$	$\frac{dF_1}{dx_1} + p_1 = 0$ $\frac{dM_1}{dx_1} + q_1 = 0$ $\frac{d^2M_2}{dx_1^2} + p_3 + \frac{dq_2}{dx_1} = 0$ $\frac{d^2M_3}{dx_1^2} - p_2 + \frac{dq_3}{dx_1} = 0$	$\begin{Bmatrix} F_1 \\ M_1 \\ M_2 \\ M_3 \end{Bmatrix} = \begin{bmatrix} S_{11} & S_{12} & S_{13} & S_{14} \\ S_{12} & S_{22} & S_{23} & S_{24} \\ S_{13} & S_{23} & S_{33} & S_{34} \\ S_{14} & S_{24} & S_{34} & S_{44} \end{bmatrix} \begin{Bmatrix} \gamma_{11} \\ \kappa_1 \\ \kappa_2 \\ \kappa_3 \end{Bmatrix}$

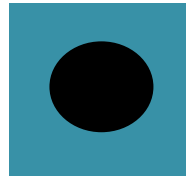
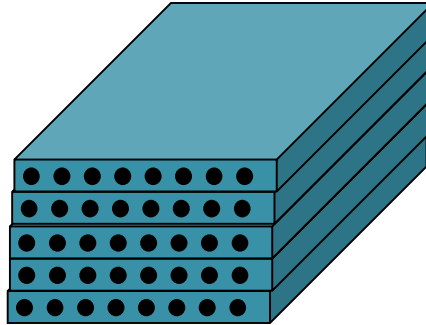
Mechanics of Structure Genome



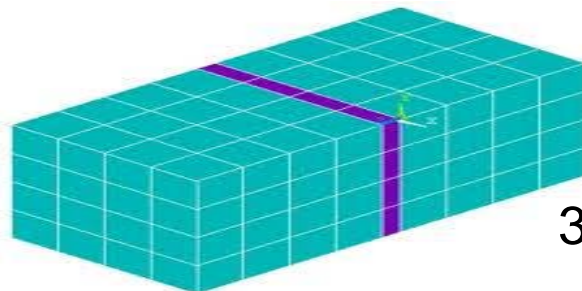
SG for 3D Structures



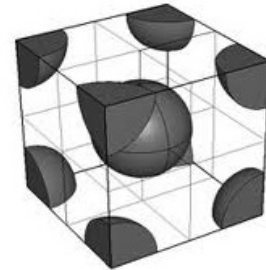
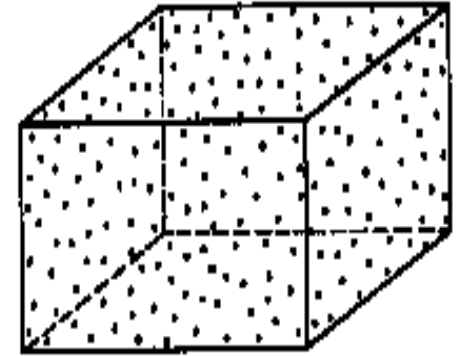
a) 1D SG



b) 2D SG

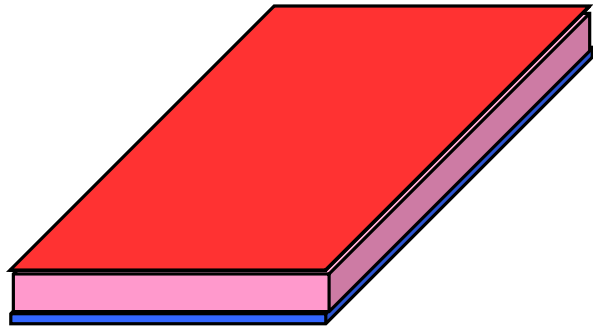


3D macroscopic structural analysis

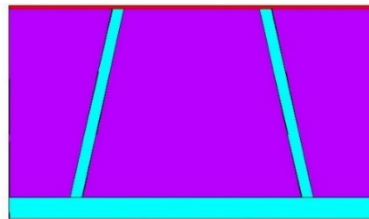
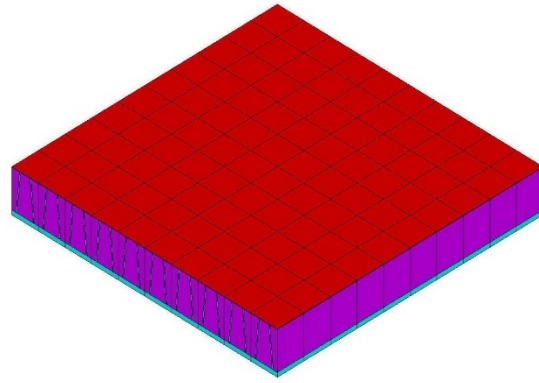


c) 3D SG

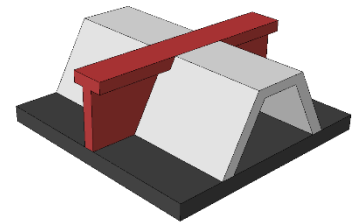
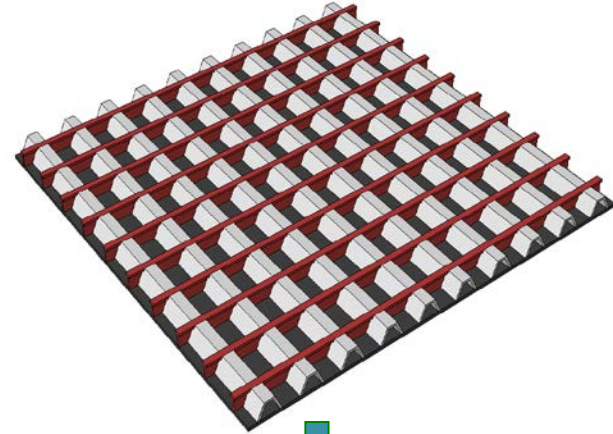
SG for Panels (Plates/Shells)



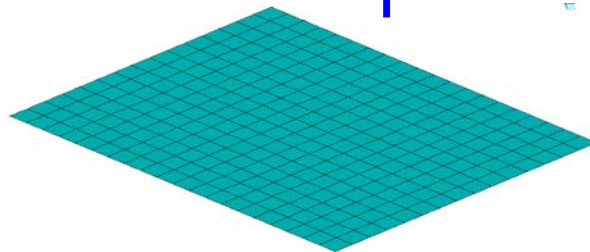
a) 1D SG



b) 2D SG

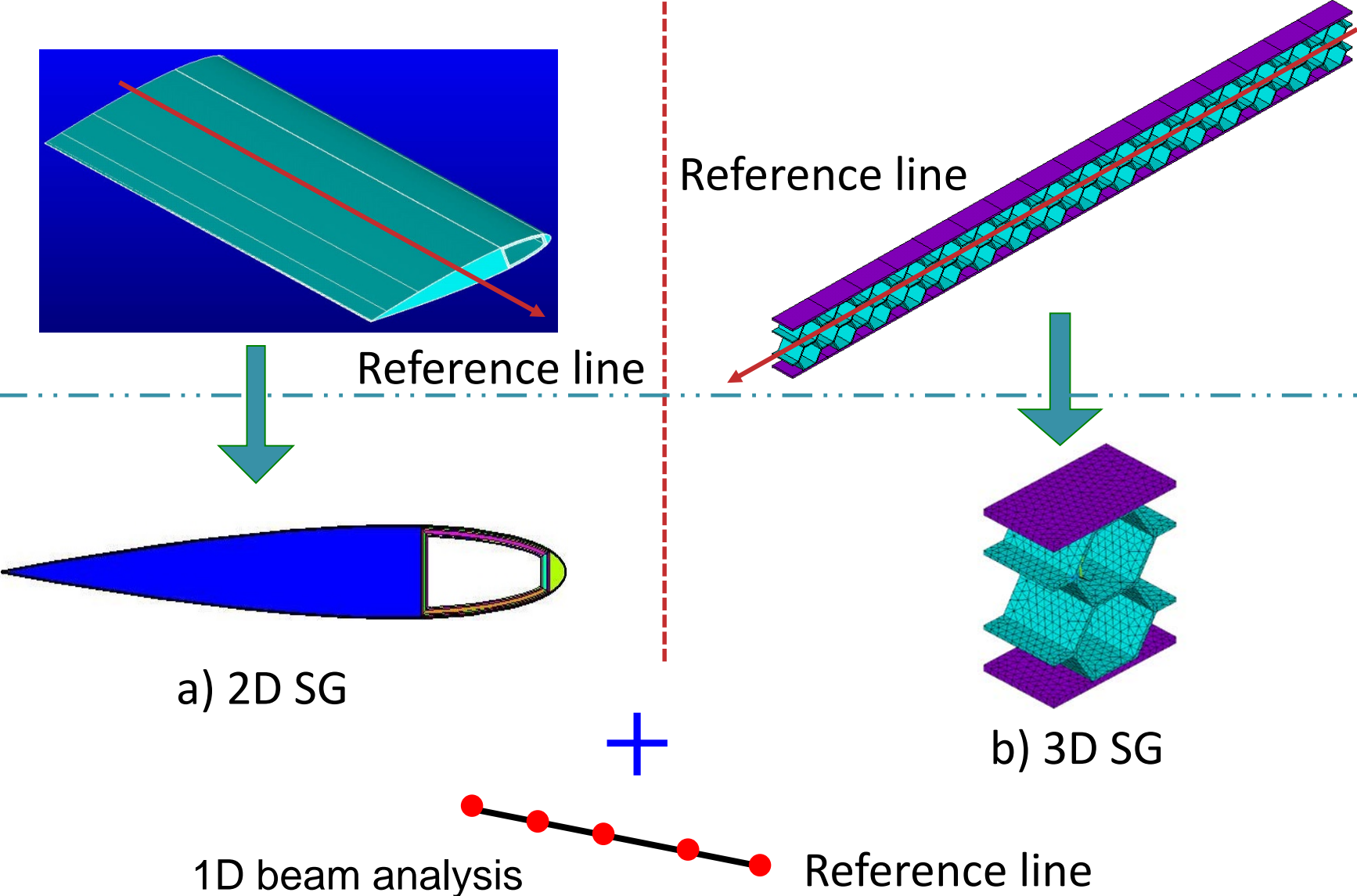


c) 3D SG

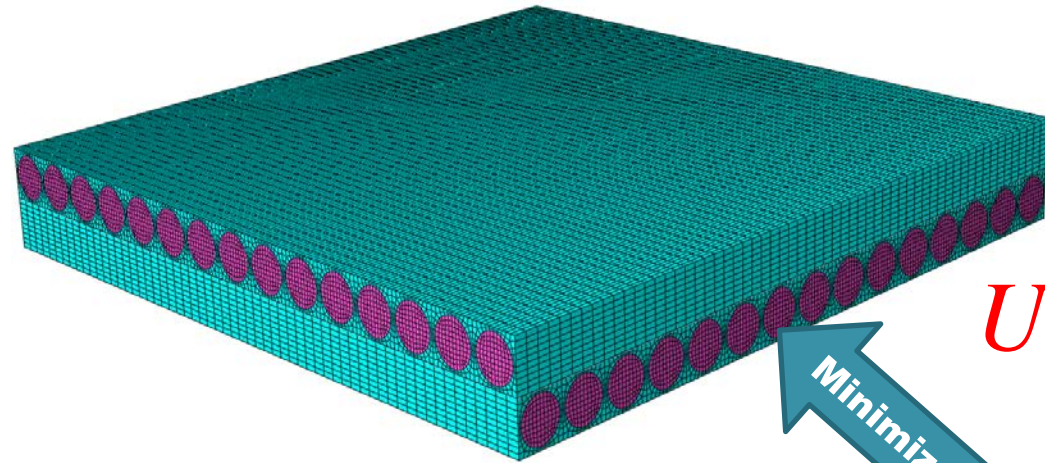


2D plate/shell analysis

SG for Beam-like Structures



MSG for CLPT



U

Minimize Energy Loss

\bar{U}

$$\sigma_{ij,j} + f_i = 0$$

$$\epsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$$

$$\begin{Bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{Bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ c_{12} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ c_{13} & c_{23} & c_{33} & c_{34} & c_{35} & c_{36} \\ c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} \\ c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} \\ c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66} \end{bmatrix} \begin{Bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ 2\epsilon_{23} \\ 2\epsilon_{13} \\ 2\epsilon_{12} \end{Bmatrix}$$

