Advances of Multiscale Modeling in LS-DYNA

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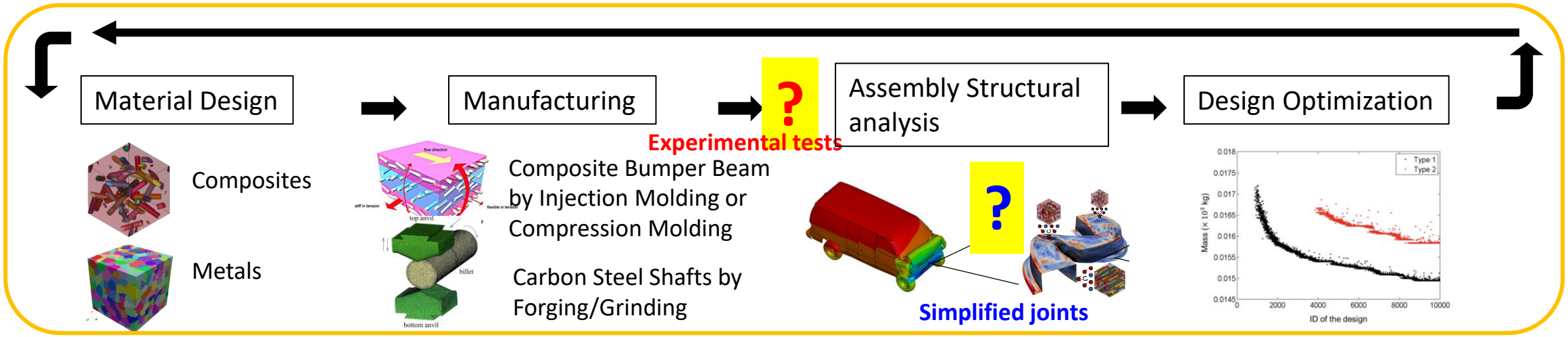
Outline

1. **Introduction of Multiscale Modeling**
2. **Geometric Multiscale Modeling**
   - Bridging the information of meso and macro scales in the assembly system (e.g., solder balls in PCB, rivets in a car model, etc.)
   - Key technology: **Two-scale co-simulation** (2021 LS-DYNA R13)
3. **Material Multiscale Modeling (Presented by Haoyan Wei)**
   - Bridging the information of micro and meso scales in the material system (e.g., fiber in composites, polycrystalline grains in metals, etc.)
   - Key technology: **Deep Material Network (DMN)** (2022 LS-DYNA R14)

Why Multiscale Modeling is Important for CAE Applications?

- After manufacturing, materials becomes heterogeneous (location-specific) and nonlinear.
- However, in structure analysis the manufactured materials are modeled by the phenomenological homogeneous material law. It requires a lot of experimental testing to obtain the material constants which can be inaccurate and time/money wasting.
  -> **Missing Manufacturing details of material in the structural analysis**
- Additionally, using the simplified joint models for the assembled structural analysis is efficient but not accurate.
  -> **Missing Geometric details of connections/joints in the structural analysis** (joints are the weakest points in a full-car model!)
- Therefore, the development of efficient multiscale modeling methods is in high demand.

Model-based simulation workflow of a car component in a full-vehicle crashworthiness



Two Multiscale Modeling Methods in LS-DYNA

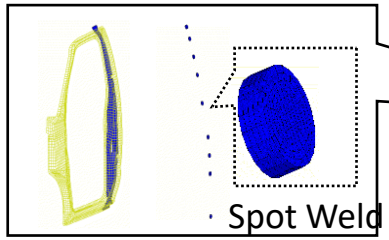
Goal: **Introduce manufacturing and geometric details to the structural analysis**

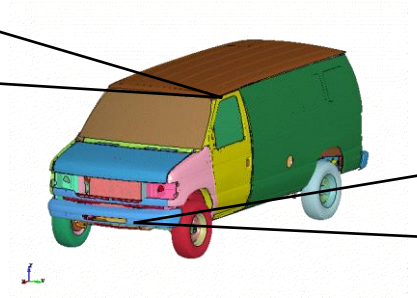
- **Deep Material Network (DMN)** for **material multiscale modeling** that bridges the **microstructures** from manufacturing simulation results with the meso-scale finite element structures for the injection molded fiber-reinforced composites
- **Two-scale Co-simulation** for **geometric multiscale modeling** that bridges the meso-scale **connections/joints** with the macro-scale assembly structure for an efficient and accurate crash simulation

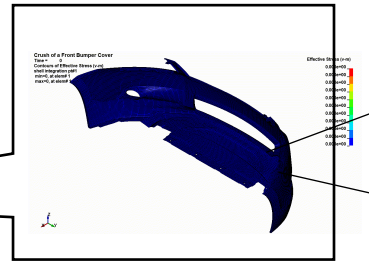
Crash Analysis of Injection Molded Composite Bumper in a Full-Vehicle Model

Assembly Structural analysis

Crashworthiness by **Two-scale Co-simulation**

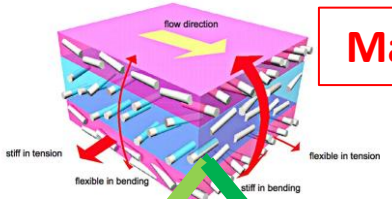






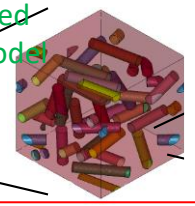
Manufacturing Processing Simulation

Simulation of injection molding of short fiber-reinforced composites by Moldex3D



phenomenological material law

Physics-based material model



Linking microstructure-performance by **ML-based DMN method**

Assembled FEM Model
Two-scale

Composite Part
Macro-scale

Finite Element
Meso-scale

RVE Model
Micro-scale

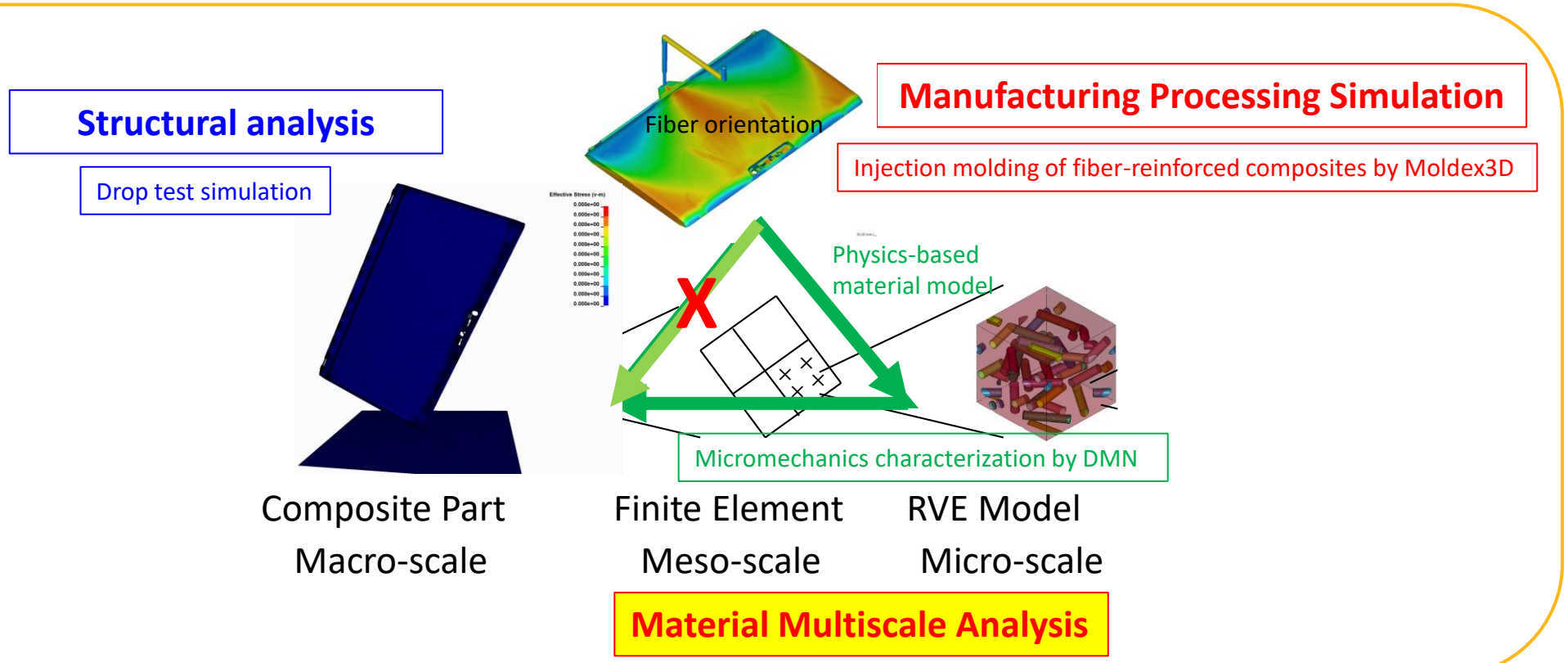
Geometric Multiscale Analysis

Material Multiscale Analysis

Application of Material Multiscale Modeling

- In real manufacturing, different process parameters produce different material properties
- Perform the **Material Multiscale** Analysis using the LS-DYNA **Deep Material Network (DMN)** method can avoid a lot of experimental tests

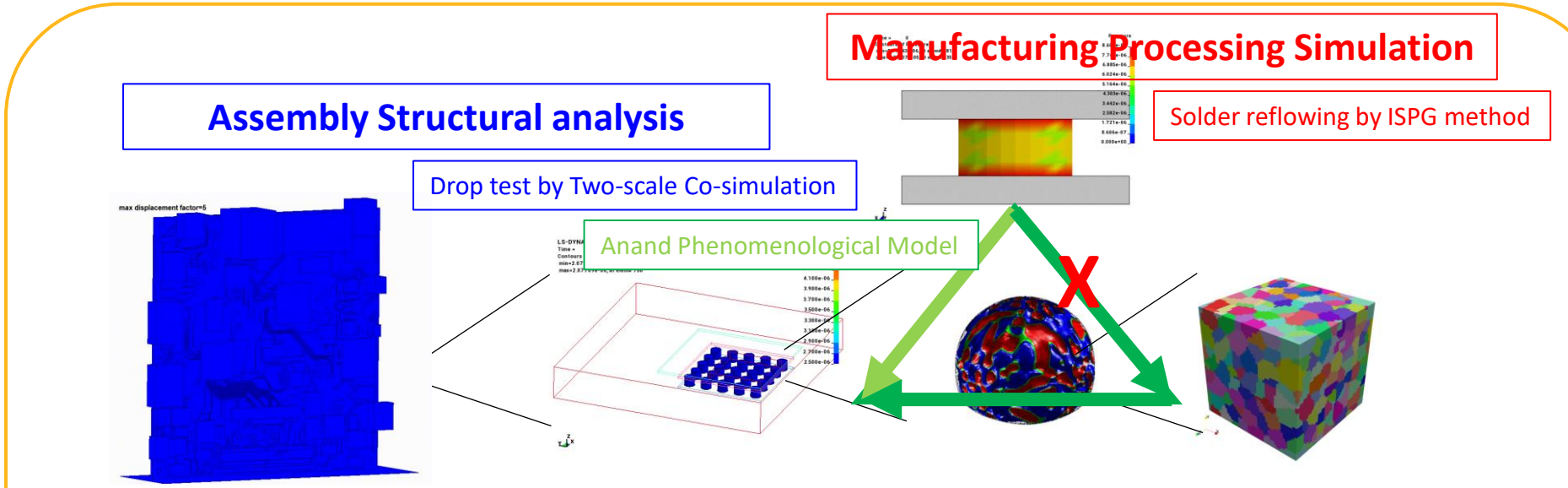
Drop Test of a Composite Notebook Cover



Application Geometric Multiscale Modeling

- In practice, solder ball reflowed geometries including defects are critical to the reliability analysis.
- Using the **ISPG method** for reflow soldering simulation and LS-DYNA **Two-scale Co-simulation** method for shock wave analysis can effectively perform the reliability analysis.

