

# Flow and Transient Phenomena in Large Scale Additive Manufacturing.

**Presenter:** Eduardo Barocio,

Composites Additive Manufacturing Group  
Composites Manufacturing and Simulation Center, Purdue University

**FLOW PROCESSES IN COMPOSITE MATERIALS - 15**

# Agenda

- ◆ Large scale additive manufacturing
- ◆ Physics-based simulation workflow ADDITIVE3D for composites additive manufacturing
- ◆ Overview of physics considered
- ◆ Examples of simulation driven design with ADDITIVE3D
- ◆ Horizons and opportunities in composites additive manufacturing

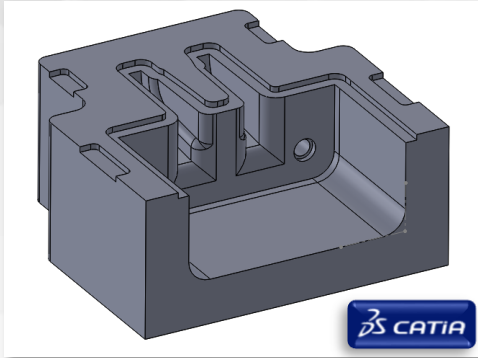
# Large Scale Additive Manufacturing (LSAM)



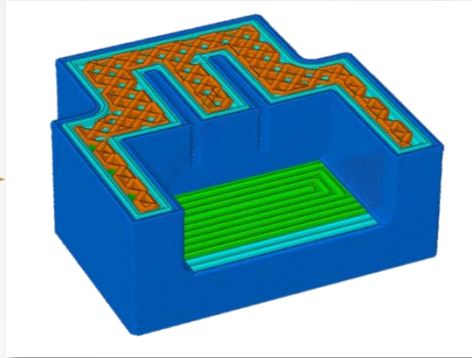
**THERMWOOD**  
**LSAM** RESEARCH  
LABORATORY