v

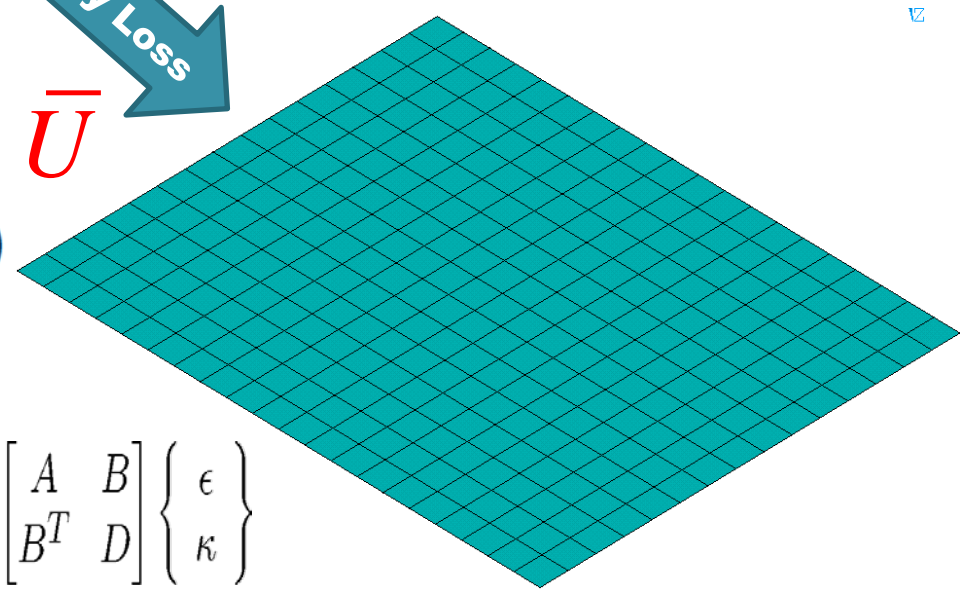
$$\epsilon_{\alpha\beta} = \frac{1}{2}(\bar{u}_{\alpha,\beta} + \bar{u}_{\beta,\alpha})$$

$$\kappa_{\alpha\beta} = -\bar{u}_{3,\alpha\beta}$$

$$N_{\alpha\beta,\beta} + p_\alpha = 0$$

$$(M_{\alpha\beta,\beta} + e_{\alpha\beta}q_\beta)_{,\alpha} + p_3 = 0$$

$$\begin{Bmatrix} N \\ M \end{Bmatrix} = \begin{bmatrix} A & B \\ B^T & D \end{bmatrix} \begin{Bmatrix} \epsilon \\ \kappa \end{Bmatrix}$$



MSG for CLPT (Cont.)

- Express kinematics of the original model in terms of that of the macroscopic model and unknown warping/fluctuating functions

$$u_i = u_i(\overline{u}, \overline{u}_{,\alpha}, w_i)$$

$$\varepsilon_{ij} = \varepsilon_{ij}(\overline{\varepsilon}_{\alpha\beta}, \overline{K}_{\alpha\beta}, w_{i,j})$$

- Define kinematics of the macroscopic model in terms of the original model

MSG for CLPT (Cont.)

- Express the energy of the original model

$$U = U(\varepsilon_{ij}) = U(\overline{\varepsilon}_{\alpha\beta}, \overline{K}_{\alpha\beta}, w_{i,j})$$

- Minimize the energy to solve fluctuating functions

$$\min_{w_i} U(\overline{\varepsilon}_{\alpha\beta}, \overline{K}_{\alpha\beta}, w_{i,j}) = \overline{U}(\overline{\varepsilon}_{\alpha\beta}, \overline{K}_{\alpha\beta})$$

MSG for Aperiodic Materials

➤ Kinematics

- Displacement

$$u_i(\mathbf{x}; \mathbf{y}) = v_i(\mathbf{x}) + \varepsilon \chi_i(\mathbf{x}; \mathbf{y})$$

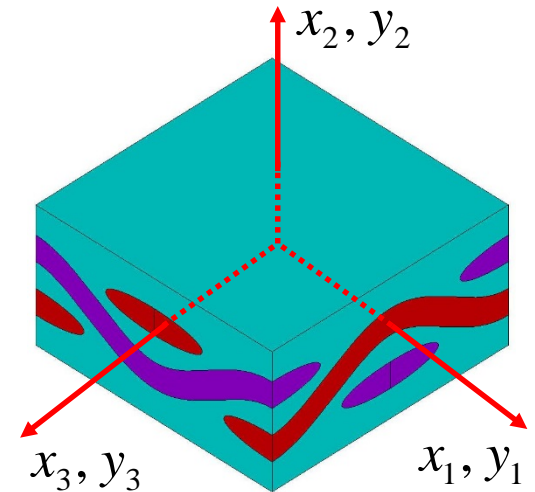
- Strain

$$\epsilon_{ij}(\mathbf{x}; \mathbf{y}) = \frac{1}{2} \left[\frac{\partial u_i(\mathbf{x}; \mathbf{y})}{\partial x_j} + \frac{\partial u_j(\mathbf{x}; \mathbf{y})}{\partial x_i} \right] = \bar{\epsilon}_{ij} + \chi_{(i|j)} + \varepsilon \chi_{(i,j)}$$

- Kinematic equivalency constraints:
average displacement and strain

$$v_i = \frac{1}{\Omega} \int_{\Omega} u_i \, d\Omega \equiv \langle u_i \rangle \quad \Rightarrow \quad \langle \chi_i \rangle = 0$$

$$\bar{\epsilon}_{ij} \equiv \langle \epsilon_{ij} \rangle \quad \Rightarrow \quad \langle \chi_{(i|j)} \rangle = 0$$



MSG for Aperiodic Materials

- Minimize energy discrepancy between the deformed heterogeneous material and the homogenized material

$$J = \Pi_{Micro} - \Pi_{Macro} - \lambda_{kl} \langle \chi_{(k|l)} \rangle - \eta_i \langle \chi_i \rangle \quad \delta J = 0$$

$$\Pi_{Micro} = \langle C_{ijkl} \epsilon_{ij} \epsilon_{kl} \rangle = \langle C_{ijkl} (\bar{\epsilon}_{ij} + \chi_{(i|j)}) (\bar{\epsilon}_{kl} + \chi_{(k|l)}) \rangle \quad \Pi_{Macro} = \langle \bar{C}_{ijkl} \bar{\epsilon}_{ij} \bar{\epsilon}_{kl} \rangle$$

- Finite Element Implementation

$$\chi(x_i; y_j) = S(y_j) V(x_i)$$

$$J = \frac{1}{2} (V^T E V + 2V^T D_{h\epsilon} \bar{\epsilon} + \bar{\epsilon}^T D_{\epsilon\epsilon} \bar{\epsilon}) - \frac{1}{2} V^T \bar{D}^* V - \lambda^T D_{h\lambda}^T V$$

$$E = \langle (\Gamma_h S)^T D (\Gamma_h S) \rangle \quad D_{h\epsilon} = \langle (\Gamma_h S)^T D \rangle \quad D_{\epsilon\epsilon} = \langle D \rangle \quad D_{h\lambda} = \langle \Gamma_h S \rangle^T$$