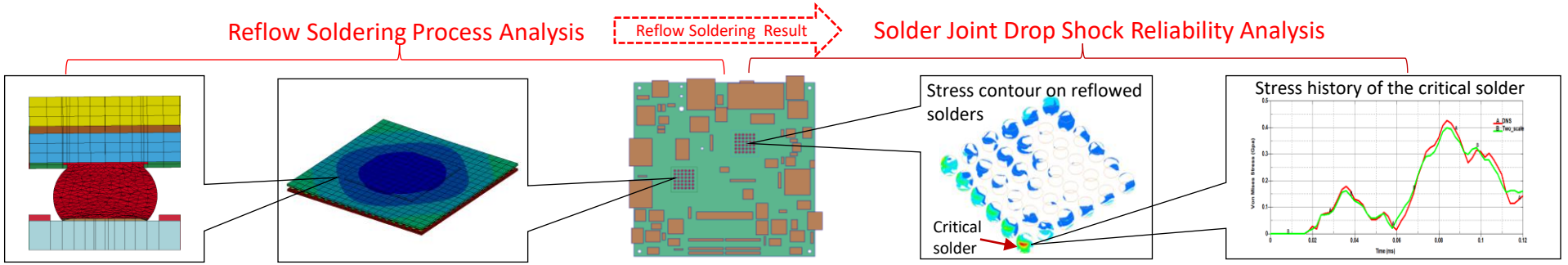
Solder Balls Reliability in a PCB Drop Test



Geometric Multiscale Modeling (1)

- **IC Packaging Concern**

Integrated Circuit (IC) packaging is the final stage of semiconductor device fabrication. **It is a multiscale problem where the small-scale reflowed solder joints are the weakest structure in assembly**. Therefore, the analysis of reflow soldering process and the solder joint reliability is critical.



- **Current CAE Market**

There is no other efficient reflow soldering solver in CAE market for the large-scale analysis (missing an appropriate numerical method)

- ✓ Most existing approaches are either analytical (e.g., reflow profile calculator) or experimental methods, thus having strong limitations in engineering practice.
- ✓ Few established numerical methods work for individual solder or small-scale problems, but they are prohibitively expensive for large-scale analysis.
- ✓ Because of that, existing drop test solvers could not consider reflow soldering solution.

Existing drop test solvers are either computationally expensive or inaccurate (missing an effective multiscale method)

- ✓ Even without reflowed solder information, the direct numerical simulation is still computationally expensive while the sub-modeling method is efficient but inaccurate.

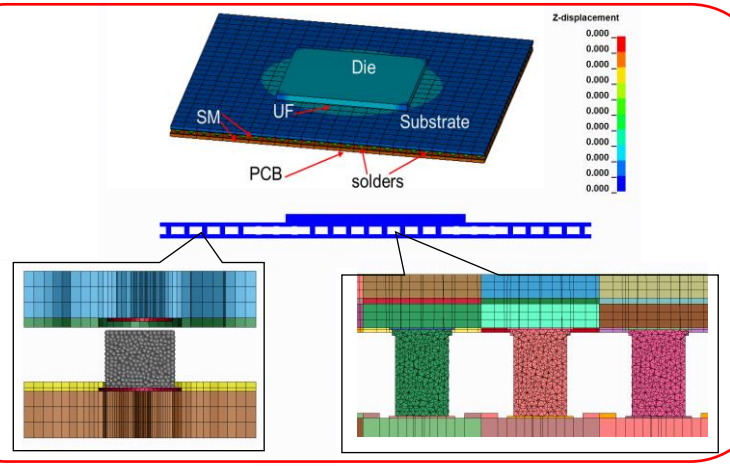
- **Importance**

IC packaging industry needs **an effective CAE tool** for the **large-scale reflow soldering process simulation**, capable of predicting dissimilar reflowed ball shapes and defects, and analyzing their influence on **drop shock reliability** due to the expanding chipmaking for consumer electronics.

Geometric Multiscale Modeling (2)

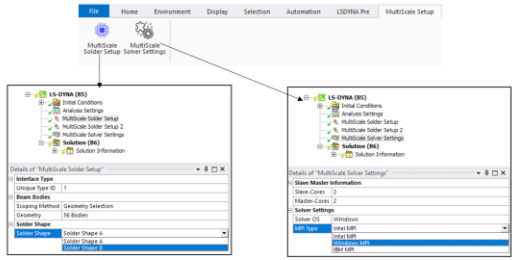
- **Workflow**
  - ➢ Available in 2021 LS-DYNA R13

Implicit Reflow Soldering Simulation by ISPG method



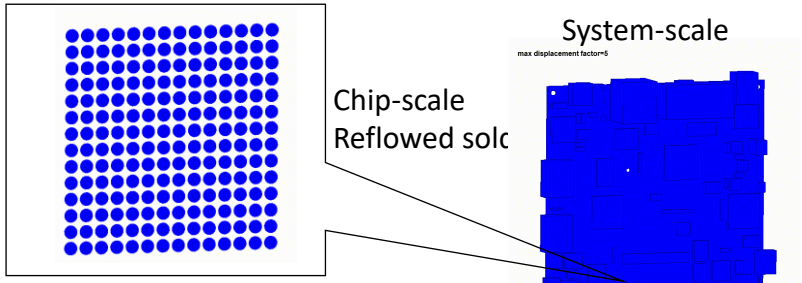
Export Reflow Soldering Results *via* Workbench

Ansys Workbench



- ✓ Dissimilar Solder Ball Shapes
- ✓ Thermal-induced PCB Warpage
- ✓ Mask and Pad Geometry
- ✓ Immerse Modeling

Explicit Multi-scale Drop Test Simulation by Two-scale Co-simulation



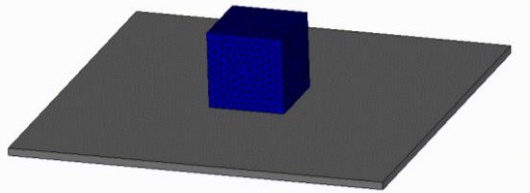
Linking Multiple Chips with a System-Scale PCB in the Drop Shock Simulation

Incompressible Smoothed Particle Galerkin (ISPG) Method

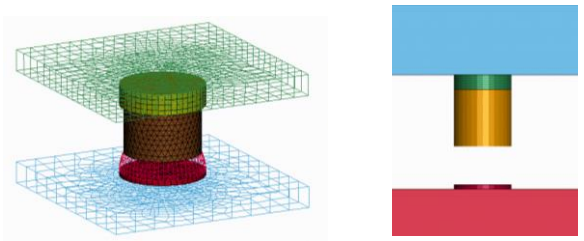
- **Objective** **Efficiently simulate the large-scale reflow soldering process**
- **Method**
  - ✓ **Technique**: **Implicit Lagrangian Particle Galerkin** approach solving Navier-Stokes equations considering **viscosity, surface tension and contact angles** in liquid
  - ✓ **Uniqueness**: Integration with structure and thermal solvers capable of modeling **tens of thousands solder balls** with **strong MPP scalability**
  - ✓ **First Release:** 2021 LS-DYNA R13; semi-implicit and full-implicit MPP versions with **ACE's Ansys Workbench** for easy large-scale solder balls setup
- **Feature**

Simulate **severe free surface flow** of solders, **predict defects** and the **variance of reflowed ball shapes** due to different solder mask/pad geometries, locations, boundary conditions, and the thermal-induced PCB warpage in **large-scale problems**

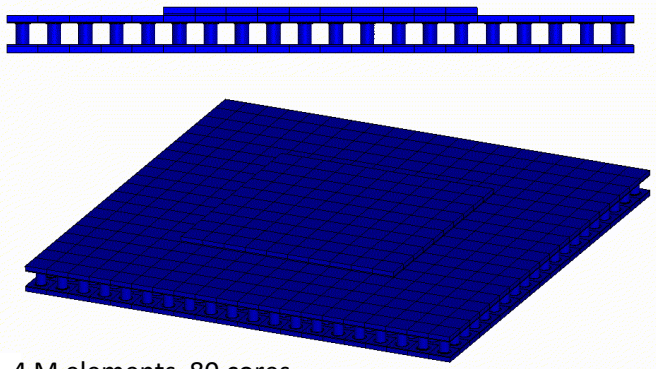
✓ Severe Solder Reflowing on Free Surface with Strong Surface Tension



✓ Defect Prediction

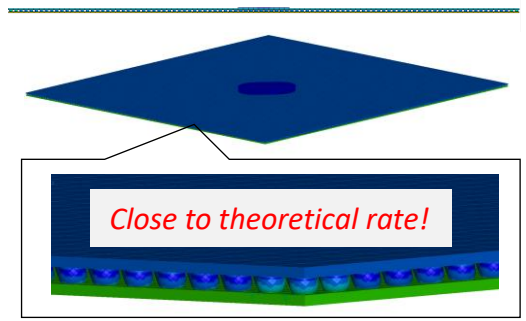


✓ 400 Dissimilar Solder Balls due to Thermal-induced PCB Warpage



~1.4 M elements, 80 cores
CPU 10 hours << Established numerical methods in weeks

✓ MPP Scalability Performance for a Large-scale Model with 10,000 Solder Balls



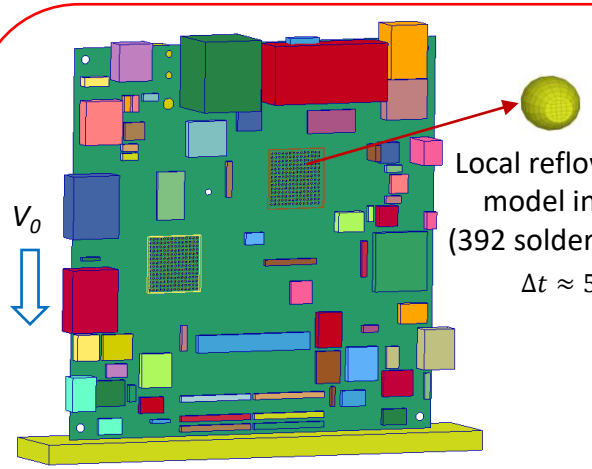
~32 M elements, 320 cores
CPU 2 days << Established numerical methods estimated in months ~ years