# Workflow for Additive Manufacturing

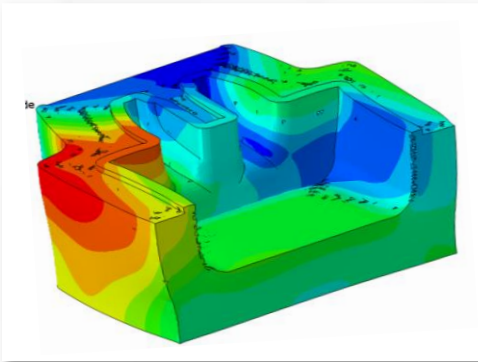
CAD Geometry



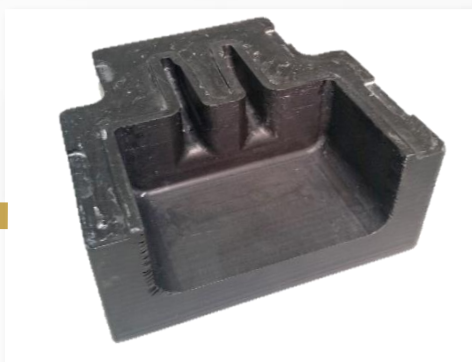
Slicing



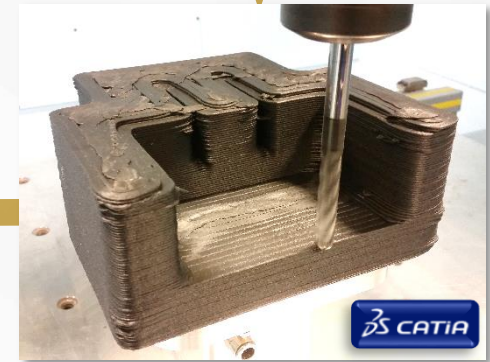
Printing



Performance

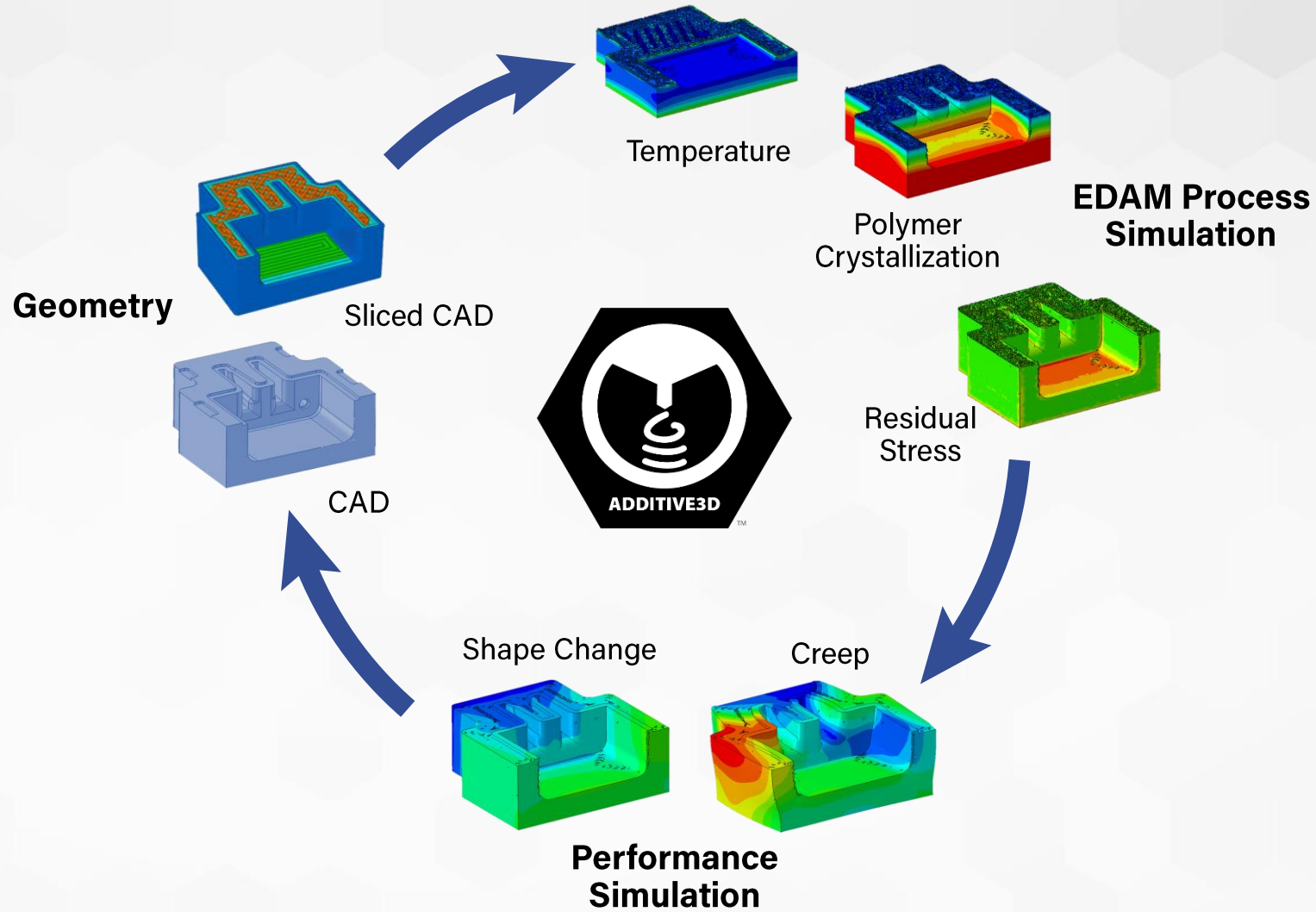


Final Part



Finishing

# ADDITIVE3D: Simulation Workflow for AM

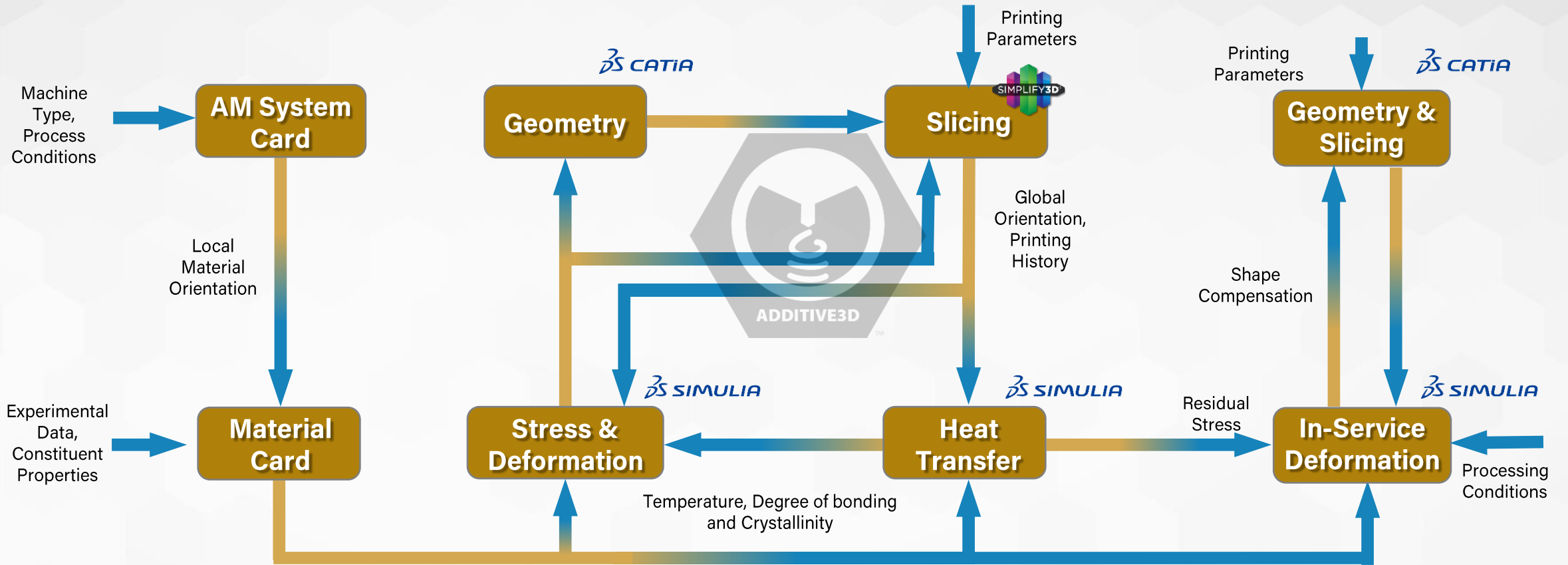


# ADDITIVE3D™ Process and Performance Simulation

## Material & Machine Characteristics

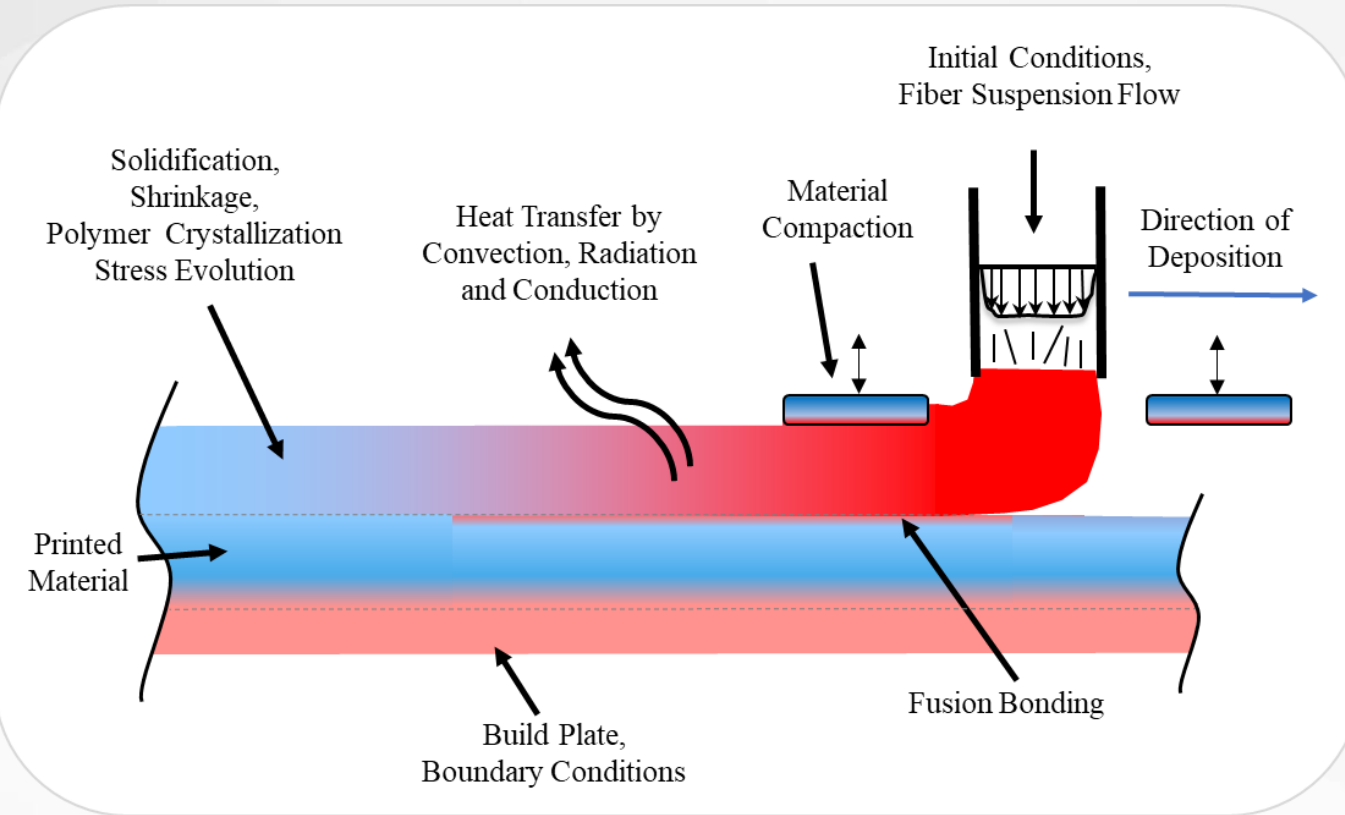
## Process Simulation

## Performance Simulation

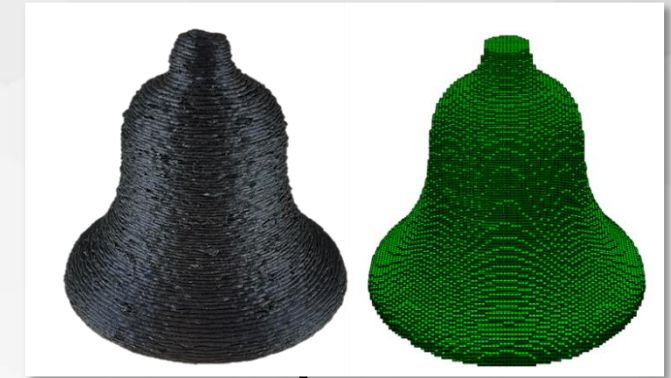


# Physics Captured in AM Process Simulation

## Multiscale and Multiphysics Process Simulations



Inactive,  
Part-Unspecific  
Mesh



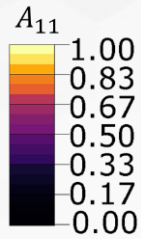
Element  
Activation  
Based  
on Machine  
Code



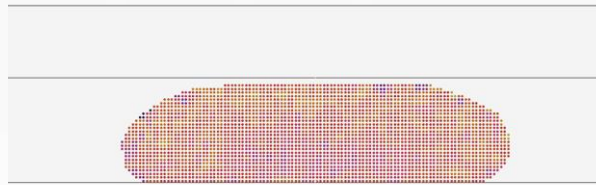
Barocio E, Brenken B, Favaloro A, Bogdanor M, Pipes RB. Extrusion Deposition Additive Manufacturing with Fiber-Reinforced Thermoplastic Polymers. In: Friedrich K, Walter R, editors. Struct. Prop. Addit. Manuf. Polym. Components. 1st ed., Woodhead Publishing; 2020, p. 450.