MSG for Aperiodic Materials

➤ The solution

$$V = V_0 \bar{\epsilon} \quad \chi = SV_0 \bar{\epsilon}$$

➤ Homogenized energy

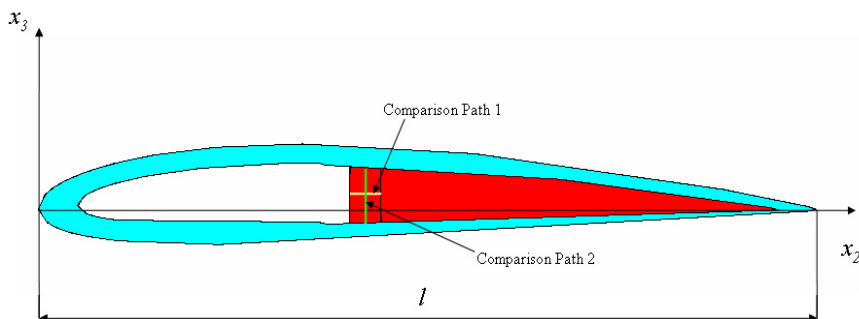
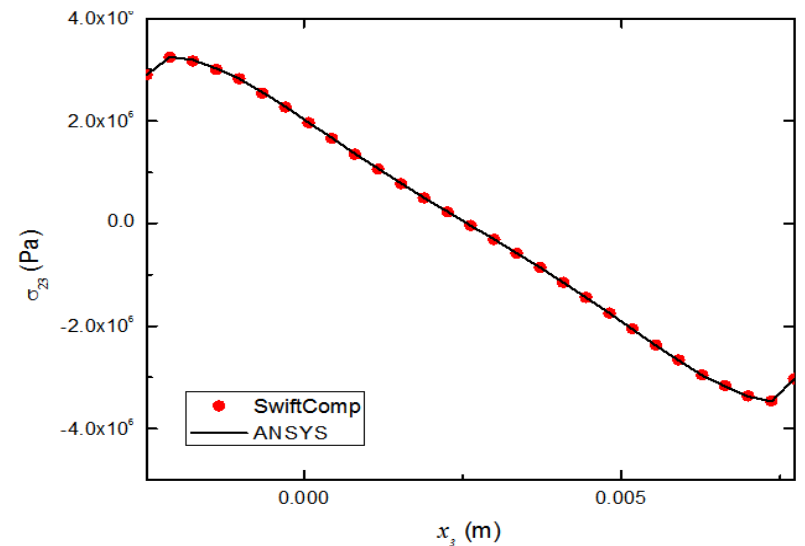
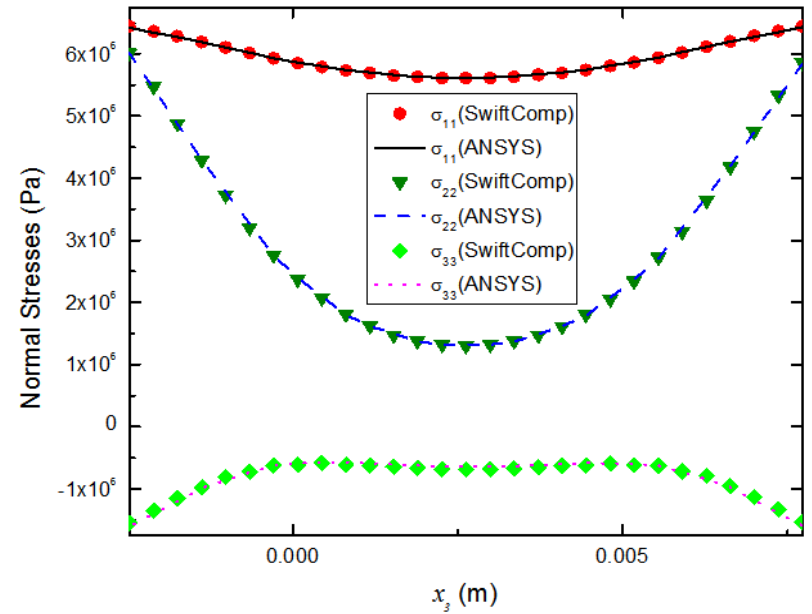
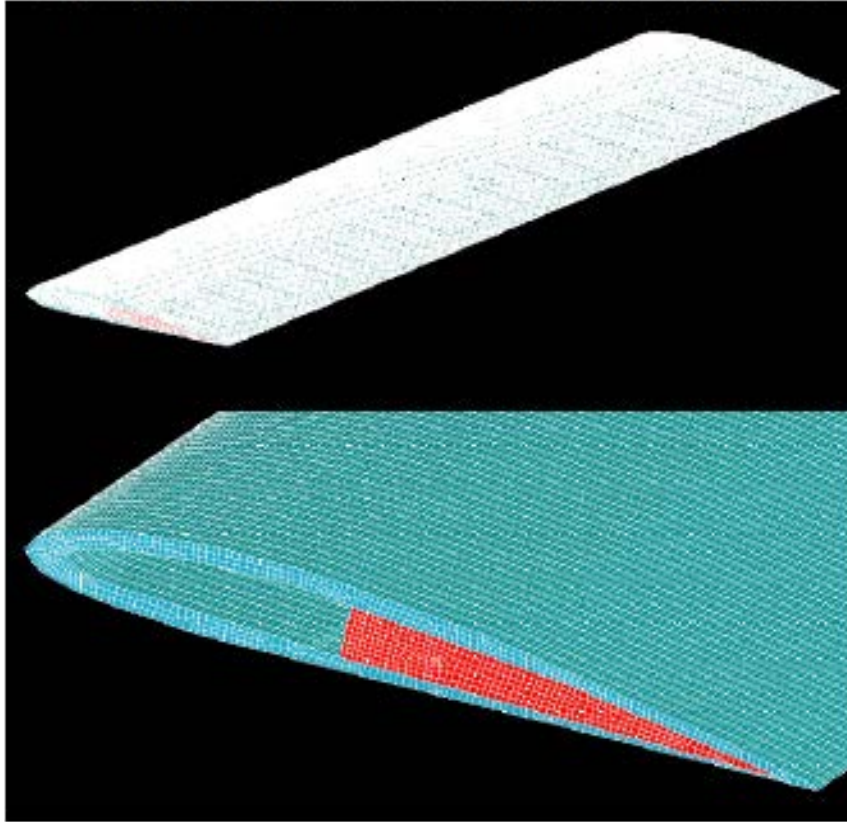
$$U = \frac{1}{2} \bar{\epsilon}^T (D_{\epsilon\epsilon} + 2V_0^T D_{h\epsilon} + V_0^T E V_0) \bar{\epsilon} \equiv \frac{\Omega}{2} \bar{\epsilon}^T \bar{D} \bar{\epsilon}$$

➤ Dehomogenization relations

$$\mathbf{u} = \mathbf{v} + \begin{bmatrix} \frac{\partial v_1}{\partial x_1} & \frac{\partial v_1}{\partial x_2} & \frac{\partial v_1}{\partial x_3} \\ \frac{\partial v_2}{\partial x_1} & \frac{\partial v_2}{\partial x_2} & \frac{\partial v_2}{\partial x_3} \\ \frac{\partial v_3}{\partial x_1} & \frac{\partial v_3}{\partial x_2} & \frac{\partial v_3}{\partial x_3} \end{bmatrix} \begin{Bmatrix} y_1 \\ y_2 \\ y_3 \end{Bmatrix} + SV_0 \bar{\epsilon}$$

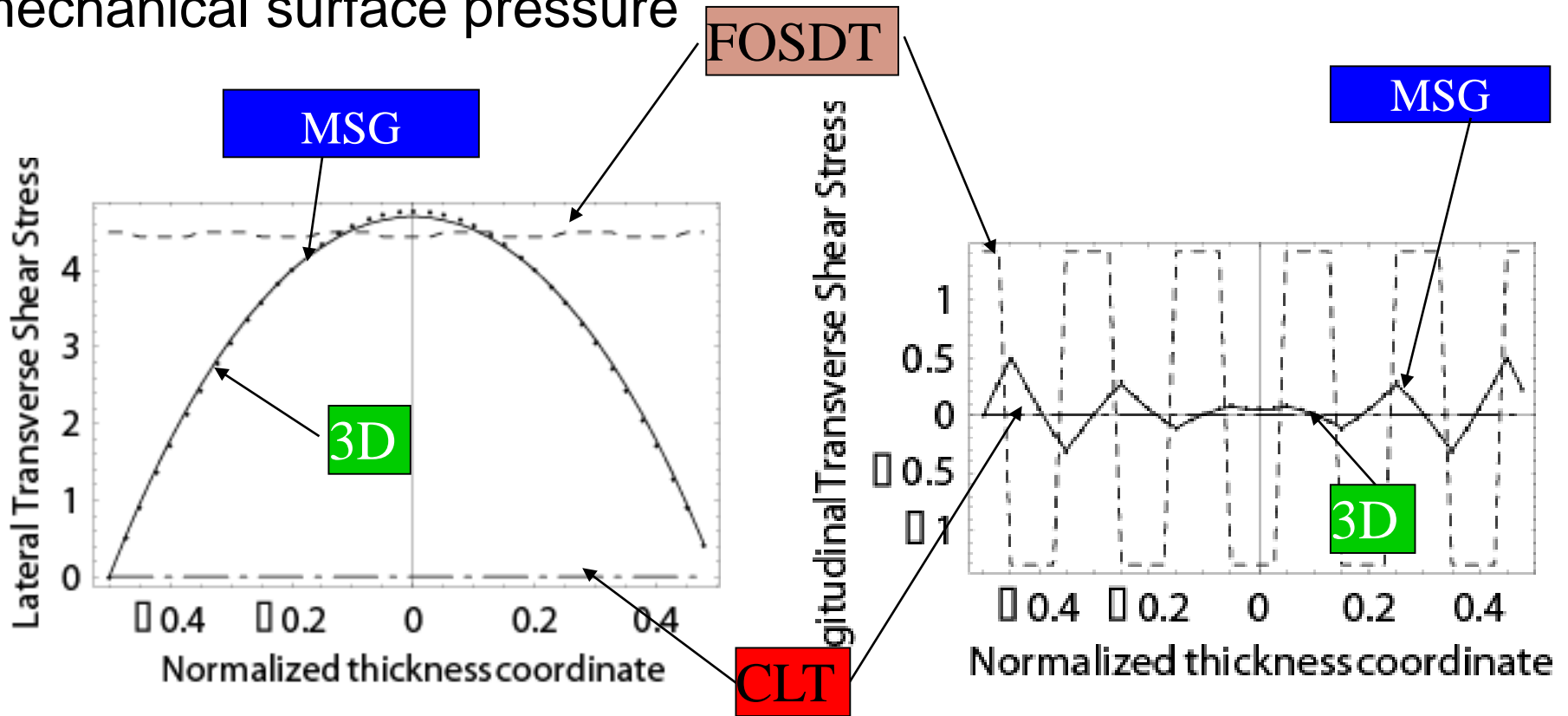
$$\epsilon = \bar{\epsilon} + \Gamma_h SV_0 \bar{\epsilon} \quad \sigma = D \epsilon$$

Realistic Rotor Blade



3D FEA Accuracy with FOSDT Cost

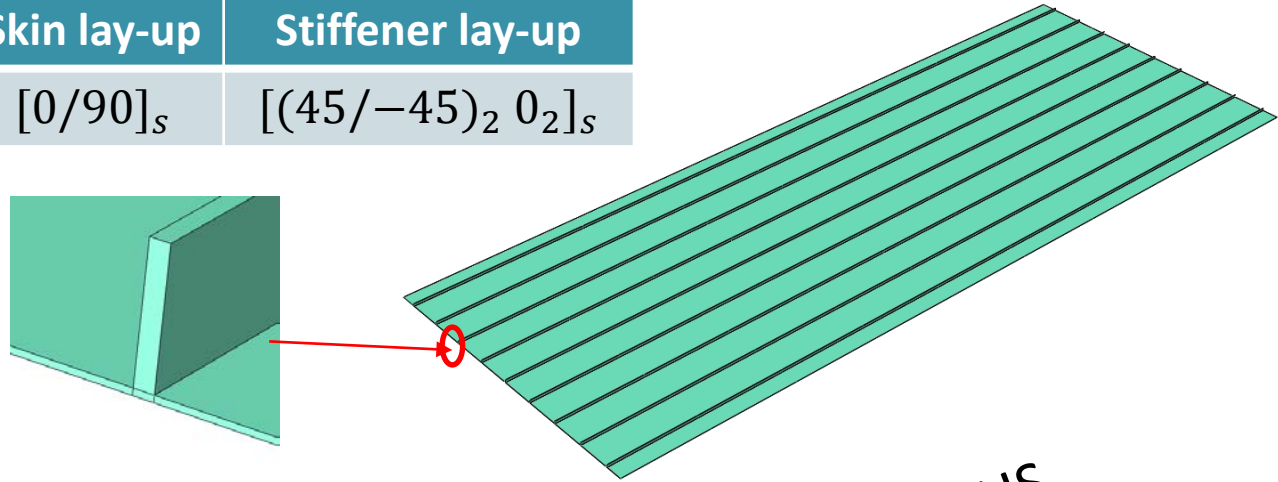
A 20-layer plate $[30^\circ / -30^\circ / -30^\circ / 30^\circ]_5$ under a sinusoidal mechanical surface pressure