Two-scale Co-simulation Method

- **Objective** **Efficiently analyze the solder joint reliability in the drop test**
- **Method**
  - ✓ **Technique: two-way sub-cycling** with independent time stepping in co-simulation for accelerated multiscale computation
  - ✓ **Uniqueness: Process-informed structural analysis** capable of importing ISPG reflow soldering solution for drop test simulation
  - ✓ **First released:** 2021 LS-DYNA R13; explicit MPP version with **ACE's Ansys Workbench** for low modeling cost and easy setup
- **Feature**

  Efficiently execute the **run-time coupling** of local reflowed solder joints model and global PCB model in the multiscale drop test

✓ Multi-scale Model for Drop Test



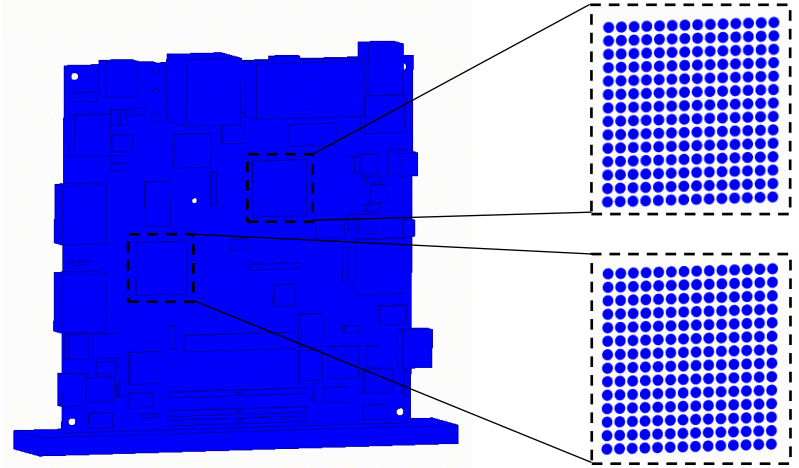
Local reflowed solder joints model in the chip-scale (392 solders, 121,520 solids)

$\Delta t \approx 5.0 \times 10^{-9} s$

Global PCB model in the system-scale (10,249 shells and 1,483 solids)

$\Delta T \approx 3.0 \times 10^{-8} s$

✓ Efficient Multi-scale Shock Wave Simulation in Drop Test

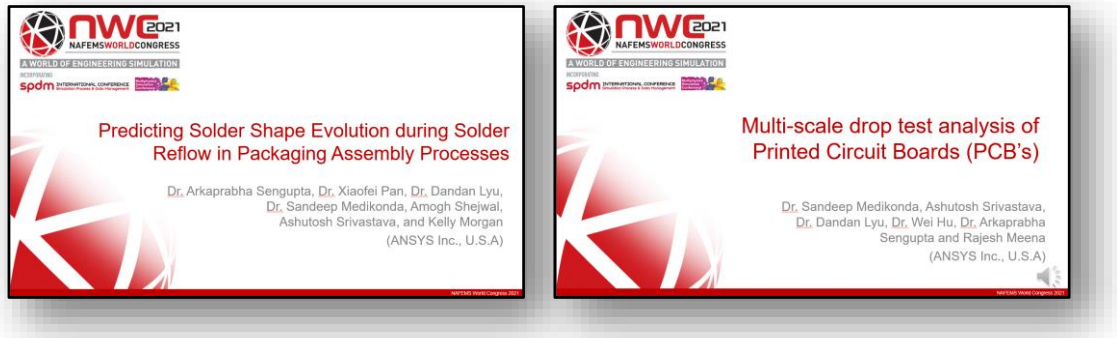


	Direct Numerical Simulation	Two-scale Co-sim
Normalized CPU time	1.0 (8 CPUs)	**0.2** (global 1 + local 7 CPUs)

Geometric Multiscale Modeling (3)

Contact

Dr. Arka Sengupta (Ansys Application Engineer)



Publication

Journal Paper

1. X.F. Pan, C.T. Wu, W. Hu, "A Semi-Implicit Stabilized Particle Galerkin Method for Incompressible Free Surface Flow Simulations", *International Journal for Numerical Methods in Engineering,* 121(17), pp.3979-4002, **2020**.
2. W. Hu, X.F. Pan, D.D. Lyu, A. Srivastava, S. Shah, C.T. Wu, "A Two-scale Approach for the Drop Shock Simulation of a Printed Circuit Board Package Considering Reflowed Solder Ball Geometries", *International Journal for Multiscale Computational Engineering,* 18(4): 455-476, **2020**.

Conference Paper

1. A. Sengupta, X.F. Pan, D.D. Lyu, S. Medikonda, A. Shejwal, A. Srivastava, K. Morgan, "Predicting Solder Shape Evolution during Solder Reflow in Packaging Assembly Processes", NAFEMS Conference, **2021**.
2. S. Medikonda, A. Srivastava, D. D. Lyu, W. Hu, A. Sengupta, R. Meena, "Multiscale Drop Test Analysis of Printed Circuit Boards (PCB's)", NAFEMS Conference, **2021**.
3. D.D. Lyu, W. Hu, X.F. Pan, C.T. Wu, "Introduction of ISPG Method and Geometric Multiscale Modeling for Electronics Solder Reflow and Shock Wave Analysis", 13th European LS-DYNA Conference **2021**.

Patent

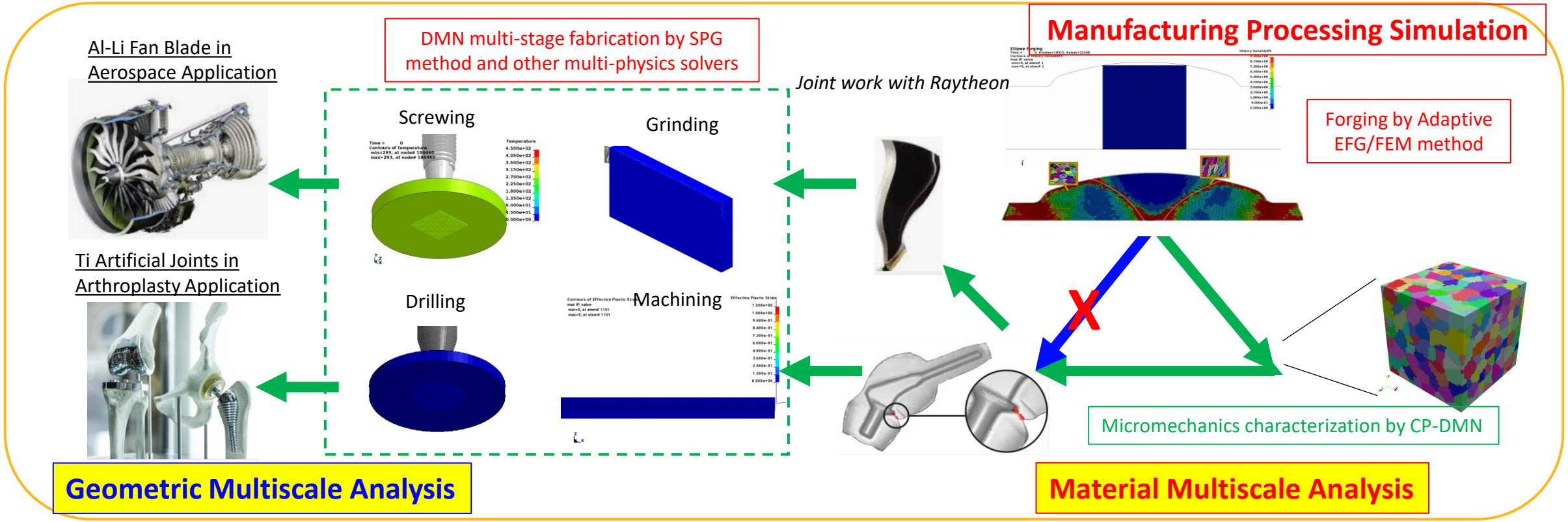
"System and Methods of Simulating Drop Shock Reliability of Solder Joints with a Multiscale Model"

US Patent Application Number: 63/056,418 filed on July 24, **2020**. Inventors: C.T. Wu, Wei Hu, Dandan Lyu, Siddharth Shah, Ashutosh Srivastava

On-going Developments for Polycrystalline Metals

- DMN Multi-stage Metal Fabrication Simulation
  1. **Crystal Plasticity in DMN** to process material heterogeneity for Forging + Heat Treatment + Machining/Griding + Screwing/Drilling processes
  2. **Global and local data transfer** between multiple multi-physics solvers (Adaptive FEM/EFG, SPG)
  3. A new **transfer learning** to speed up on-line computation
  4. **Material failure**

Multi-stage Multiscale Metal Fabrication Analysis



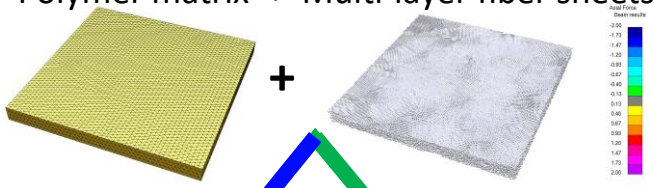
Long-term Developments for Other Composites

- DMN for various composite systems
  1. Randomly-Oriented chopped fiber Composites, Randomly-Oriented long fiber Composites, Woven fiber Composites, Particle-Reinforced Composites, etc.
  2. **Geometrical descriptors** linking process-structure
  3. **Transfer learning**
  4. **Material Failure**

Multiscale Long-fiber Composite Analysis

Manufacturing Processing Simulation

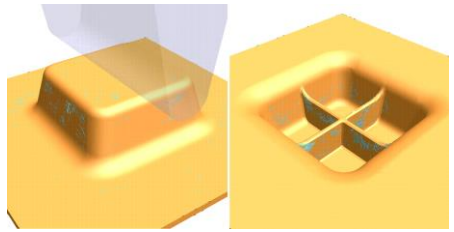
Polymer matrix + Multi-layer fiber sheets

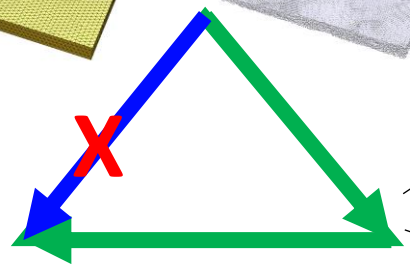


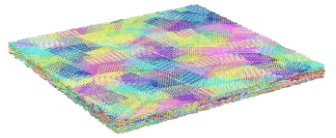
Compression Molding by Adaptive EFG/FEM method

Structural analysis

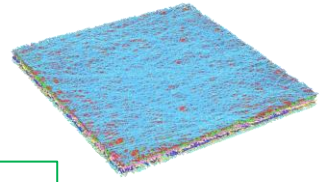
Compression test by a direct numerical simulation using SPG method







Chopped fiber



Long fiber

Micromechanics characterization by DMN

Joint work with JSOL

Material Multiscale Analysis

Summary

1. Two multiscale methods, **Two-scale co-simulation** (2021) and **DMN** (2022), were developed to include the manufacturing information and geometric details in the LS-DYNA Explicit Dynamics solver for the advanced assembly structural analysis, *suggesting a saving of expensive experiments in material characterization and time-consuming simulation for multiscale problems.*

2. A successful multiscale modeling not only relies on the effective multiscale methods, but also the accurate manufacturing simulation results.