# Anisotropic Flow of Fibers Polymer Suspension

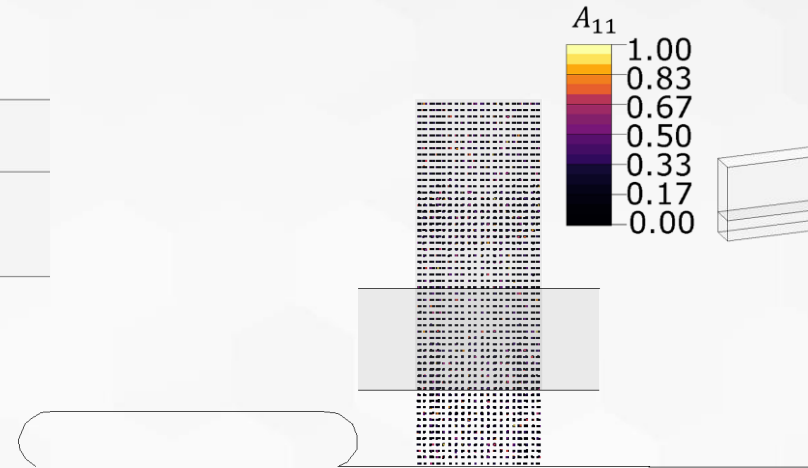
Single Bead  
Deposition



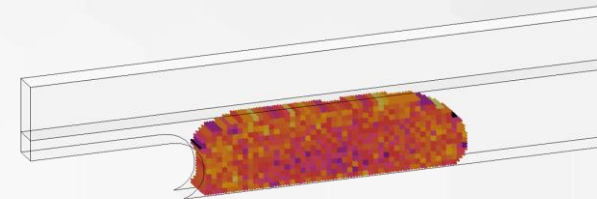
Single Bead  
Compaction



Second Bead  
Deposition



Second Bead  
Compaction



Pibulchinda P, Barocio E, Favaloro AJ, Pipes RB. Influence of printing conditions on the extrudate shape and fiber orientation in extrusion deposition additive manufacturing. Compos Part B Eng 2023;261:110793. <https://doi.org/10.1016/j.compositesb.2023.110793>.

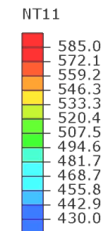
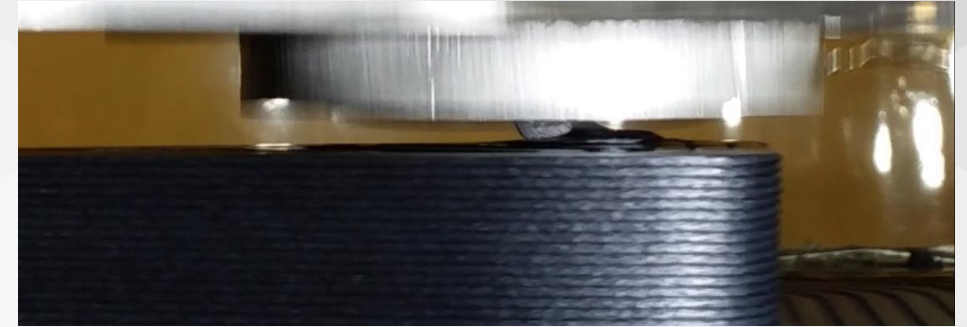
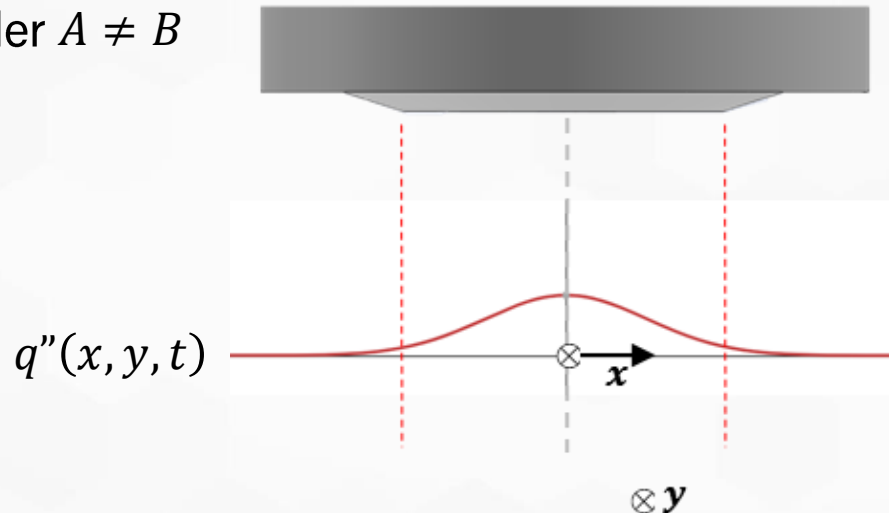


# Heat Losses in Material Compaction

- ◆ Actively cooled compacter
- ◆ Modeled as a moving heat flux with double gaussian distribution

$$q''(x, y, t) = \frac{Q^c \sqrt{AB}}{\pi} e^{-A(x+v_x t)^2} e^{-B(y+v_y t)^2}$$

- ◆ Tamper  $A = B$
- ◆ Roller  $A \neq B$

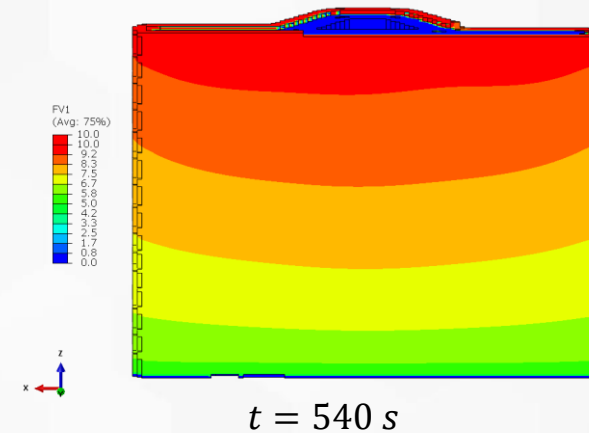
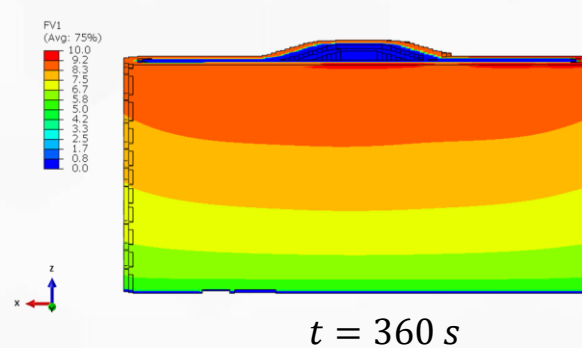
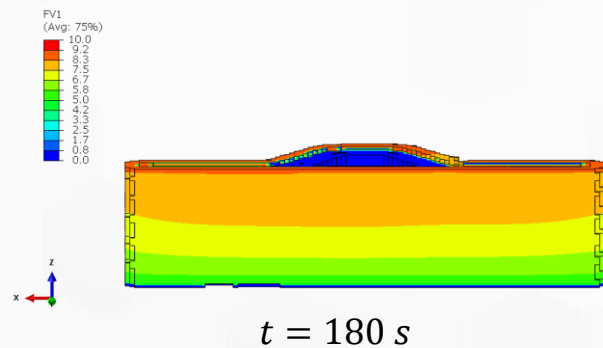
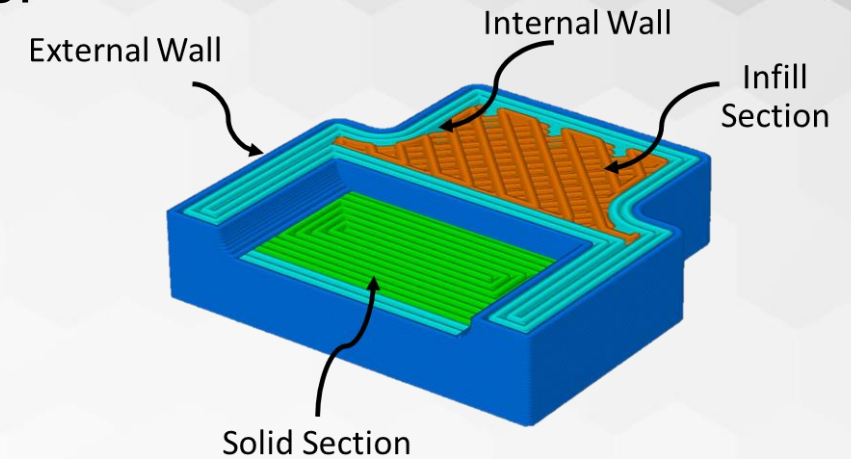