Achieving 3D elasticity accuracy at efficiency of FOSDT (Reissner-Mindlin Theory)

Buckling Analysis of Stiffened Composite Panels

Skin lay-up	Stiffener lay-up
$[0/90]_s$	$[(45/-45)_2 0_2]_s$



Constitutive modeling
using SwiftComp

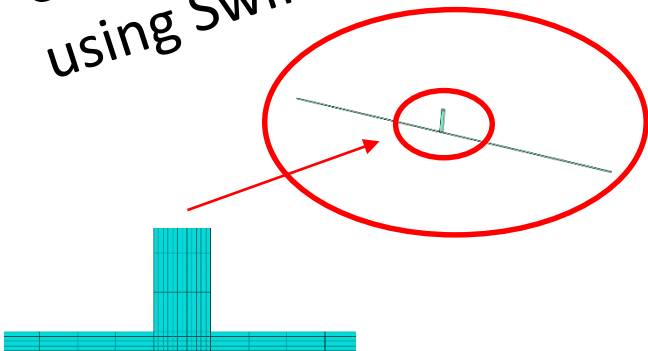
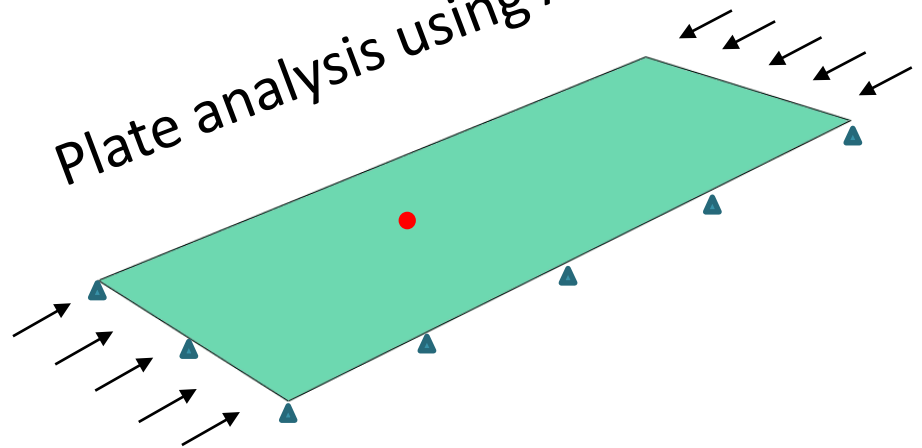


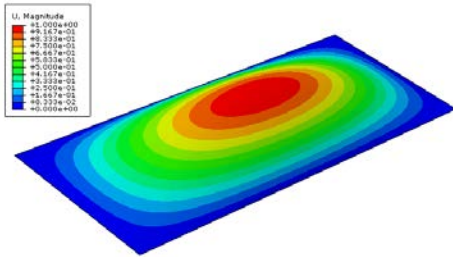
Plate analysis using ABAQUS



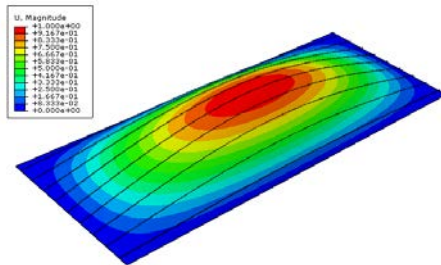
Buckling Analysis of Stiffened Composite Panels

1st mode

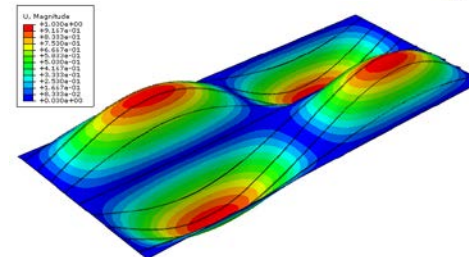
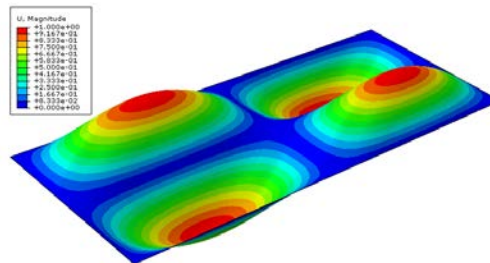
SwiftComp
based plate



3D FEA

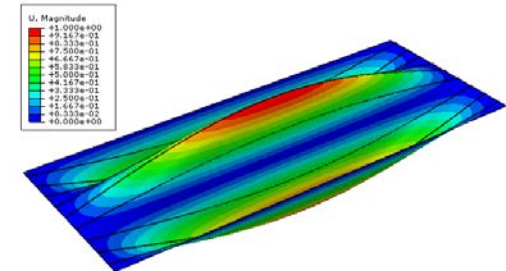
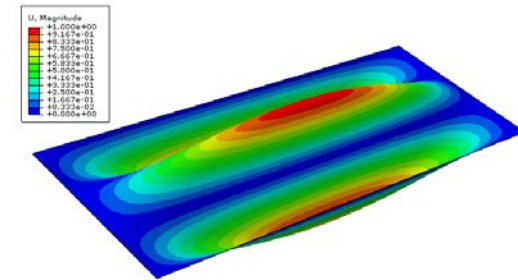


4th mode



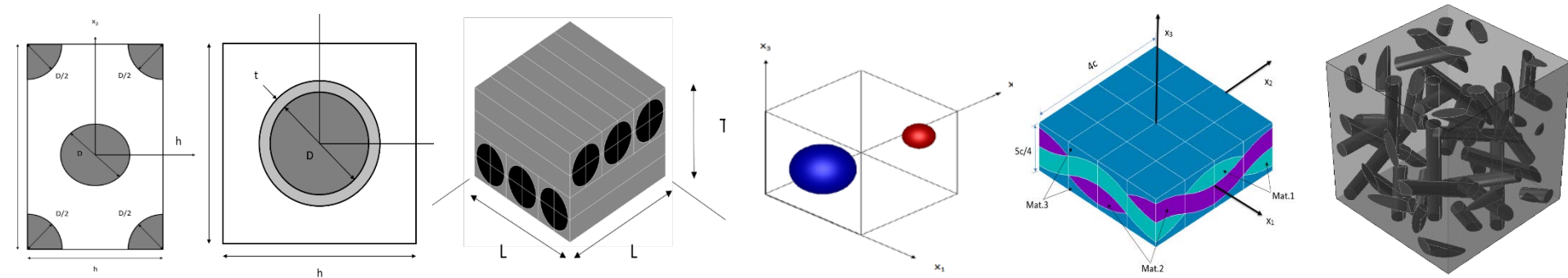
Half wave number	MSG-based plate analysis	3D FEA
m=1 n=1	930 (0.11%)	931
m=1 n=2	1799 (0.55%)	1809
m=2 n=1	3348 (1.42%)	3301
m=2 n=2	3743 (1.19%)	3699
m=2 n=3	4836 (0.71%)	4802
m=1 n=3	5009 (0.50%)	5034