3. Various LS-DYNA Multi-physics solvers are available to perform many manufacturing process simulations. (Adaptive FEM/EFG, SPH/ISPH, SPG/ISPG, S-ALE, ICFD, EM, etc.)

Our Developers in attendance
Wei Hu (Two-scale Co-simulation, Adaptive FEM/EFG)
Xiaofei Pan (SPG, ISPG)
Yong Guo (Adaptive FEM/EFG)
Haoyan Wei (DMN for injection molded composites)

Advances of Multiscale Modeling in LS-DYNA:

Part II – Material Multiscale Modeling

Machine Learning Approach to Simulate Injection-Molded Composites

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C. T. Wu
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Outline

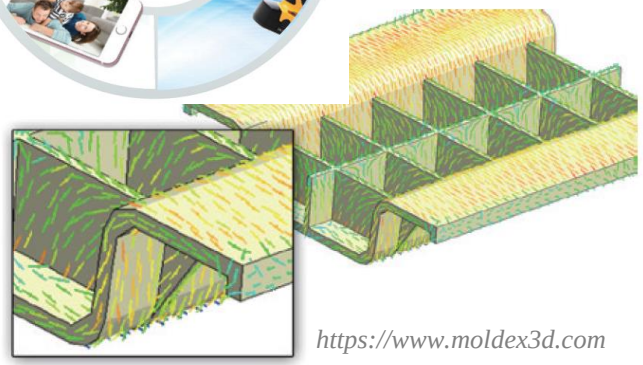
1. **Challenges in Modeling Short-Fiber-Reinforced Composites**
2. **AI-based LS-DYNA Multiscale Simulation of Composite Structures**
   - DMN (Deep Material Network)
   - Application Examples
3. **Summary**

Problem

- **Short-fiber-reinforced composites (SFRC)** are widely used in the automotive and electronics industries. SFRC are manufactured by **injection molding**, which induces **heterogeneous microstructures**.
- Conventional numerical models are either too **expensive** (e.g., *FE^2, direct numerical simulation*) or **inaccurate/difficult to calibrate** (e.g., *phenomenological models*) for nonlinear analysis of SFRC structures
- **Multiscale models** bridge the micro-scale (*where the deformation mechanisms occur*) and the macro-scale (*which is of interest to engineering structural applications*). There is a demand to develop **an effective multiscale model** to capture the **nonlinearity** and **anisotropy** of SFRC composite structures.

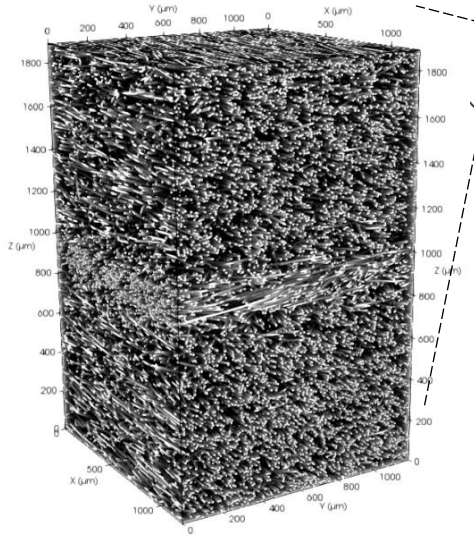
injection-molded short-fiber composites

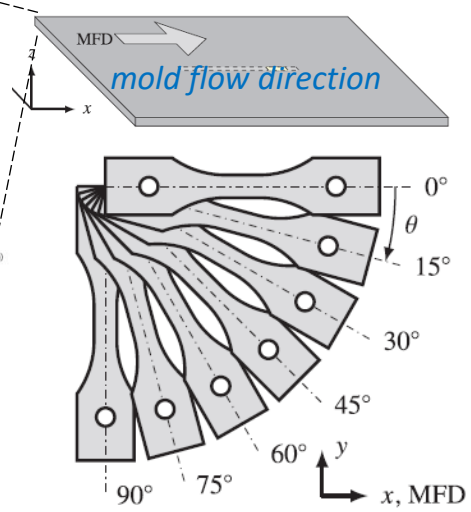
Wang, M-L., Chang, R-Y. , Hsu, C-H. (2018). Hanser.

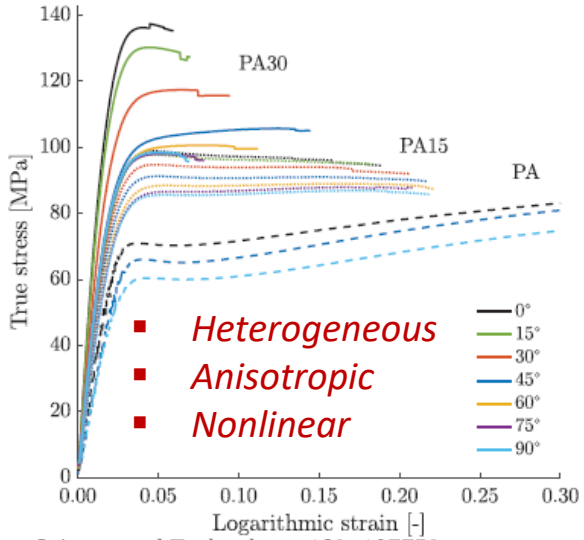


https://www.moldex3d.com

skin-core structures







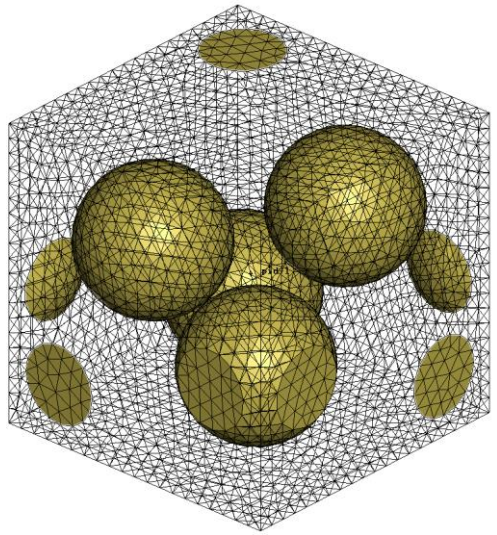
Hessman, P. A., Riedel, T., Welschinger, F., Hornberger, K., Böhlke, T. (2019). Composites Science and Technology, 183, 107752.

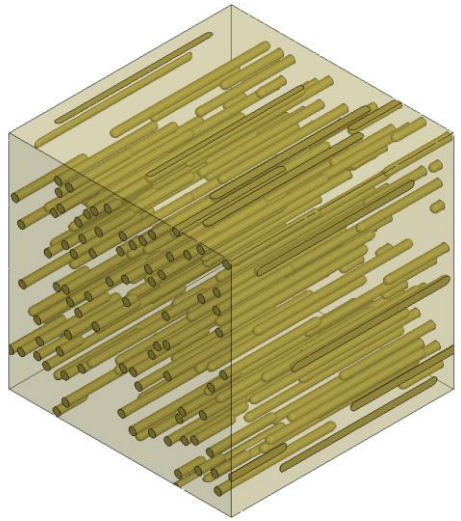
Multiscale material modeling of composites: RVE Analysis

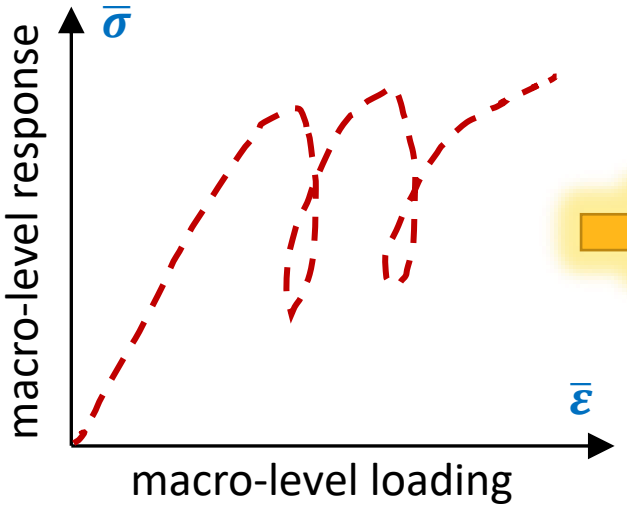
❑ Computational Homogenization

❖ *Keyword ***RVE_ANALYSIS_FEM** in **LS-DYNA***

- ✓ Virtual testing of materials
- ✓ Calibration of constitutive laws
- ✓ Accelerated design & analysis for composite materials