\* Convection and radiation disabled

# Local Convection Conditions

Feature dependent convection coefficients assumes:

- ◆ Convection occurs instantaneously
- ◆ Features are non-interactive
- ◆ Analogies made:
  - ◆ Solid section → Horizontal surface
  - ◆ External wall → Vertical surface
  - ◆ Internal wall and Infill section → Neglect or same as external wall



Convection coefficient at internal and external features

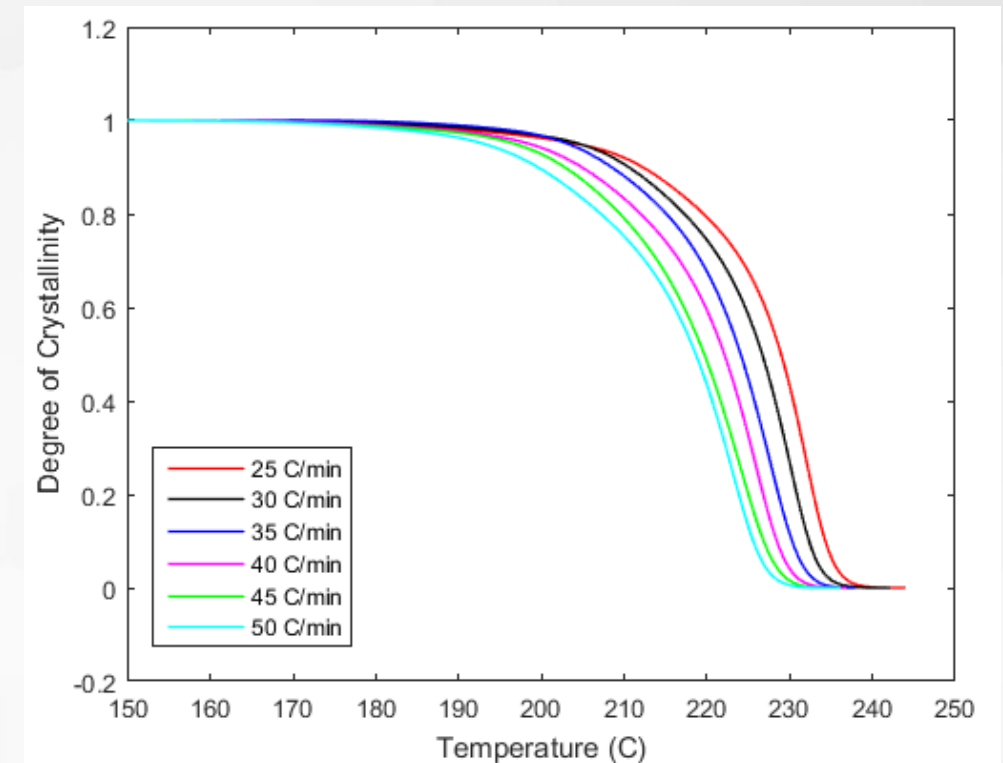
# Polymer Crystallization Kinetics

- ◊ Polymer crystallization is cooling rate dependent
- ◊ Dual crystallization mechanisms observed in CF-PPS → Crystallization model developed by Velisaris and Seferis

$$X_{vc}(T, t) = X_{vc\infty}(w_1 F_{vc1} + w_2 F_{vc2})$$

$$F_{vc_i} = 1 - \exp\left[-C_{1i} \int_0^t T \cdot \exp\left[\frac{-C_{2i}}{(T-T_g+T_{ci})} - \frac{C_{3i}}{(T(T_{m_i}-T)^2)}\right] n_i \tau^{n_i-1} d\tau\right] \quad i = 1,2$$

$X_{vc}$  - crystallinity volume fraction,  $w_1$  and  $w_2$  are weight factors  
 $C_{1i}$  - pre-exponential factors capturing the temperature dependence  
 $C_{2i}$  - parameters associated with the temperature dependence of diffusion  
 $C_{3i}$  - parameters associated with the free enthalpy of nucleation  
 $n_i$  - Avrami coefficients for each crystallization mechanism



Barocio E, Brenken B, Favaloro A, Bogdanor M, Pipes RB. Extrusion Deposition Additive Manufacturing with Fiber-Reinforced Thermoplastic Polymers. In: Friedrich K, Walter R, editors. Struct. Prop. Addit. Manuf. Polym. Components. 1st ed., Woodhead Publishing; 2020, p. 450.

# Polymer Melting

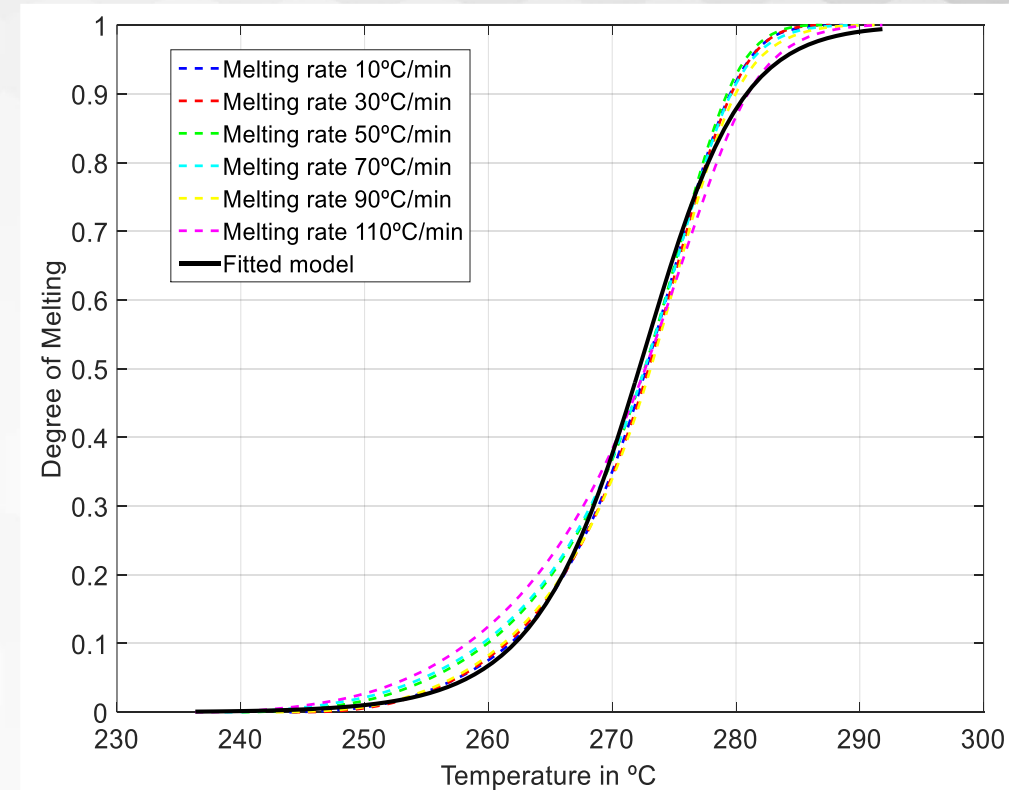
- Melting model assumes statistical distribution of lamellar thicknesses (Greco & Maffezzoli) -> Only temperature dependent

$$T_m = T_m^\circ - \frac{2\gamma_e T_m^\circ}{l\Delta H_f}$$

$$\frac{dX_{vc}}{dT} = k_{mb} \left\{ \exp[-k_{mb}(T-T_c)] \right\} \cdot \left( 1 + (d-1)\exp[-k_{mb}(T-T_c)] \right)^{\frac{d}{1-d}}$$

$T_c$  - crystallization temperature  
 $k_{mb}$  - sharpness of the distribution of lamellar thicknesses  
 $d$  - shape factor of the distribution of lamellar thicknesses

$\gamma_e$  - lateral surface energy  
 $T_m^\circ$  - thermodynamic melting temperature  
 $\Delta H_f$  - enthalpy of fusion  
 $l$  - lamellar thickness



Barocio E, Brenken B, Favaloro A, Bogdanor M, Pipes RB. Extrusion Deposition Additive Manufacturing with Fiber-Reinforced Thermoplastic Polymers. In: Friedrich K, Walter R, editors. Struct. Prop. Addit. Manuf. Polym. Components. 1st ed., Woodhead Publishing; 2020, p. 450.