6th mode

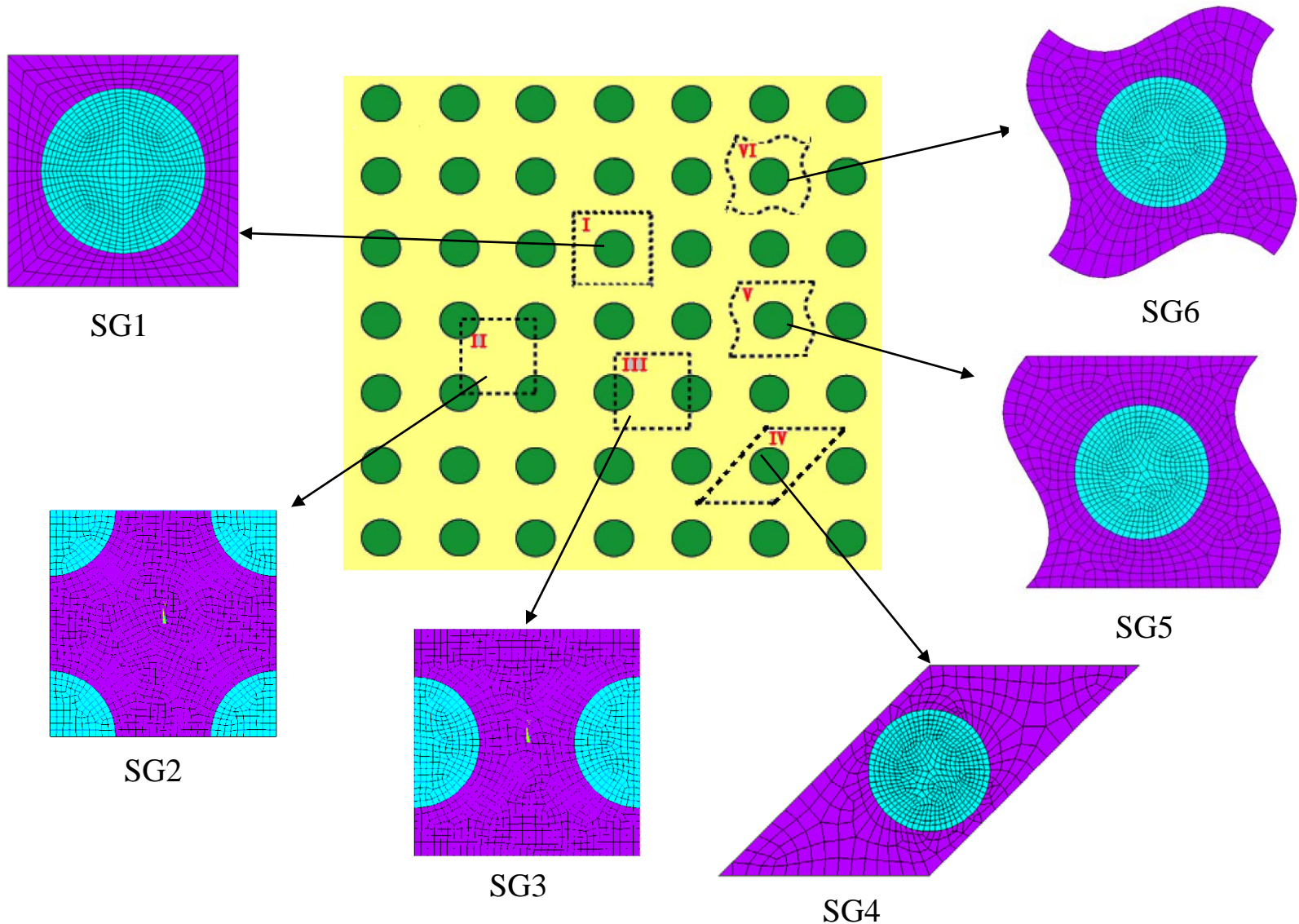


Micromechanics Simulation Challenge

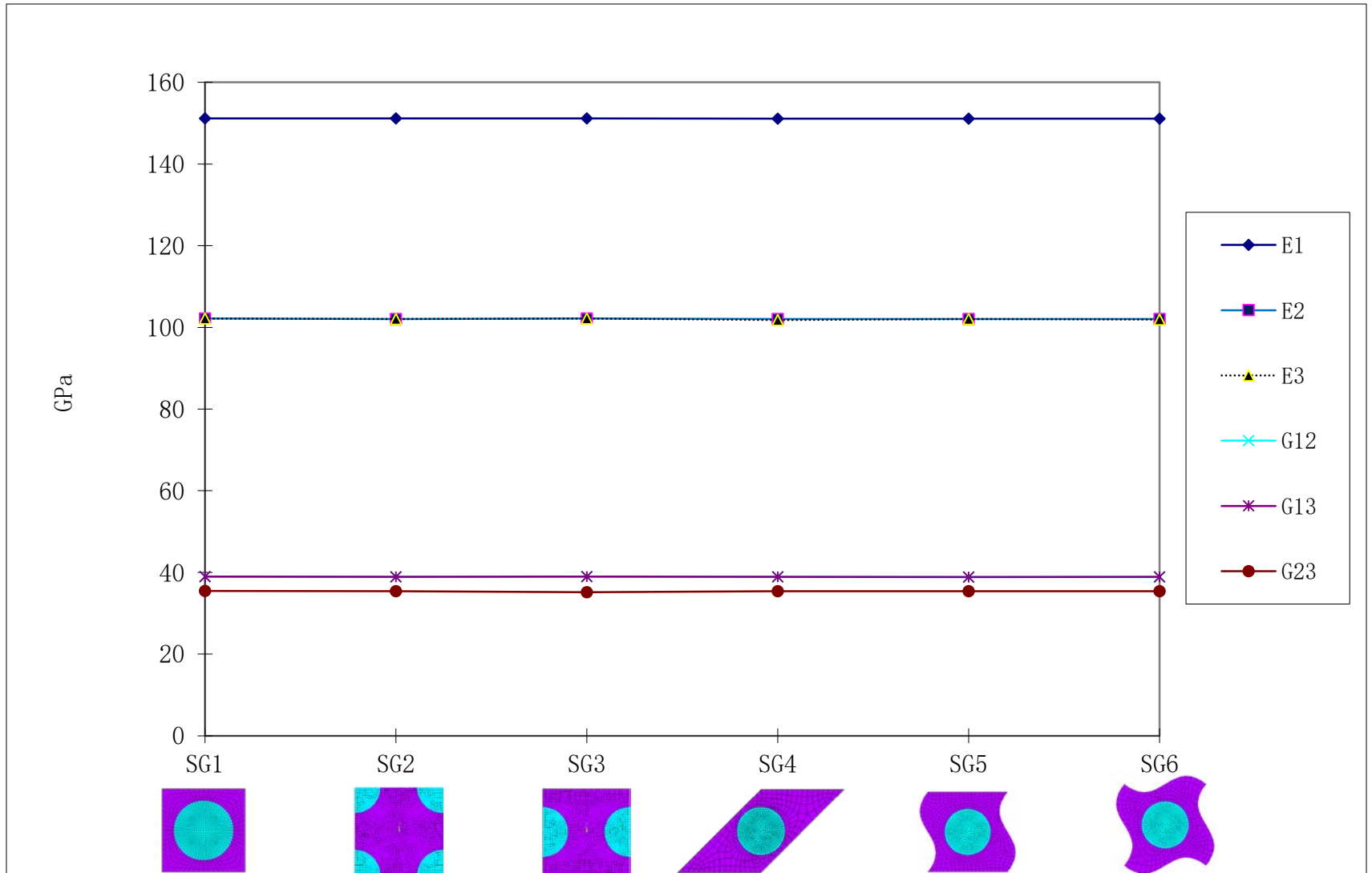
- MAC/GMC, MAC/HFGMC, DIGIMAT, Altair MDS, FVDAM, ESI/VPS, SwiftComp, 3D FEA of RVE with periodic BCs.
- Final report: cdmhub.org/resources/948.
- All data needed for reproducing the results: cdmhub.org/members/project/mmsimulationchalleng/view.
- Level I: accuracy and efficiency of linear thermoelastic properties and local fields.
- SwiftComp achieves versatility and accuracy as 3D FEA with a small fraction of its computing time.



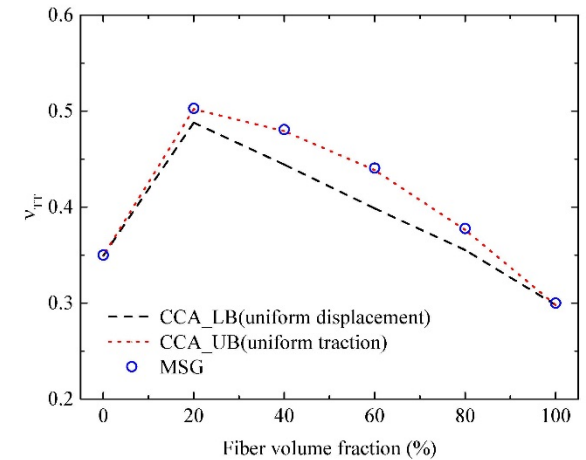
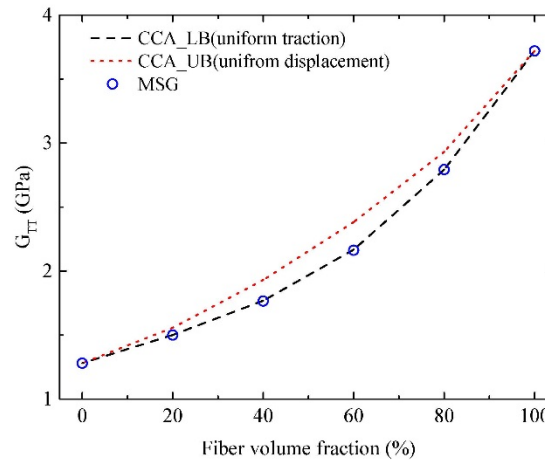
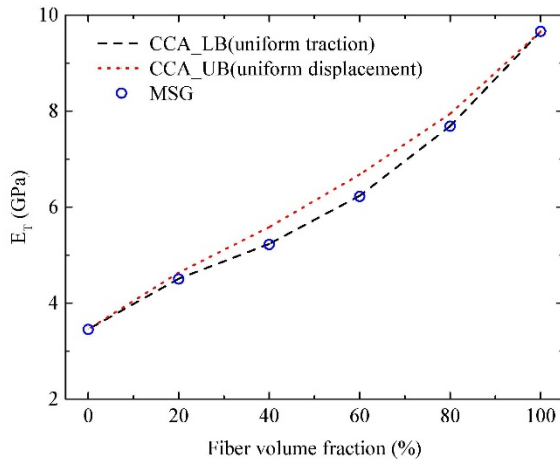
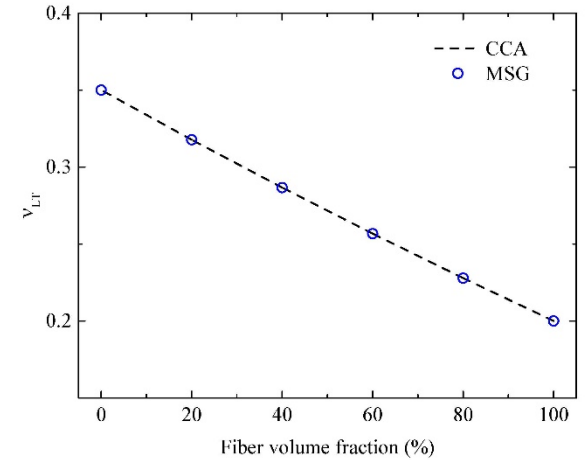
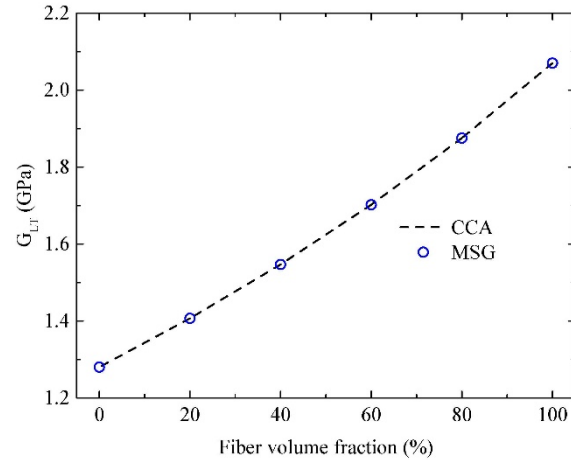
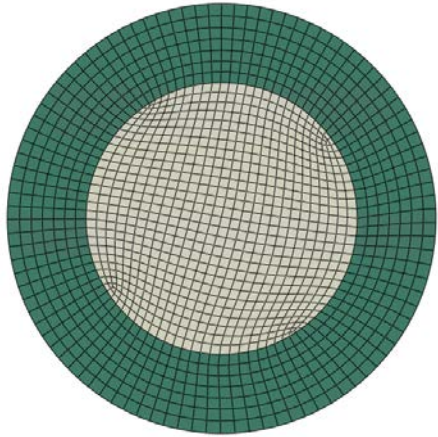
Choice of SG