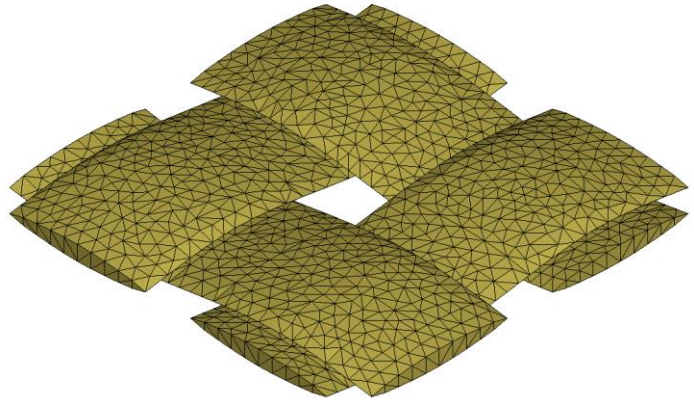


- Linear model

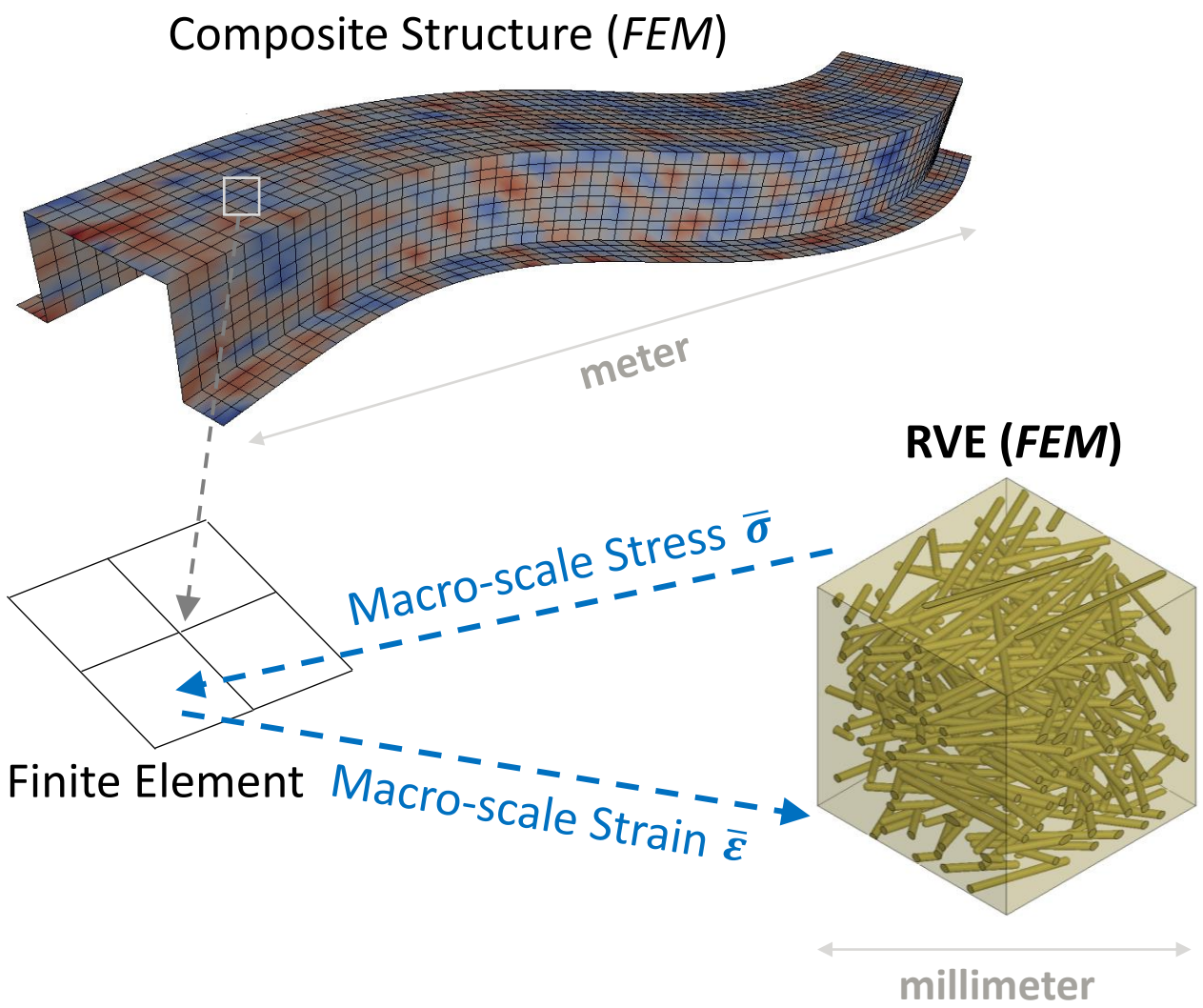
$\bar{\sigma} = \bar{C} : \bar{\varepsilon}$

- Non-linear model

$\bar{\sigma} = f(\bar{\varepsilon}, \beta_1, \beta_2, \beta_3, \cdots)$



Multiscale structural simulation: FEM-based method



❑ Pros

- No macro-constitutive approximation
- High-fidelity multiscale simulation

❑ Cons

- Too expensive for large-scale structures

- **Macroscale S-rail Model:**

2340 shell elements, 4 integration points per element

- **Microscale RVE Model:**

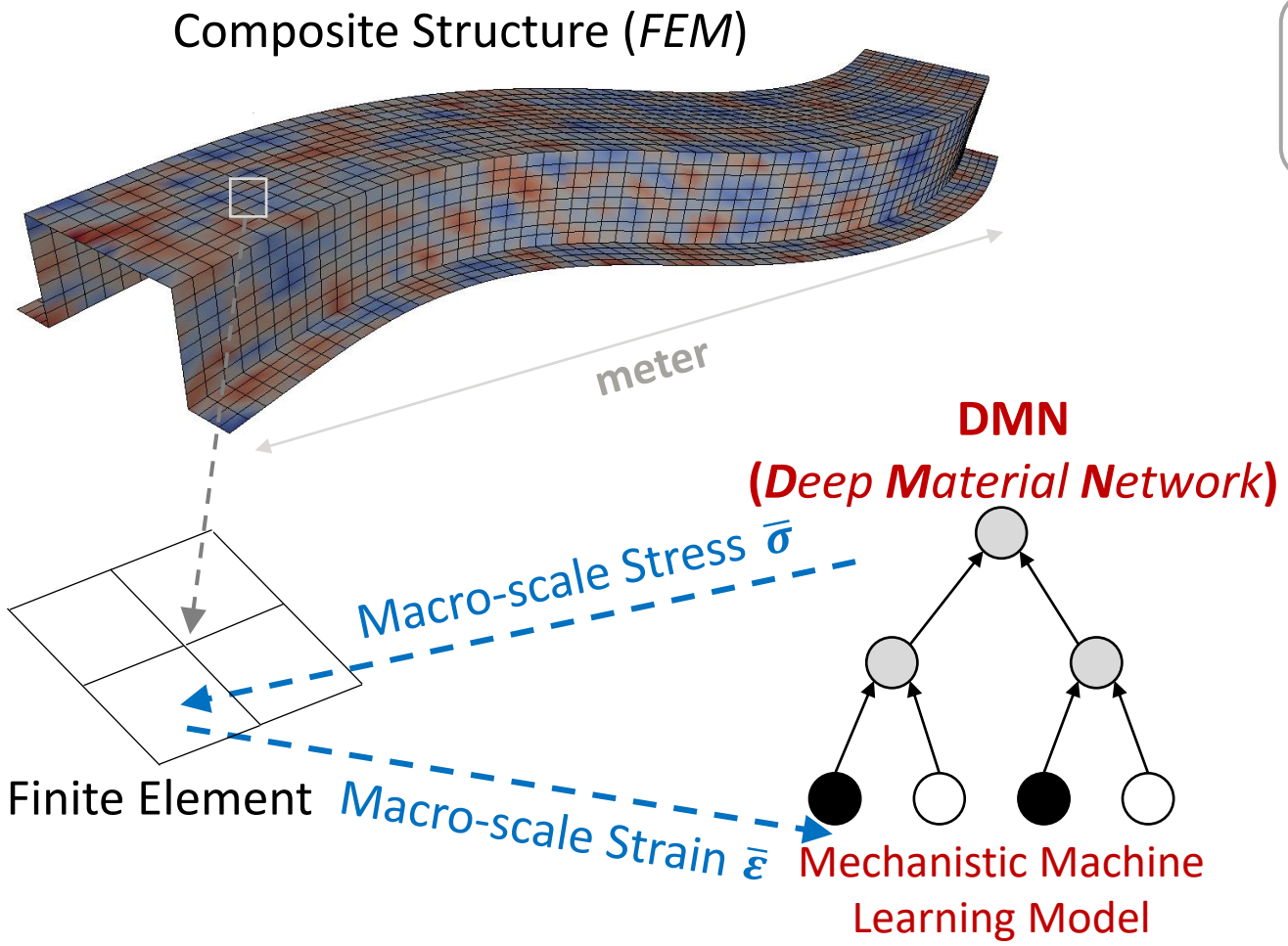
~360K solid elements

- **Total number of Degrees of Freedom (DOF):**

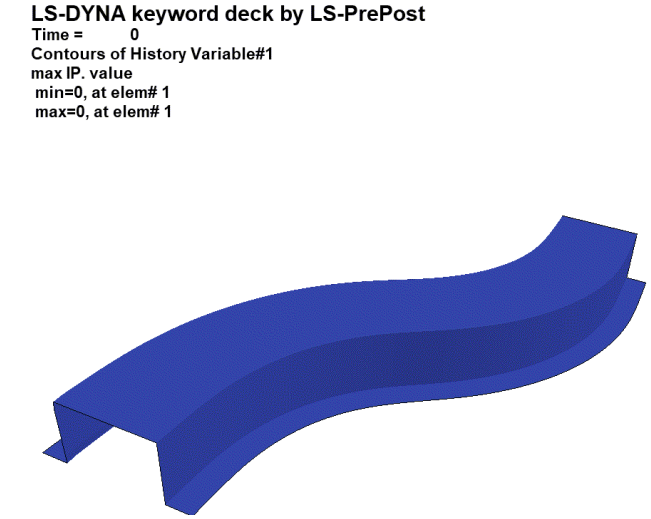
$N_{DOF} = 2340 \times 4 \times 360{,}000 = 3.4\text{B}$

➢ **1 job may take 36 days on 16 CPUs**

Multiscale structural simulation: DMN-based method



- No macro-constitutive approximation
- Accelerated multiscale simulation



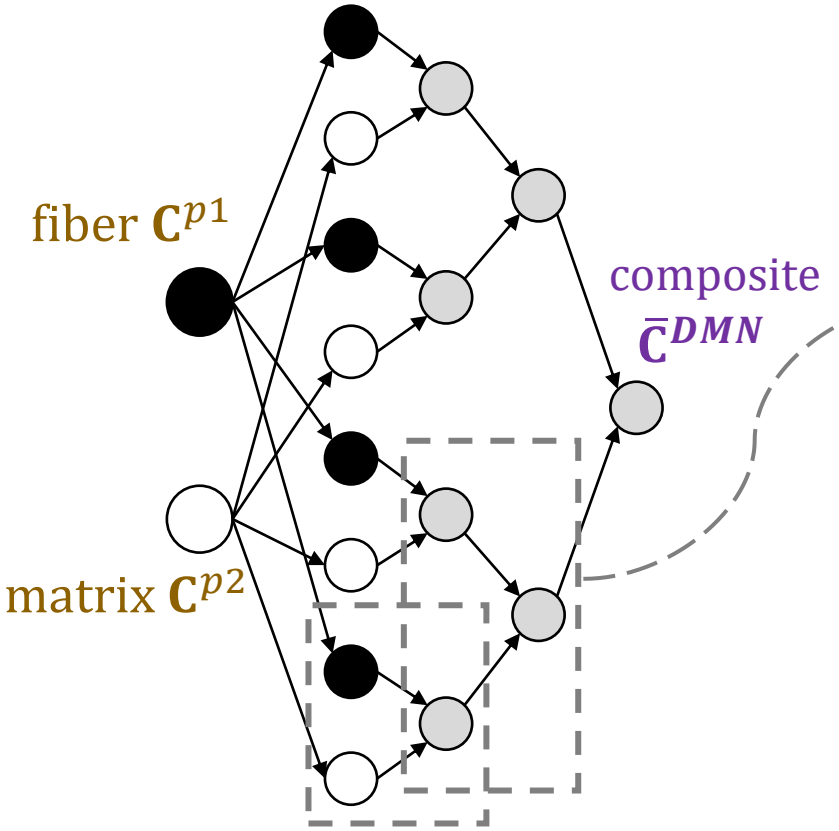
Loading cycles	$N_{CPU} = 1$	$\boldsymbol{N_{CPU} = 16}$
17372	224.0 min	**18.1 min**

Reference: Liu, Z., Wu. C.T. (2019). Exploring the 3D architectures of deep material network in data-driven multiscale mechanics. Journal of the Mechanics and Physics of Solids, 127, 20-46.