# Thermoviscoelastic Material Behavior

Anisotropic linear constitutive equation:

$$\sigma_i = \int_0^t C_{ij}(T, X, t - \tau) \frac{\partial \varepsilon_j^{eff}}{\partial \tau} d\tau, \quad i, j = 1, 2, \dots, 6$$

$T$ : Temperature,  $X$ : Crystallinity,  $t$ : Time

$\varepsilon_j^{eff} = \varepsilon_j - \varepsilon_j^{inel}$ : Effective strain

Time-Temperature-Superposition (TTS):

$$\xi_{ij}(t) = \int_0^t \frac{1}{a_T(T(\tau))} d\tau$$

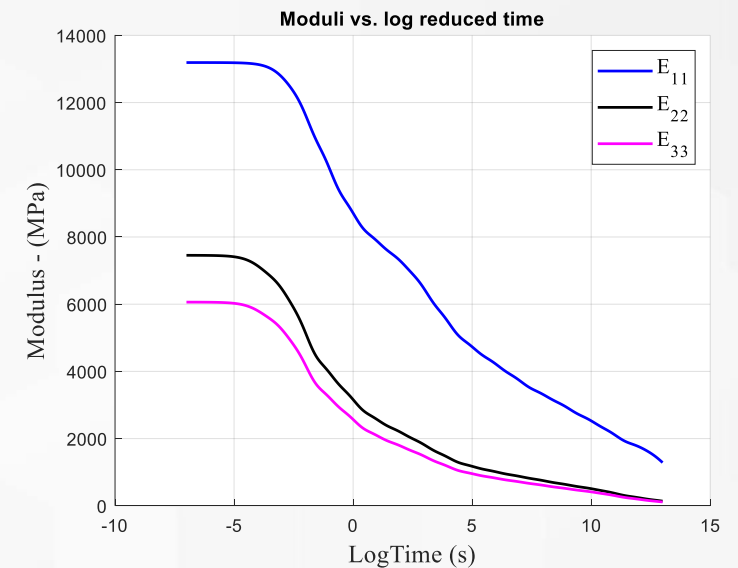
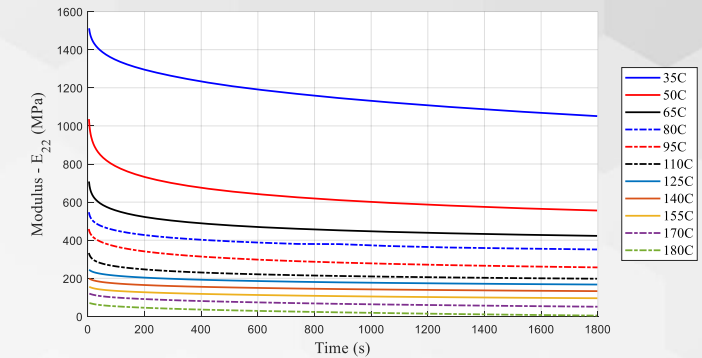
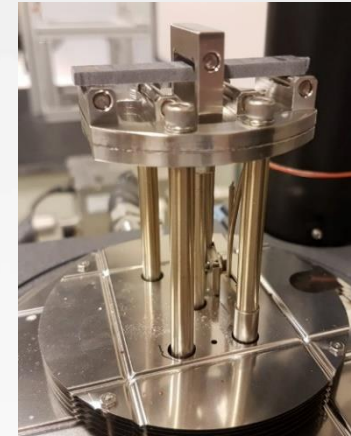
$\xi_{ij}(t)$ : Reduced time,  $a_T(T)$ : Shift factor (WLF Equation)

$$C_{ij}(T_0, X, \xi_{ij}(t) - \xi'_{ij}(\tau)) = f(X) \cdot \left[ C_{ij0} + \sum_{w=1}^N C_{ijw} \exp\left(-\frac{\xi_{ij}(t) - \xi'_{ij}(\tau)}{\lambda_{ijw}}\right) \right]$$

$\lambda_{ijw}$ : Relaxation times

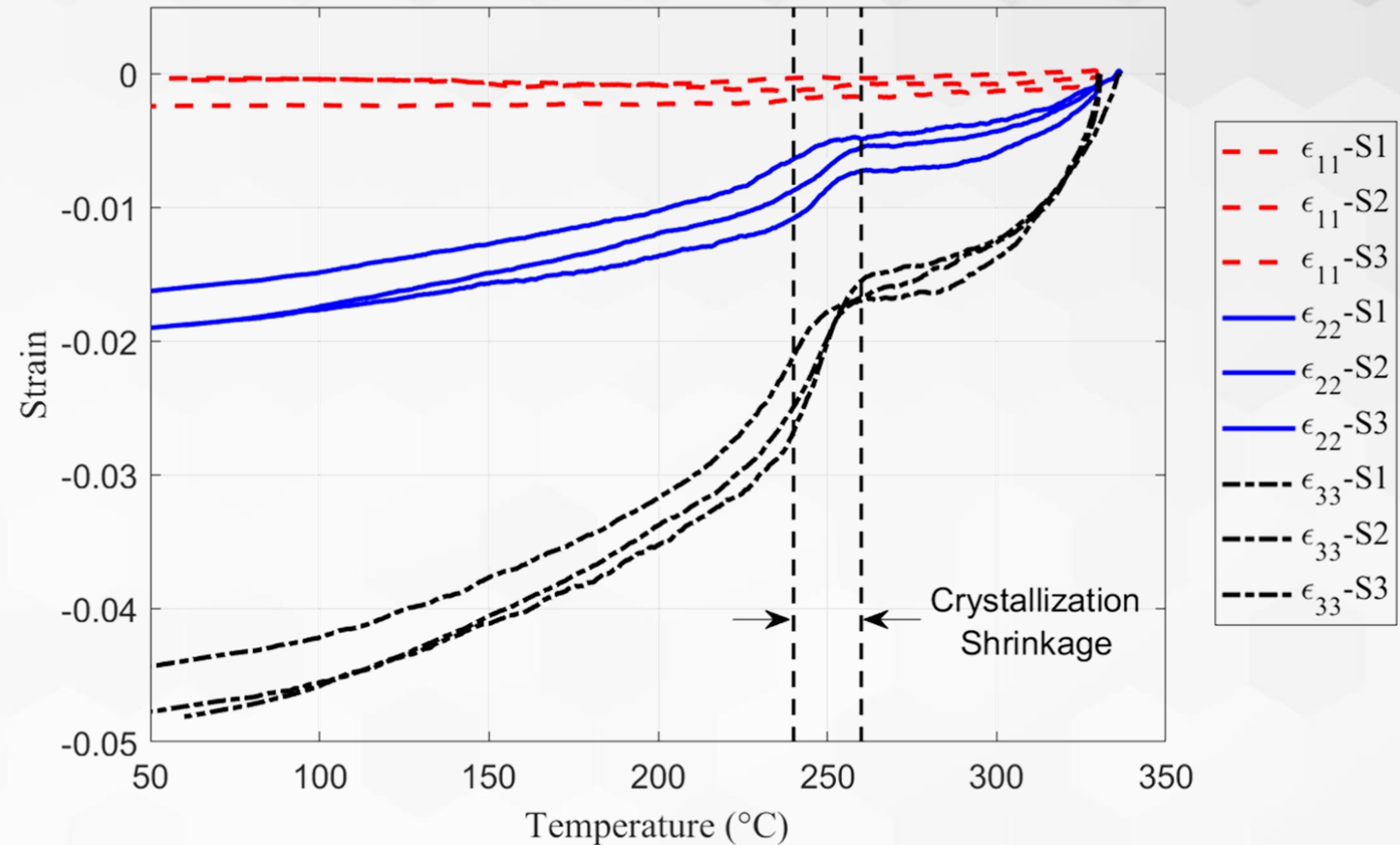
$f(X)$ : Crystallization factor

$C_{ij0}, C_{ijw}$ : Relaxed/Unrelaxed stiffness parts



# Anisotropic Shrinkage

- ◆ Contribution from both thermoelastic and crystallization shrinkage
- ◆ Thermoelastic shrinkage: Governed by  $\alpha(T)$
- ◆ Strain developed before crystallization does not contribute significantly to build up stresses