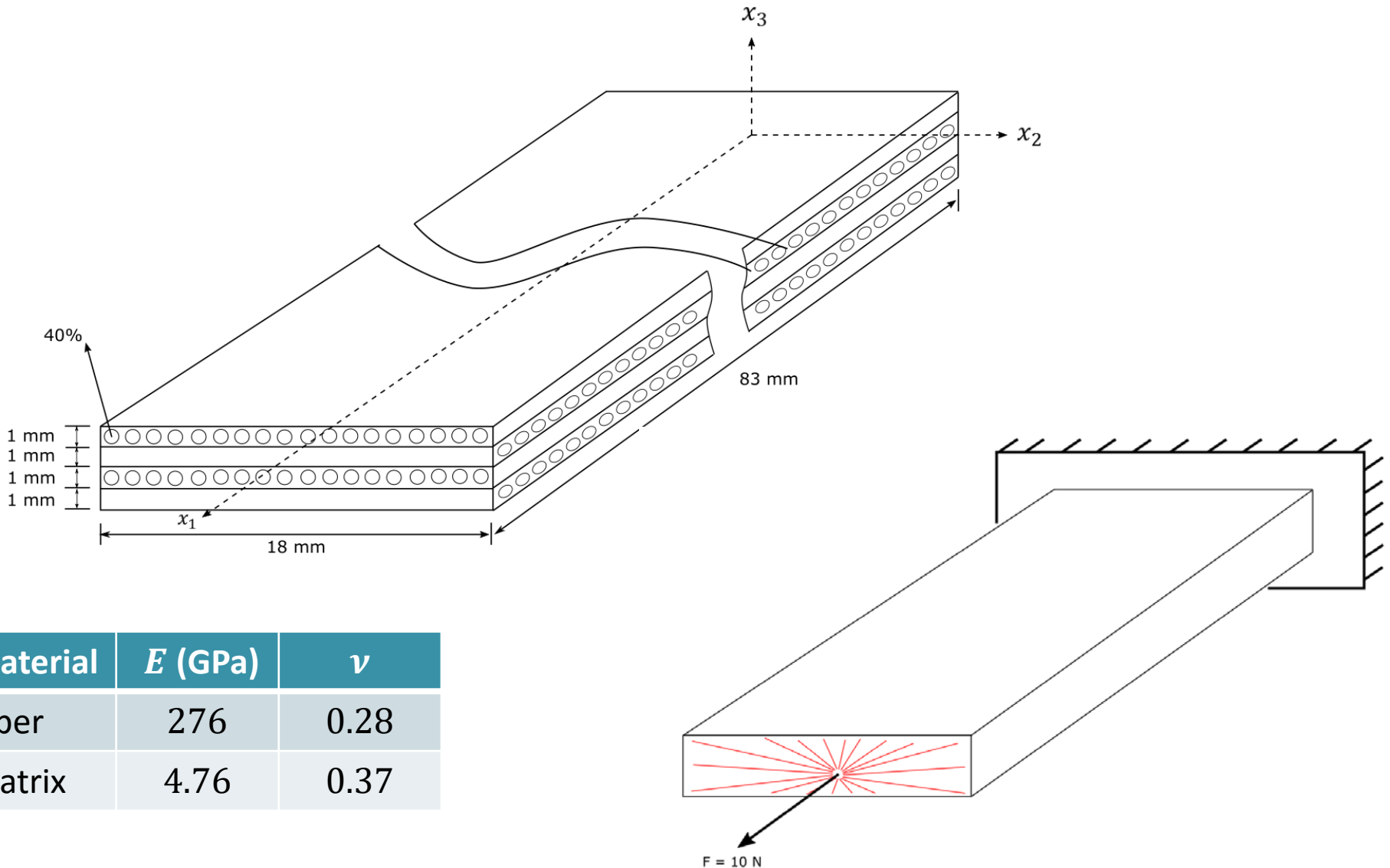
Choice of SG (cont.)