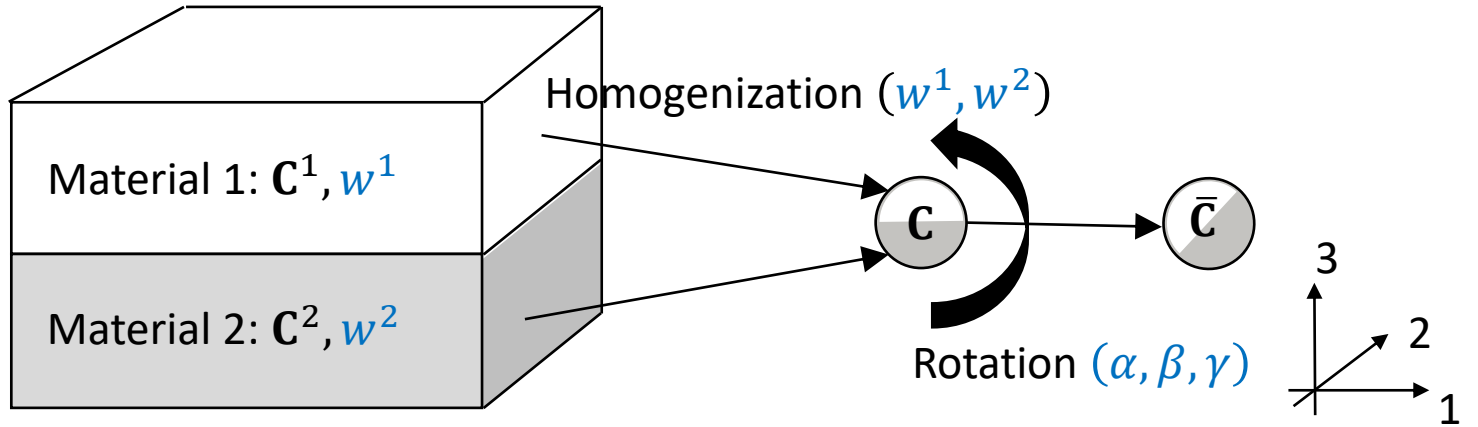
DMN (Deep Material Network)

$$\bar{\mathbf{C}}^{DMN} = \mathbf{f}\left(\mathbf{C}^{p1}, \mathbf{C}^{p2}; \boldsymbol{z}, \boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\gamma}\right)$$

Homogenized Stiffness | Microscale Stiffness | Fitting Parameters



Physics-embedded Building Block



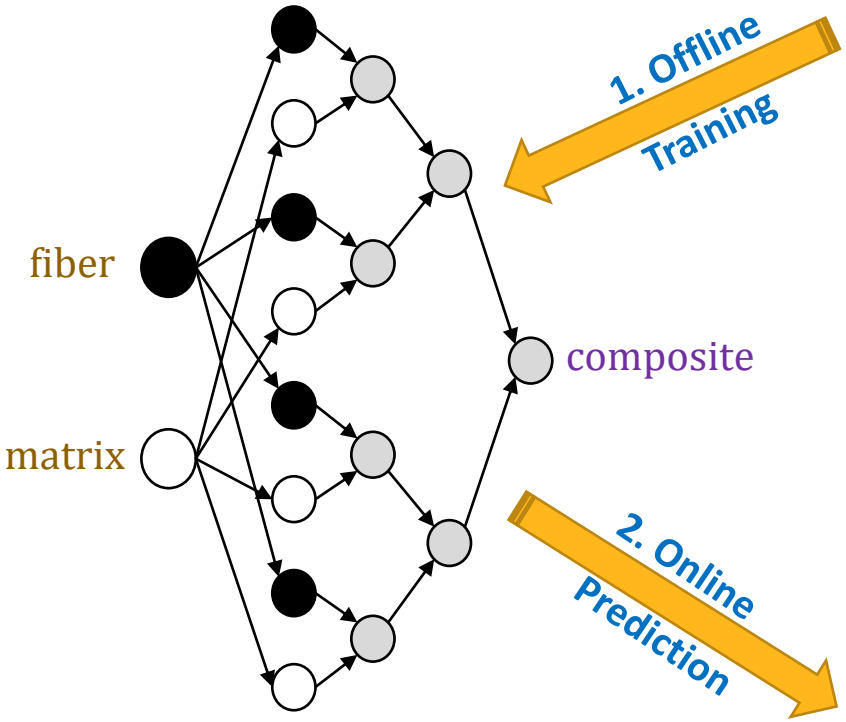
- Interfacial equilibrium conditions: $\sigma_{13}^{(1)} = \sigma_{13}^{(2)}, \quad \sigma_{23}^{(1)} = \sigma_{23}^{(2)}, \quad \sigma_{33}^{(1)} = \sigma_{33}^{(2)}$
- Interfacial kinematic constraints: $\varepsilon_{11}^{(1)} = \varepsilon_{11}^{(2)}, \quad \varepsilon_{22}^{(1)} = \varepsilon_{22}^{(2)}, \quad \varepsilon_{12}^{(1)} = \varepsilon_{12}^{(2)}$
- Weights (w^1, w^2) determined by the activations z in the bottom layer

Z. Liu, C.T. Wu, M. Koishi. CMAME 345 (2019): 1138-1168 ;

Z. Liu, C.T. Wu. JMPS 127 (2019): 20-46.

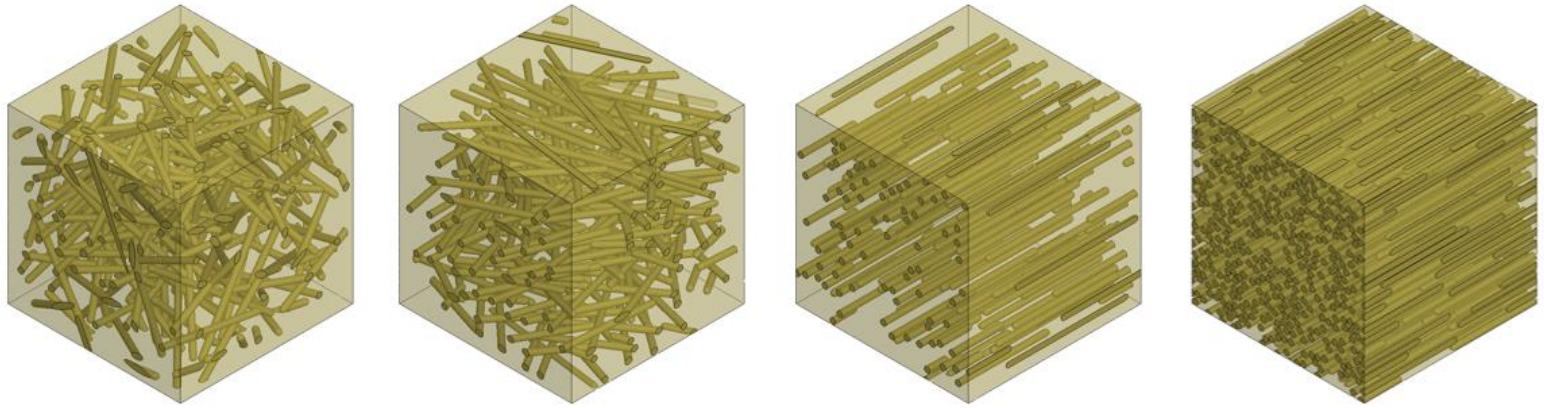
LS-DYNA Machine Learning-based Multiscale Analysis of Composites

DMN (Deep Material Network)



- ✓ **Multiscale** – *predict composite responses based on heterogeneous microstructures*
- ✓ **Nonlinear** – *capture effects of fiber orientations, volume fractions, aspect ratios on nonlinear material responses*

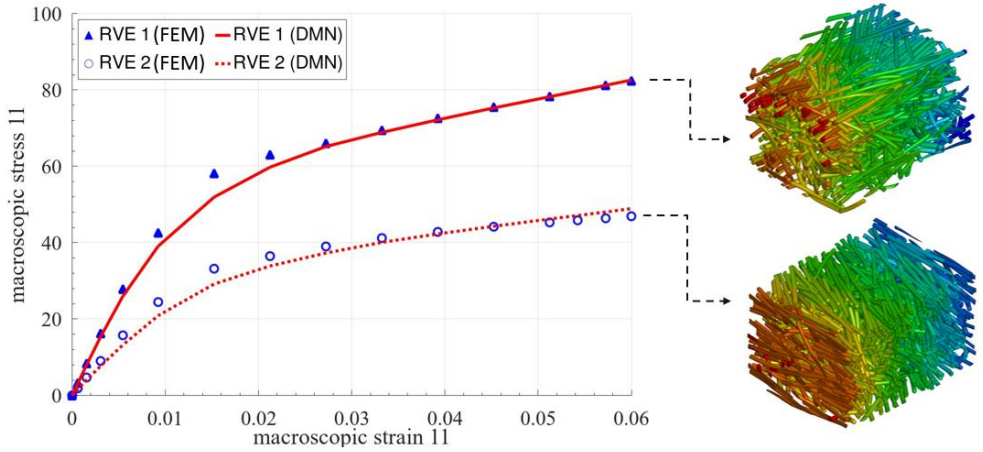
Transfer Learning



DMN vs FEM

Computational time

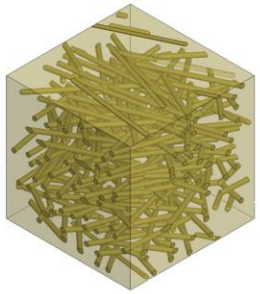
FEM	30-40 hours on 8 CPUs
DMN	1 second on 1 CPU



Reference: Wei H., Wu CT, Hu W., Su M., et al. (2022). Journal of Engineering Mechanics.