Barocio E, Brenken B, Favaloro A, Bogdanor M, Pipes RB. Extrusion Deposition Additive Manufacturing with Fiber-Reinforced Thermoplastic Polymers. In: Friedrich K, Walter R, editors. Struct. Prop. Addit. Manuf. Polym. Components. 1st ed., Woodhead Publishing; 2020, p. 450.

# Interlayer and Fusion Bonding

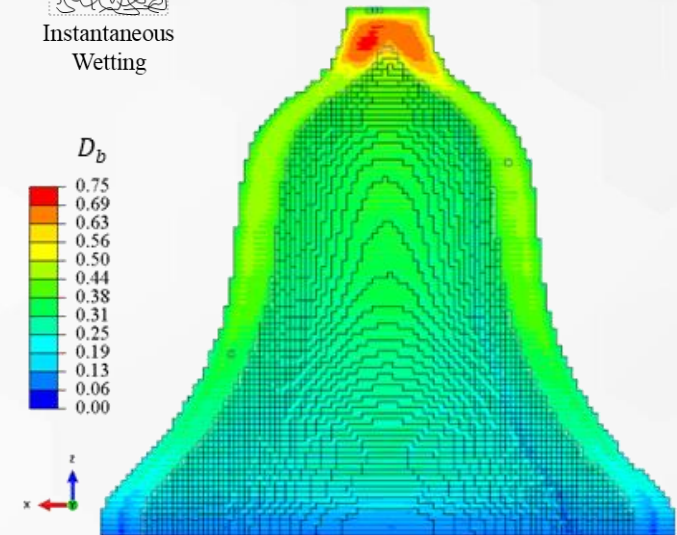
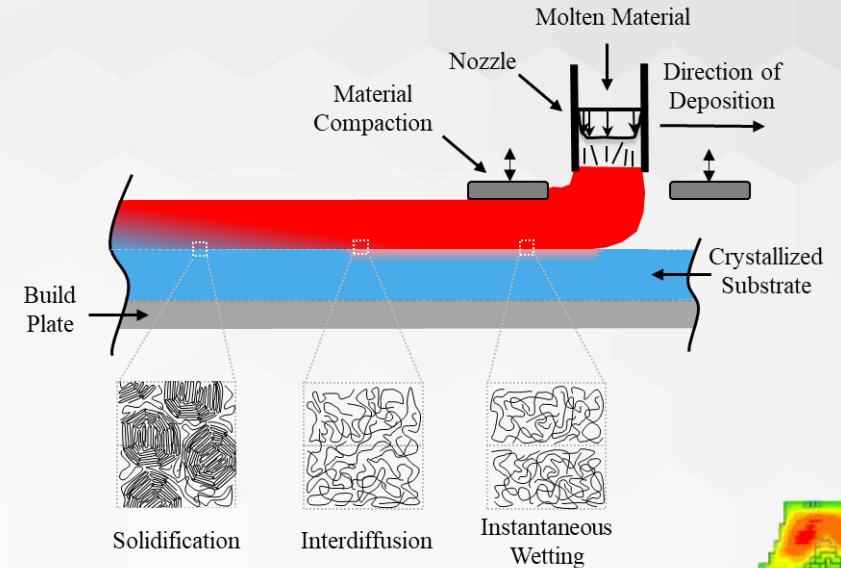
- ◆ Non-isothermal fusion bonding model provides prediction of fracture properties
- ◆ Integrates effect of polymer crystallization on precluding reptation of polymer chains
- ◆ Model extended to inter-bead fusion bonding

$$D_b(t) = \frac{G_{1C}(t)}{G_{1C\infty}} = \left[ \int_0^{t_c} \frac{1}{t_w(T(\tau))} d\tau \right]^{\frac{1}{2}}, t_c \in \{t \text{ s.t. } X_{vc} < X_{vc}^{crit}\}$$

$$t_w(T(\tau)) = A \cdot \exp\left(\frac{E_A}{RT(\tau)}\right)$$

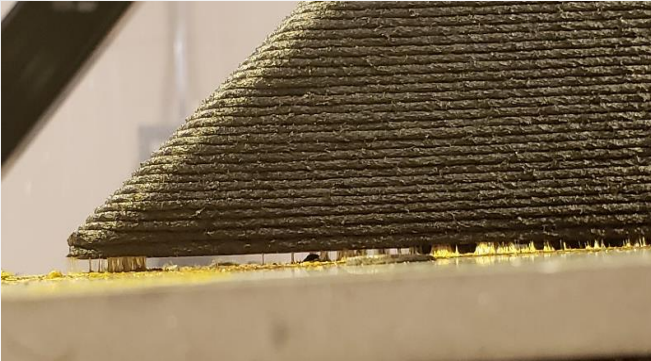
$t_w$  - welding time  
 $E_A$  - activation energy  
 $A$  - pre-exponential factor  
 $G_{1C\infty}$  - critical energy release rate of a perfectly bonded interface

Barocio E, Brenken B, Favaloro A, Pipes RB. Interlayer fusion bonding of semi-crystalline polymer composites in extrusion deposition additive manufacturing. Compos Sci Technol 2022;109334. <https://doi.org/10.1016/j.compscitech.2022.109334>.



# Interaction with Print Substrate

## Adhesive / Beadboard



### Boundary Conditions

#### Thermal

$$q_s'' = 0 \mid T_s = T_{bp} \mid R_\theta$$

#### Mechanical

#### Cohesive Contact

$$t_n(\delta_1, D), t_s(\delta_s, D), t_t(\delta_t, D)$$

## Build Sheets



### Boundary Conditions

#### Thermal

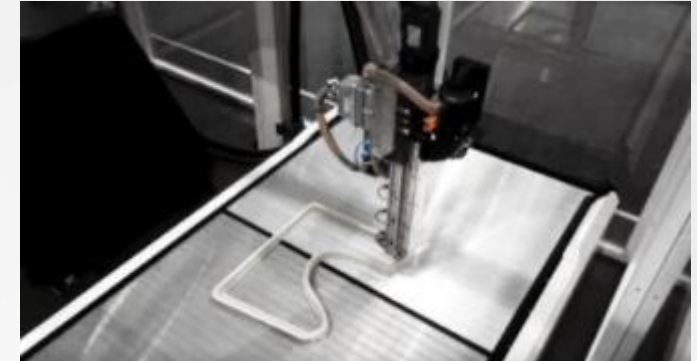
$$T_{bs} = T_{bp} \mid R_\theta$$

#### Mechanical

#### Spring Connectors

$$F_i = F_i^0 + D_{ij} u_j$$

## Rigid Constraint



### Boundary Conditions

#### Thermal

$$T_s = T_{bp} \mid R_\theta$$

#### Mechanical

#### All DOF Constrained

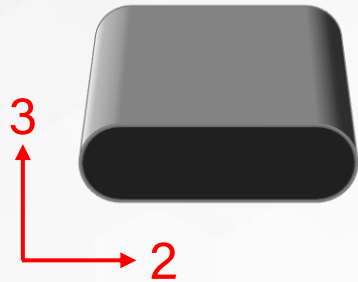
$$u_i = 0$$

Barocio E, Thomas AJ, Pipes RB. Virtual Investigation of Residual Part Deformation Due to Build Plate Support Characteristics in Material Extrusion Additive Manufacturing. CAMX 2020 – Compos. Adv. Mater. Expo, VIRTUAL EXPERIENCE: CAMX 2020; 2020.