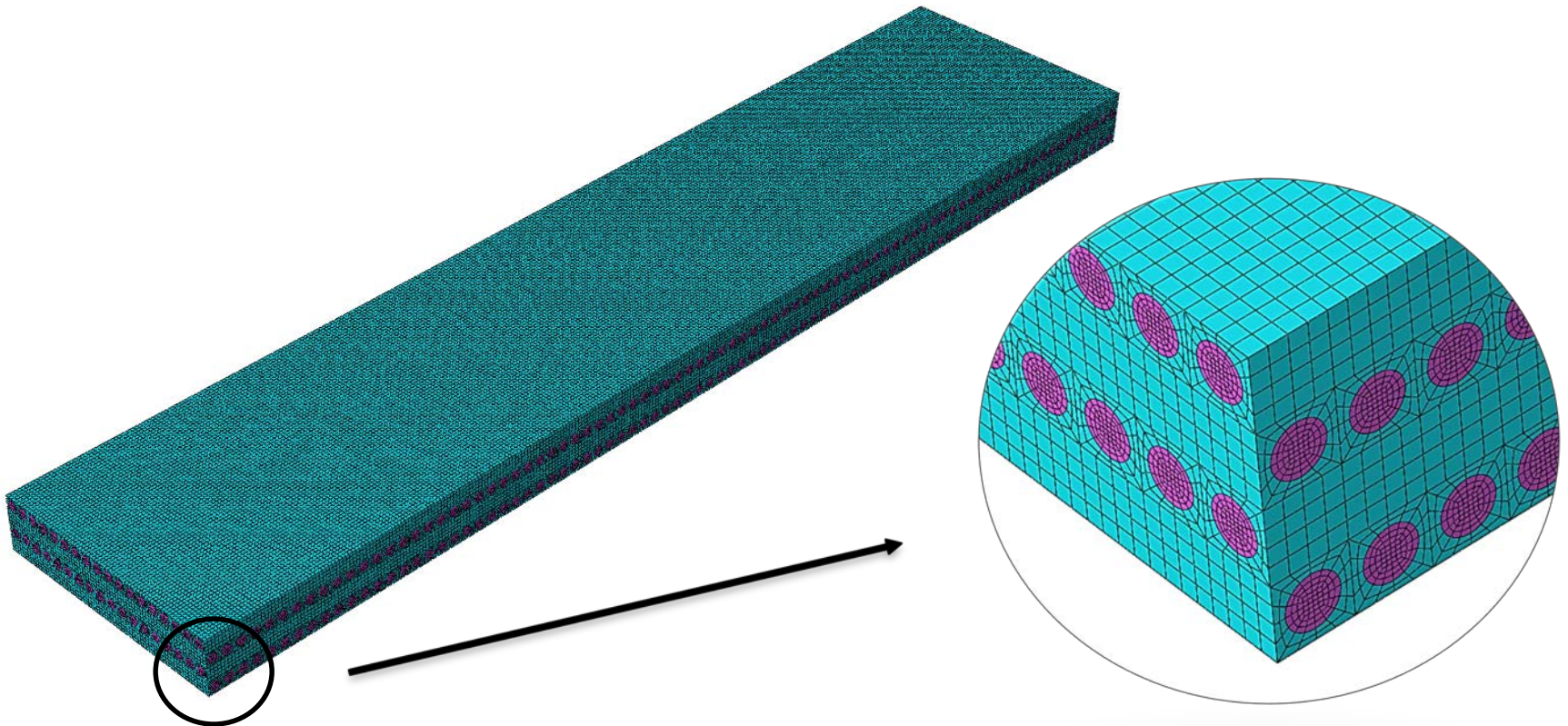
Compare with CCA model



Four Layer Cross-Ply Laminate



3D FEA



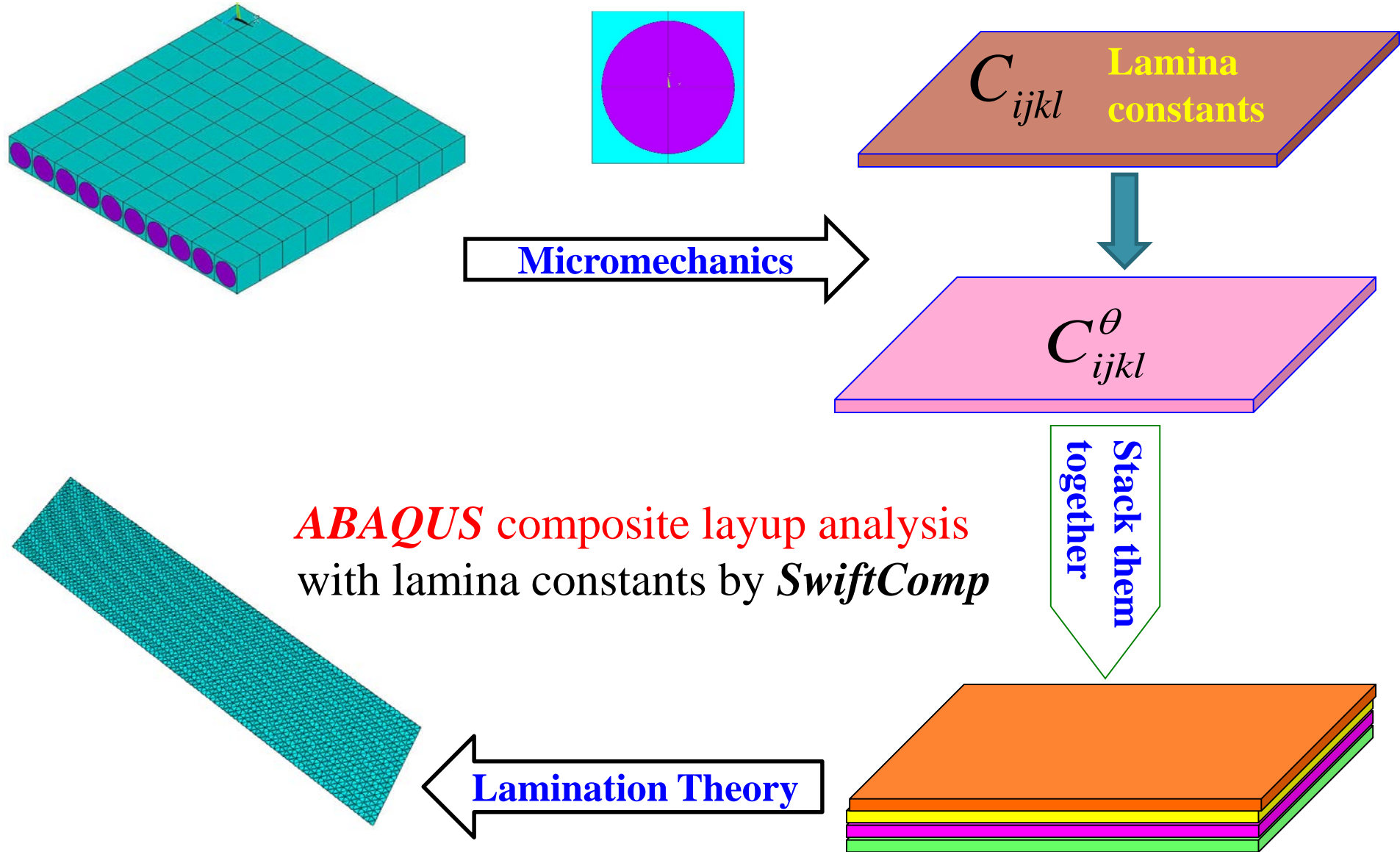
3D FEA

C3D20R

2,294,784

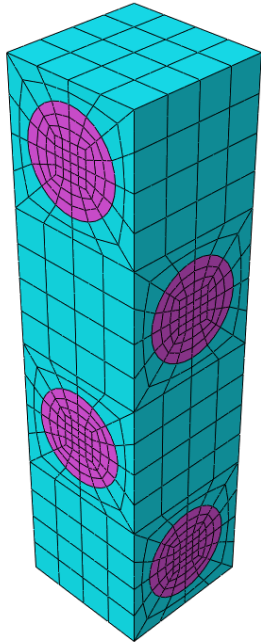
9,319,562

Two-Step Approach



SwiftComp Plate Analysis

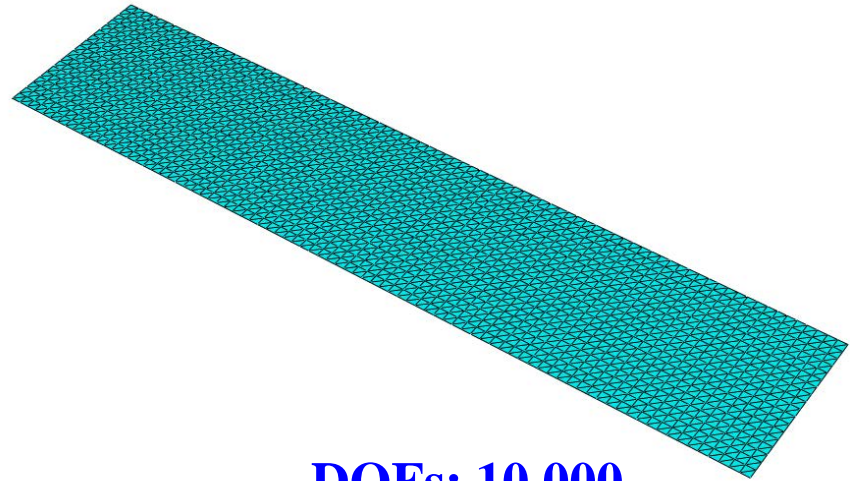
Plate SG



DOFs: 23,000



Mesh for plate analysis

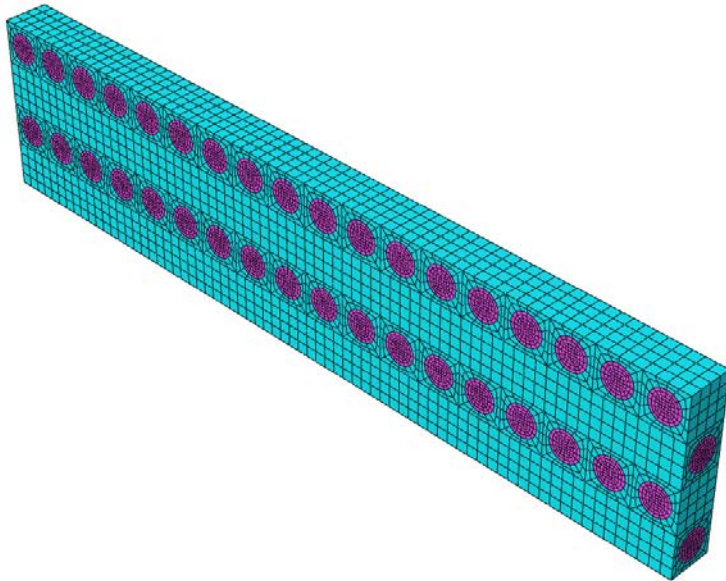


DOFs: 10,000

Same mesh is also used for ABAQUS composite layup analysis

SwiftComp Beam Analysis

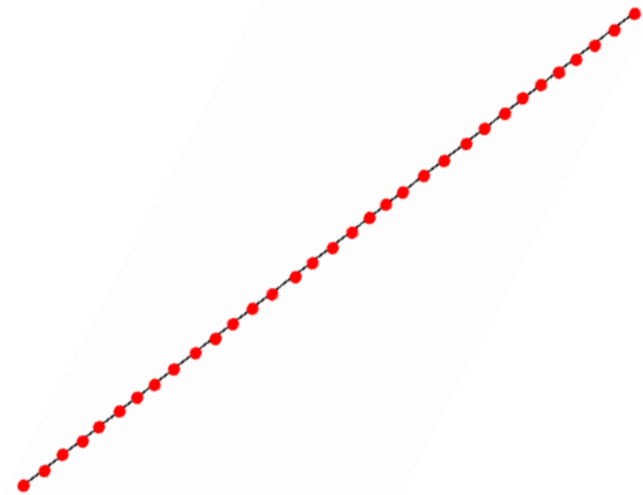
Beam SG



DOFs: 373,000

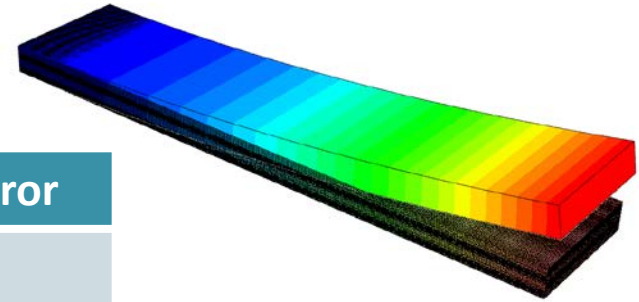
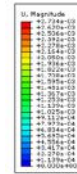


Mesh for beam analysis



DOFs: 500

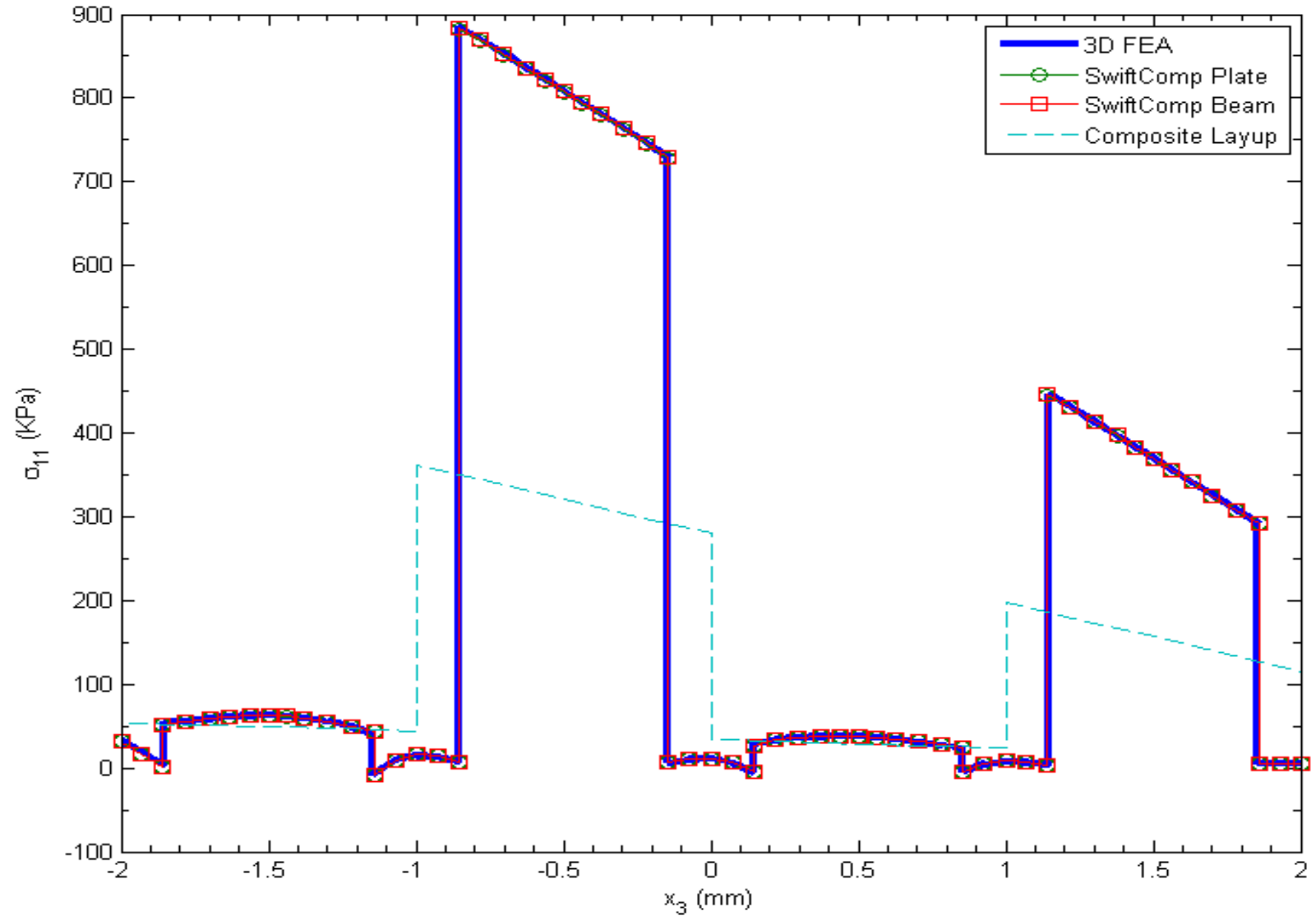
Global Behavior



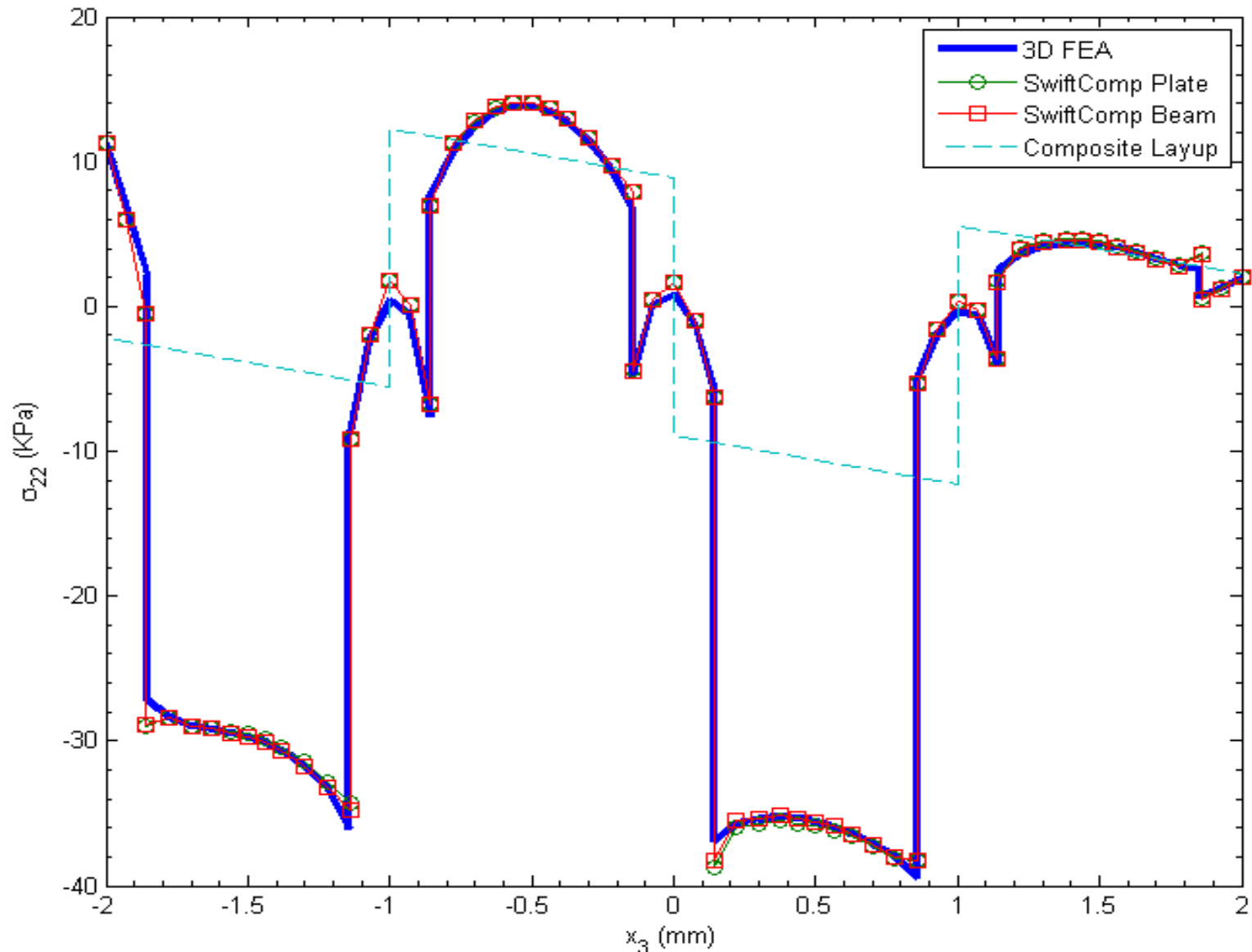
Method	U_1	Absolute error
3D FEA	2.0849×10^{-4}	
SwiftComp Beam	2.0873×10^{-4}	0.1151%
SwiftComp Plate	2.0832×10^{-4}	0.0815%
ABAQUS Composite layup	2.0804×10^{-4}	0.2158%