DMN-based manufacturing-informed multiscale simulation for SFRC

DMN (Deep Material Network) Offline Training

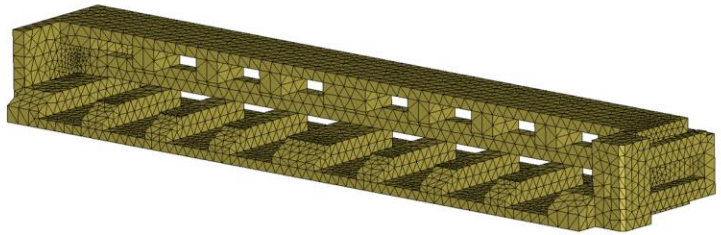


LS-PrePost
microstructural distribution mapping

2. Keyword Creation

Structural Mesh

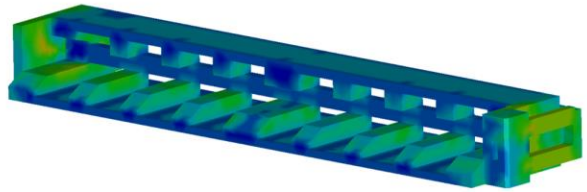
● fiber (elasticity) ○ matrix (plasticity)



3. Multiscale Structural Simulation

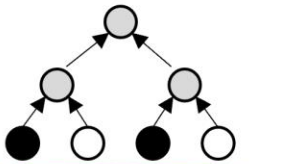
Molding Mesh

- fiber orientation
- volume fraction



1. Manufacturing Process Simulation

Moldex3D
injection molding simulation



DMN Database

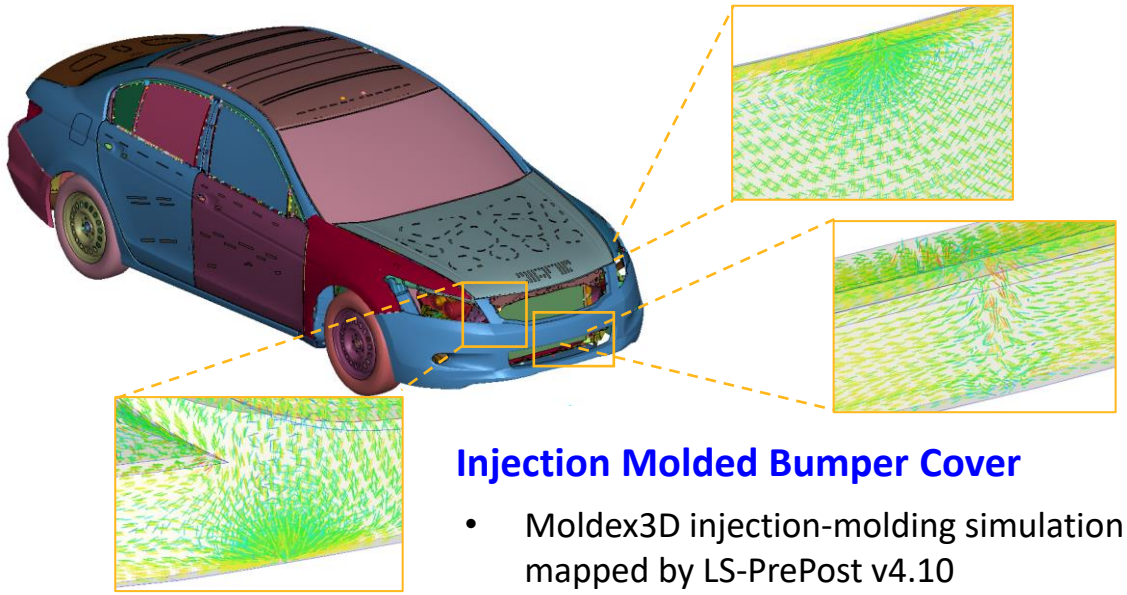
LS-DYNA
multiscale nonlinear structural simulation

DMN Online Prediction Module

Ref: Wei H, Wu CT, Lyu D, Hu W, Rouet FH, Zhang K, Ho P, Oura H, Nishi M, Naito T, Shen L. (2021). LS-DYNA European Conference (paper available).

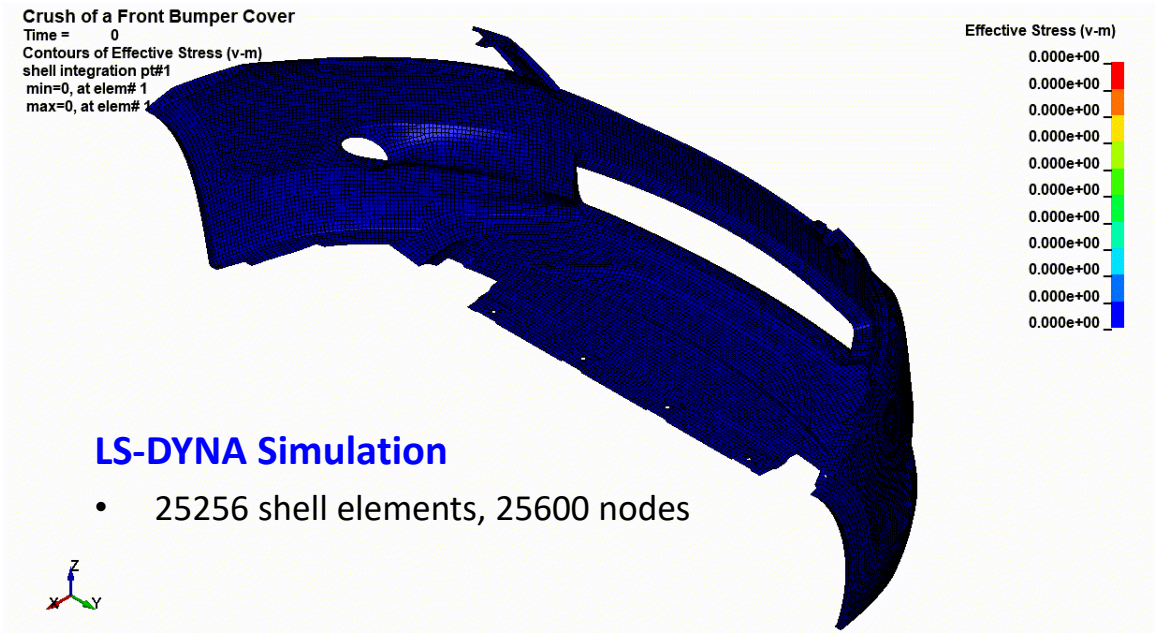
DMN-based manufacturing-informed multiscale simulation for SFRC

❖ *Keyword ***MAT_DMN_COMPOSITE_FRC** in **LS-DYNA R14***



Injection Molded Bumper Cover

- Moldex3D injection-molding simulation mapped by LS-PrePost v4.10



LS-DYNA Simulation

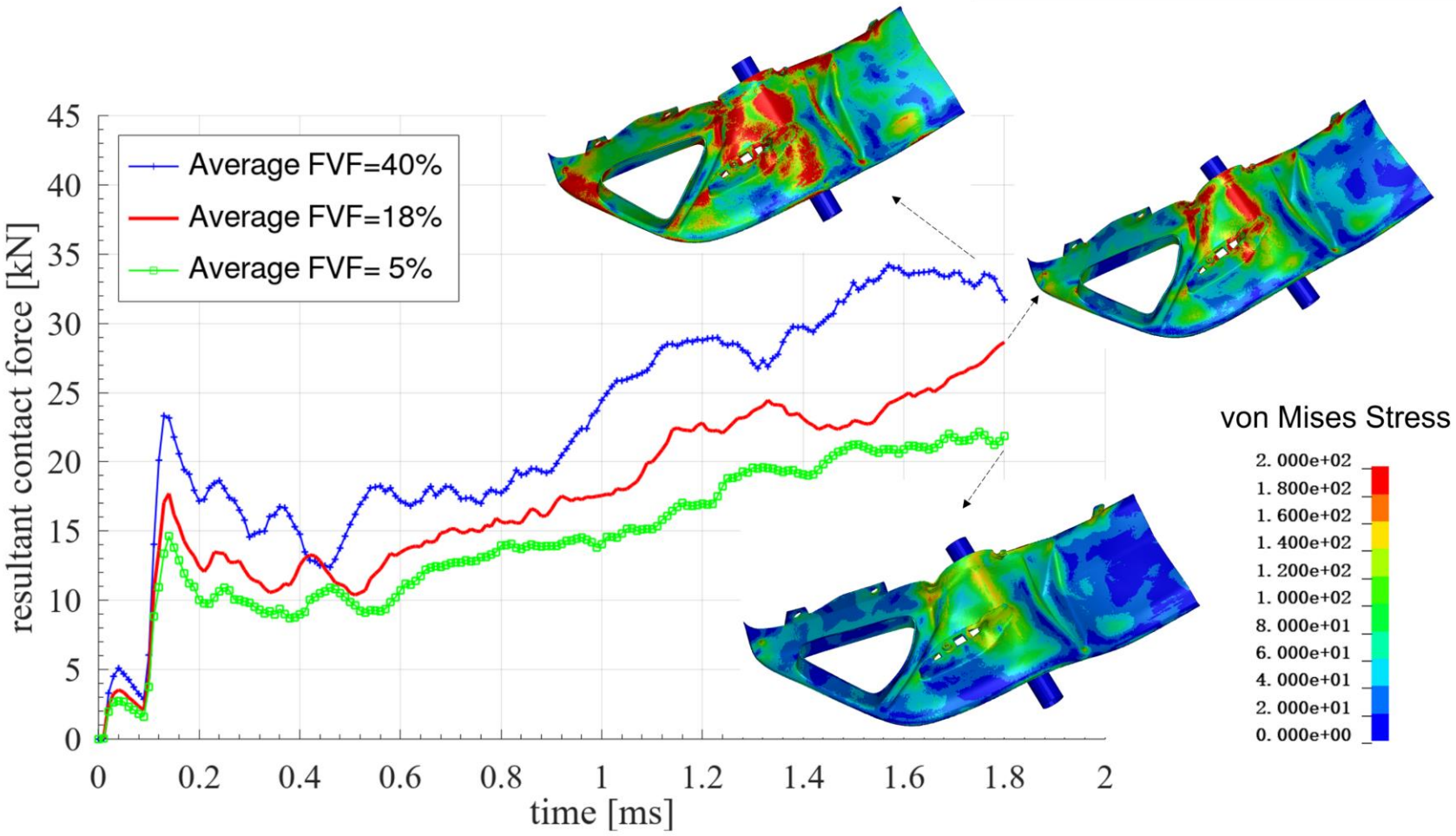
- 25256 shell elements, 25600 nodes

CPU time
8 processors (MPP LS-DYNA)

Impact time	1.92ms
Total CPU time	33 min 25 sec

✓ $10^3 \sim 10^5$ times faster than conventional FEM-based concurrent multiscale methods

DMN-based manufacturing-informed multiscale simulation for SFRC



- ✓ Predict ***anisotropic*** composite behaviors based on *isotropic* properties of fiber & matrix
- ✓ Capture the ***nonlinear*** structural response incorporating *material microstructural effects*

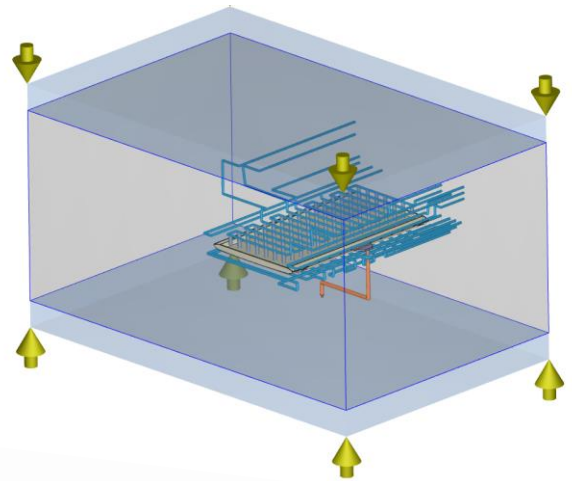
Reference: Wei H., Wu CT, Hu W., Su M., et al. (2022). Journal of Engineering Mechanics.