# Material Card Characterization

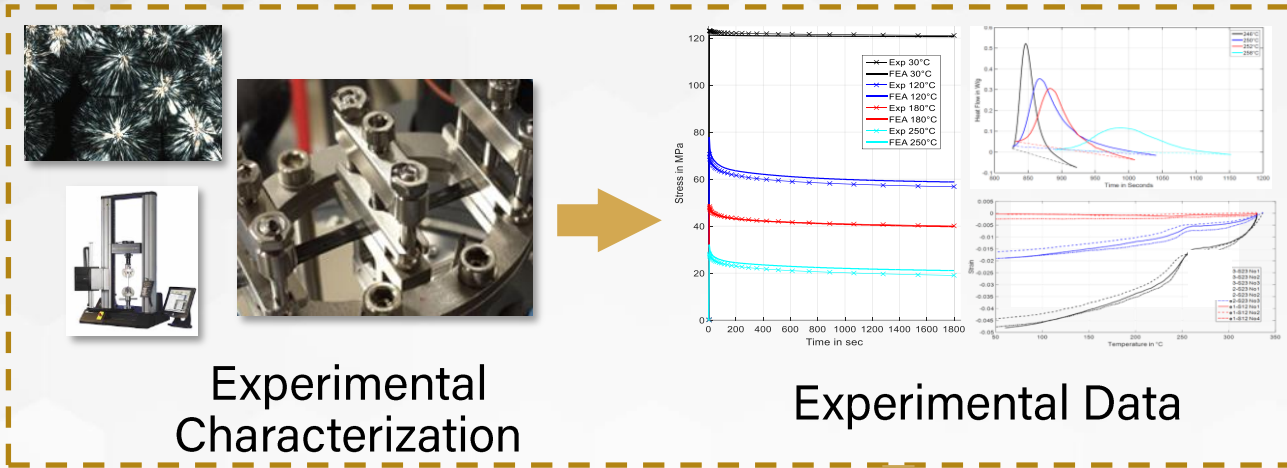
**Bead-Level Effective Properties**



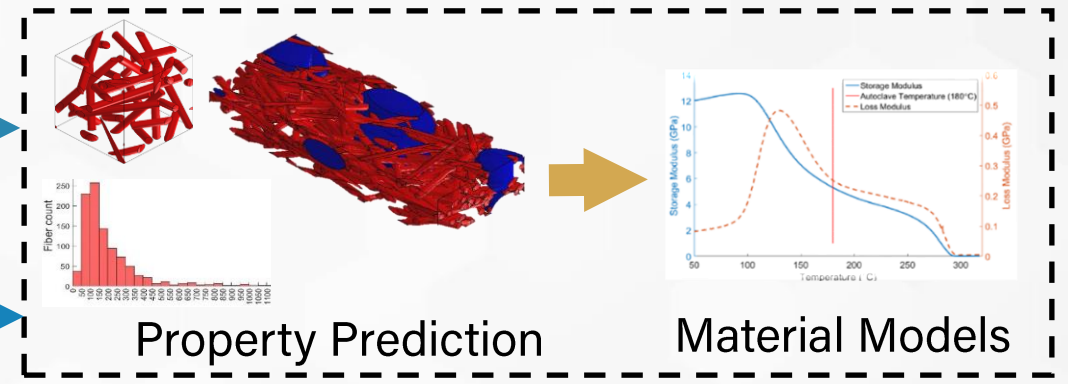
Material Property	Relevant Standard
Glass Transition Temperature	ASTM D7028
Fiber Orientation Distribution	
Fiber Length Distribution	
Elastic Properties (9 components)	ASTM D3039 ASTM D5379
Coefficient of Thermal Expansion (3 directions)	ASTM E831
Crystallization Kinetics and Melting	
Thermoviscoelastic Behavior (9 Prony series)	ASTM D5023
Thermal Conductivity (3 directions)	ASTM E1461
Heat Capacity	ASTM E1269
Fusion Bonding Time	

# Material Card Generation

## User Input



## Material Card Generation



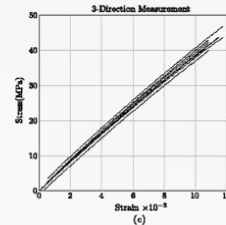
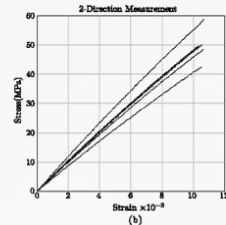
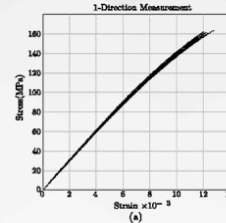
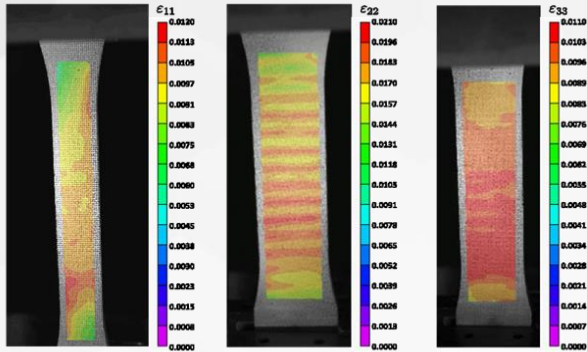
## Digital Material Card