Method	U_3	Absolute error
3D FEA	2.7124×10^{-3}	
SwiftComp beam	2.7146×10^{-3}	0.0811%
SwiftComp plate	2.7084×10^{-3}	0.1475%
ABAQUS Composite layup	2.5264×10^{-3}	6.8574%

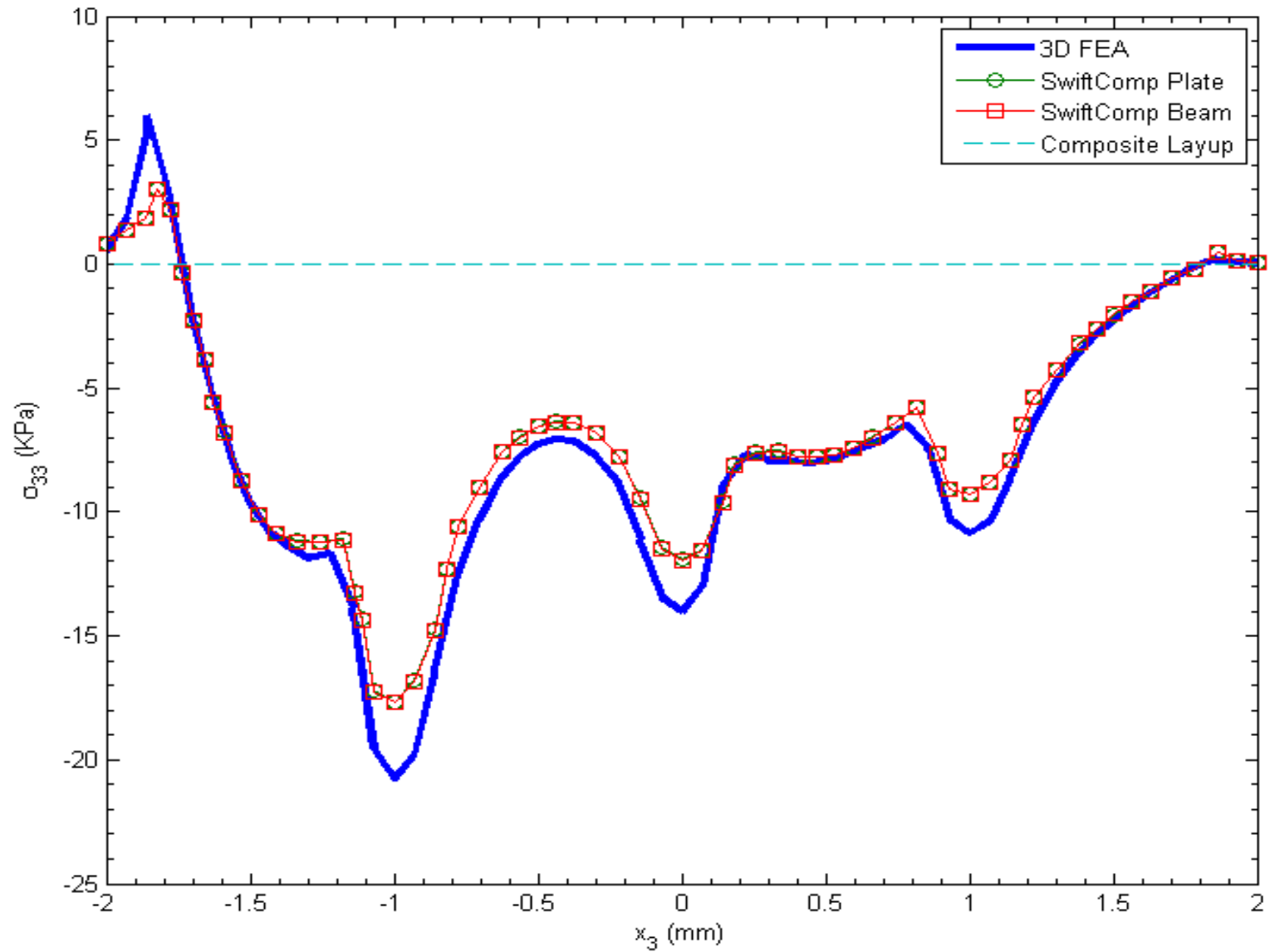
Local Stress Distribution



Local Stress Distribution



Local Stress Distribution



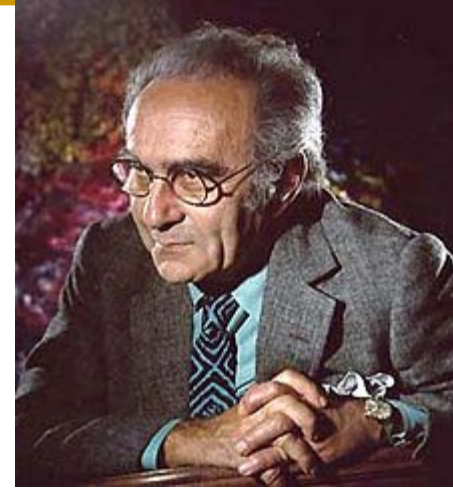
Efficiency

Method		CPU's	Time	
3D FEA		48	7 days 11 hr 37 min	
ABAQUS Composite Layup		1	30 sec	
SwiftComp Plate Analysis	Homo.	1	6 sec	40 sec
	2D plate analysis	1	28 sec	
	Dehomo.	1	6 sec	
SwiftComp Beam Analysis	Homo.	1	3 min 14 sec	4 min 35 sec
	1D beam analysis	1	0.02 sec	
	Dehomo.	1	1 min 21 sec	

Mechanics of SG & SwiftComp

- **Directly connects** materials genome with structural analysis
- **Achieves** accuracy of 3D detailed FEA at efficiency of simple engineering models
- Models composites as **black aluminum**, capturing details as **needed** and **affordable**
- Power conventional structural tools with accurate composites modeling

Unifies Structural Mechanics & Micromechanics

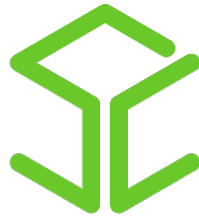


Jacob Bronowski
**The Creative
Aspects of
Science**

The progress of science is the discovery at each step of a new order which gives unity to what had long seemed unlike. Faraday did this when he closed the link between electricity and magnetism. Clerk Maxwell did it when he linked both with light. Einstein linked time with space, mass with energy,

Science is nothing else than the search to discover unity in the wild variety of nature — or more exactly, in the variety of our experience.

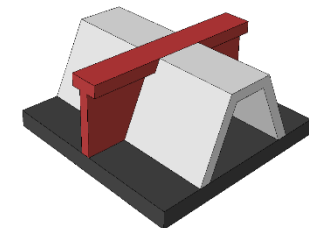
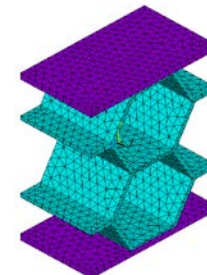
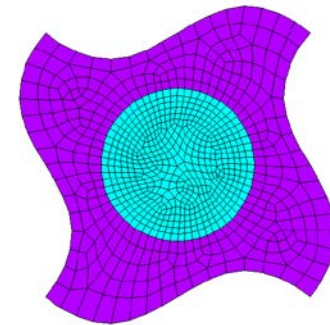
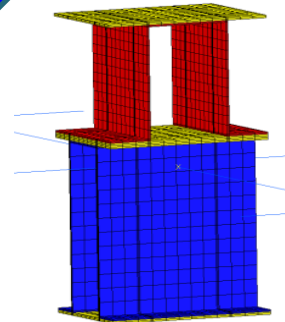
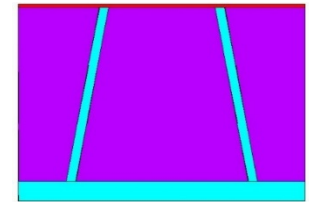
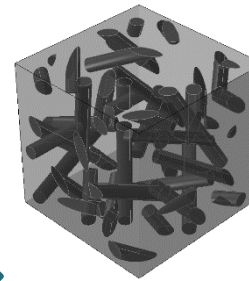
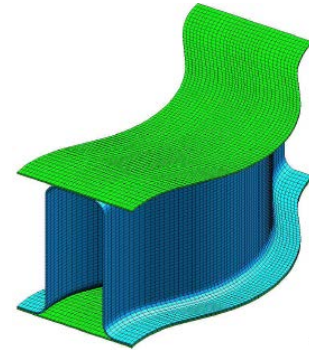
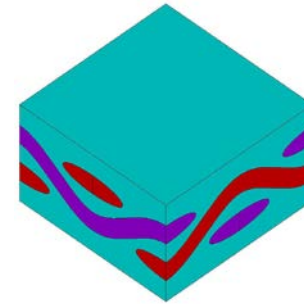
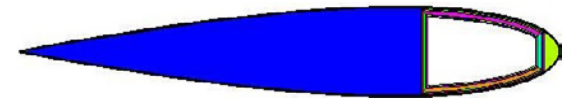
Right Results Right Away



SwiftComp™
A Purdue Technology

Principle of Minimum Information Loss

- **Virtual testing of materials**
 - Mechanical properties
 - Multifunctional properties
- **Multiscale modeling of structures**
 - Composite structures
 - Stiffened structures
 - Build-up structures



Structure Genome vs RVE

- Structure Genome (SG): **smallest mathematical** building block; structural properties (beams/plates/shells/3D bodies)
- RVE: volume entirely typical of material on average and contains a **sufficient number of inclusions** for effect properties independent of BCs; 3D RVE required for 3D properties
- Equivalent: 3D bodies featuring 3D periodicity

MSG, Asymptotic Homogenization (AH), & RVE Analysis

- RVE analysis with periodic BCs is the same as AH, same as MSG for 3D RVEs (in theory)
- MSG: no BCs in terms of displacements/tractions, automatically satisfying Hill-Mandel condition
- No assumptions for SG and local fields
- MSG unifies structural modeling and micromechanics
- MSG can handle partially periodic or aperiodic structures
- MSG can directly construct models for beams/plates/shells