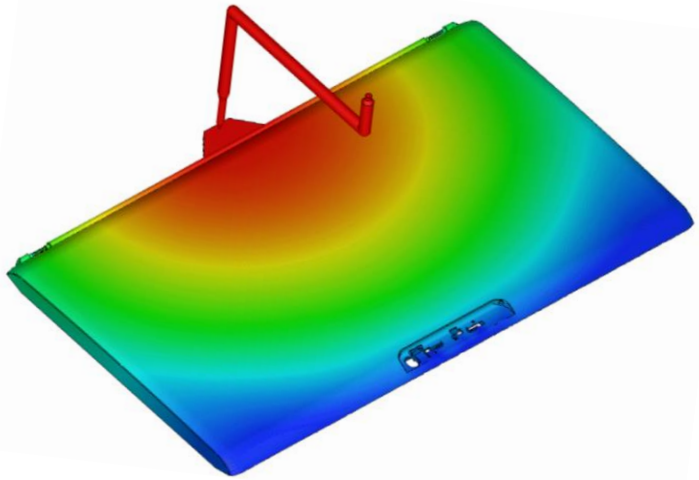
DMN-based manufacturing-informed multiscale simulation for SFRC

EXAMPLE:

Notebook/Laptop Cover

- ***MOLDING DESIGN***
  - *gate location*
  - *temperature*
  - *pressure*
  - *fiber concentration*
- ***MATERIAL SELECTION***
  - *thermoplastics (PC, PA6. …)*
  - *fibers (glass/carbon fiber)*
- ***STRUCTURAL OPTIMIZATION***
  - *shape*
  - *thickness*
  - *hole position*





Moldex3D

Injection Molding Simulation

LS-PrePost

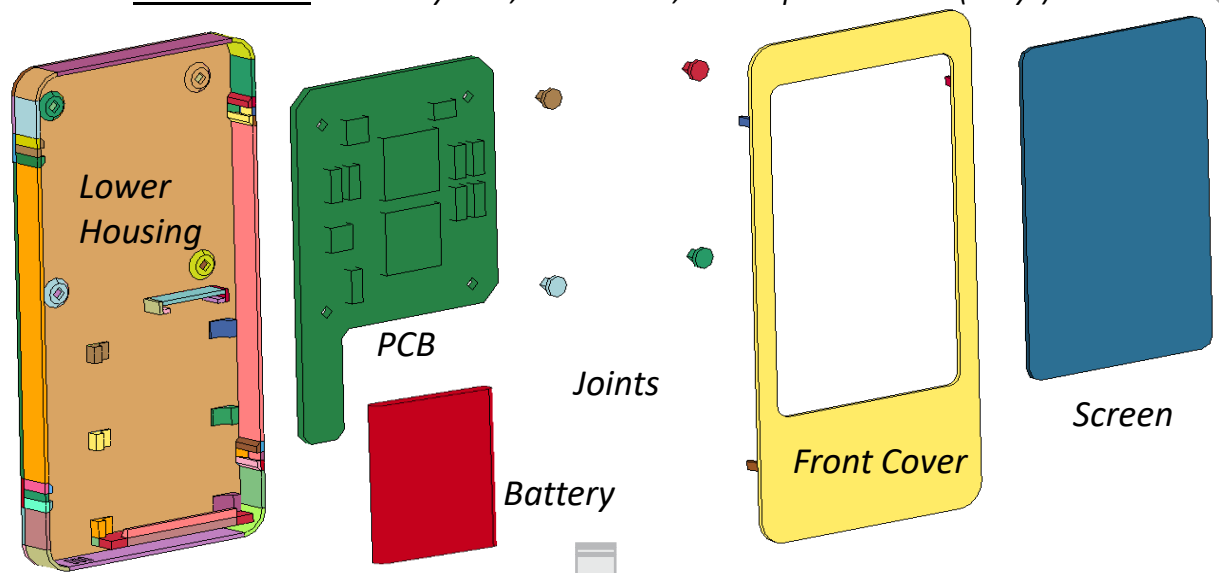
LS-Dyna

Multiscale Drop Test Simulation

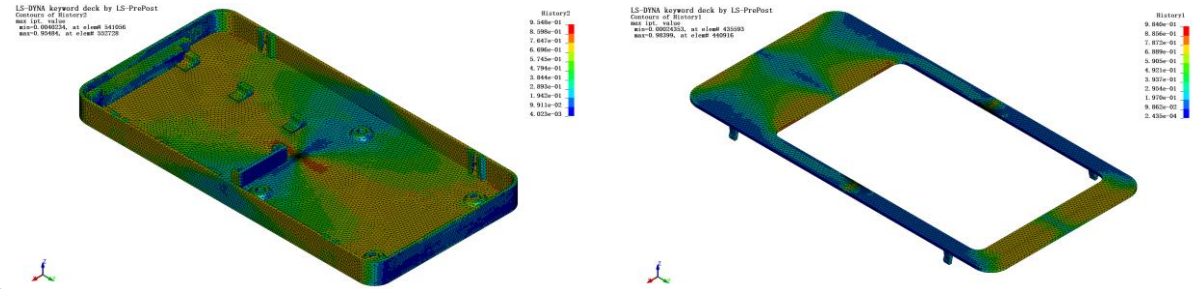
DMN-based manufacturing-informed multiscale simulation for SFRC

EXAMPLE: *Cellphone*

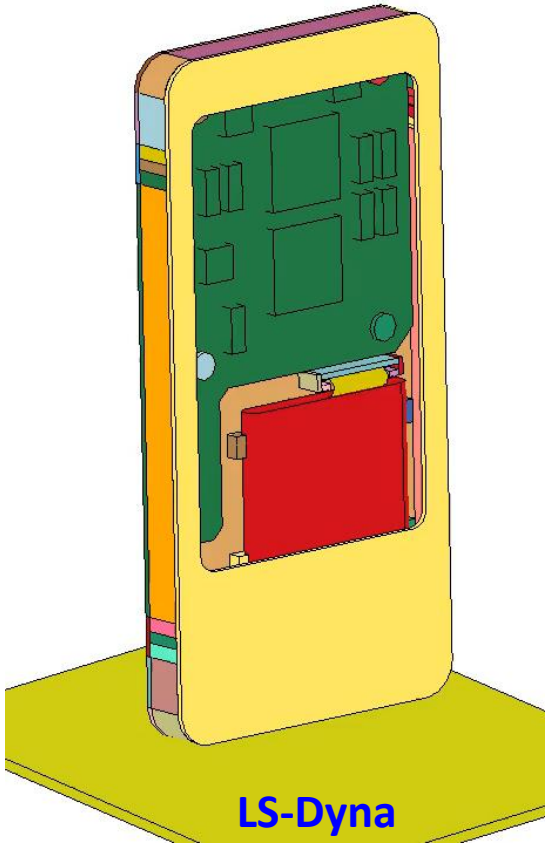
Collaborator: *Daniel Vilyatser, Fabio Pavia, Sandeep Medikonda (Ansys)*



Moldex3D Injection Molding Simulation



LS-PrePost

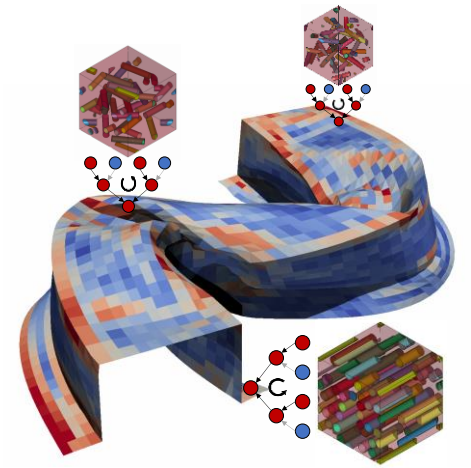


Multiscale Drop Test Simulation

- ✓ Capture effects of injection molding
- ✓ Identify critical regions for better design

Summary

DMN-based Intelligent Multiscale Simulation for SFRC Structures



Liu, Z., Wei, H., Huang, T. Wu, C. T. Intelligent multiscale simulation based on process-guided composite database. 16th International LS-DYNA Users Conference.(2020).

Wei, H., Wu, C.T., Lyu, D., Hu, W., Rouet, F.H., Zhang, K., Ho, P., Oura, H., Nishi, M., Naito, T. and Shen, L. Multiscale simulation of short-fiber-reinforced composites: from computational homogenization to mechanistic machine learning in LS-DYNA. 13th European LS-DYNA Conference. (2021).

- **Multiscale Modeling of Composites**
  - Multi-scale models bridge the micro-scale (*where the deformation mechanisms occur*) and the macro-scale (*which is of interest to engineering structural applications*).
- **RVE (Representative Volume Element) Analysis** – *LS-DYNA R13 or newer*
  - High-fidelity virtual testing of materials with complex microstructures
- **DMN (Deep Material Network)-based Multiscale Simulation** – *LS-DYNA R14*
  - Mechanistic machine learning model for nonlinear concurrent multiscale simulation of composite structures
  - Order-of-magnitude faster than traditional FEM-based concurrent multiscale methods
  - Manufacturing-informed nonlinear multiscale simulation workflow for injection-molded short-fiber composite structures will be released in 2022


Ansys
Thank you!