AM System Card

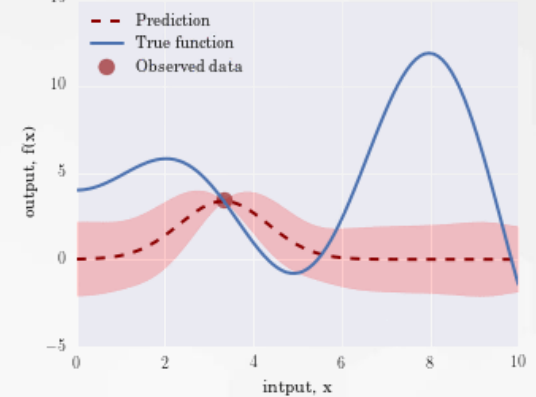


# Accelerating Material Card Generation

## 1. Three Tensile Tests

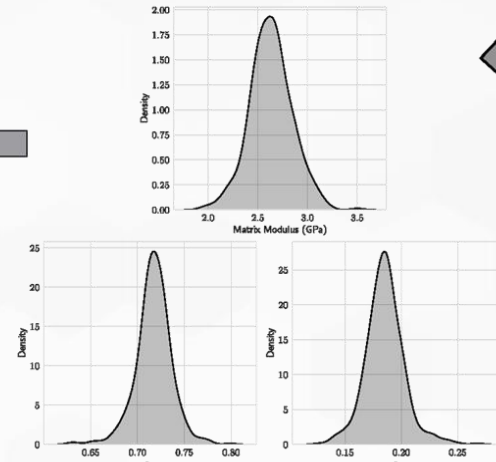


Approximating true function with more data

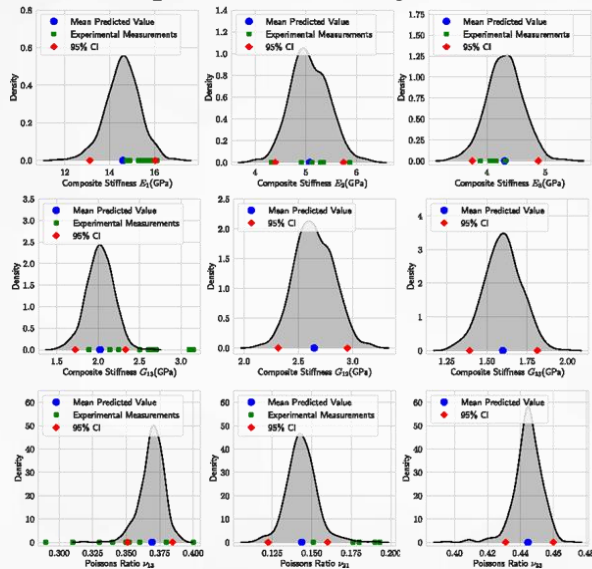


Bayesian Inference

## 2. Uncertainty Quantification



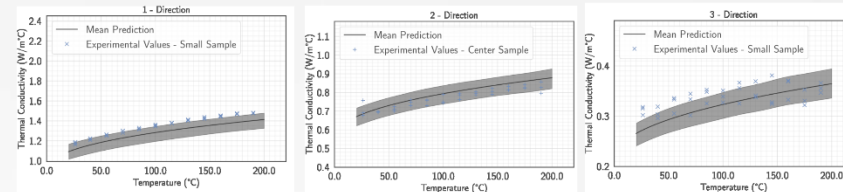
## 3. Populate Elasticity Tensor



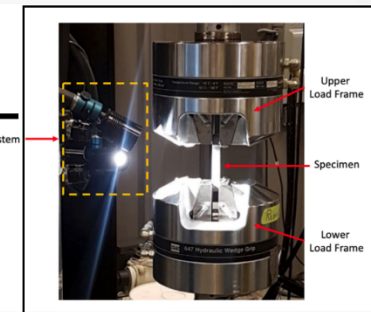
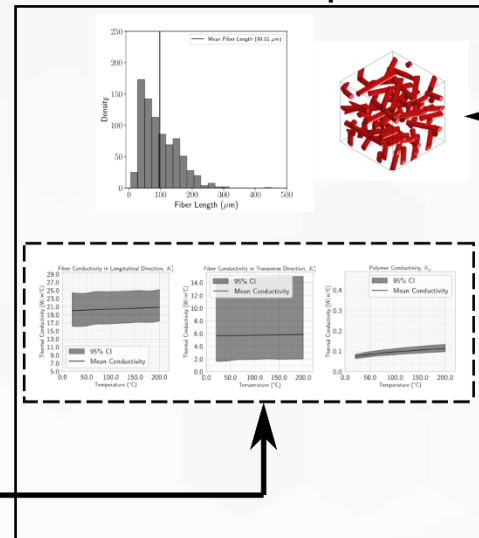
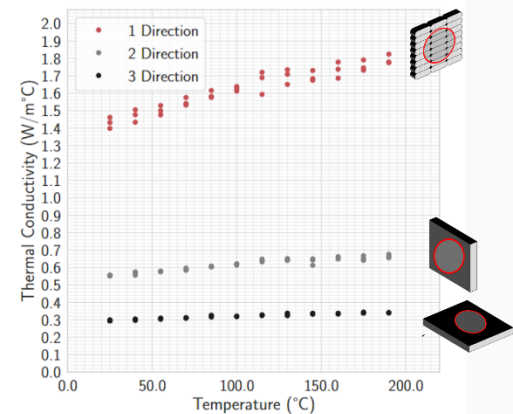
- 1) Thomas AJ, Barocio E, Pipes RB. A machine learning approach to determine the elastic properties of printed fiber-reinforced polymers. *Compos Sci Technol* 2022;109293.
- 2) Thomas AJ, Barocio E, Billionis I, Pipes RB. Bayesian inference of fiber orientation and polymer properties in short fiber-reinforced polymer composites. *Compos Sci Technol* 2022;228:109630. <https://doi.org/10.1016/j.compscitech.2022.109630>.

# Transferring Material Cards Across AM Systems

Predictions in System 2



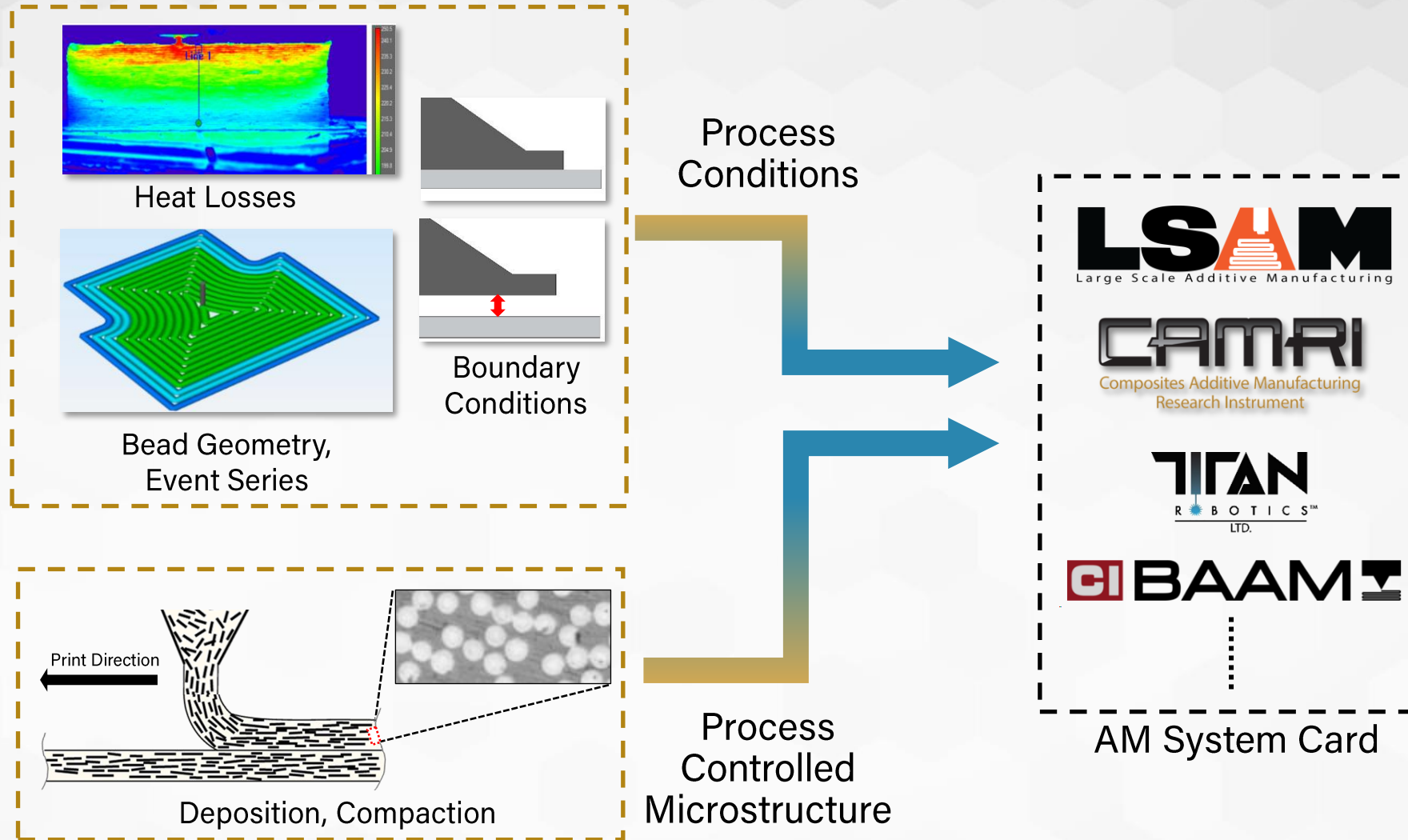
Measurements in System 1



Tensile Tests in System 2

Infer Microstructural Properties

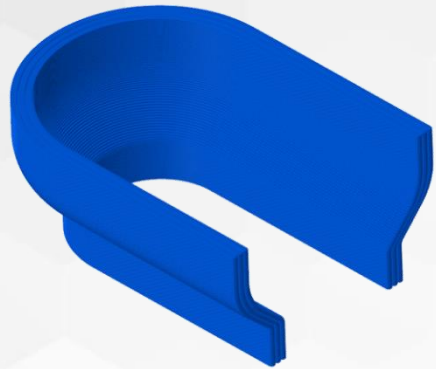
# Machine Card Characterization



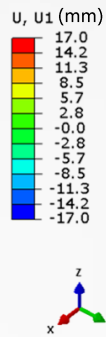
# Simulation Driven Design with ADDITIVE3D

# Simulation-Driven Shape Compensation of Autoclave Tool

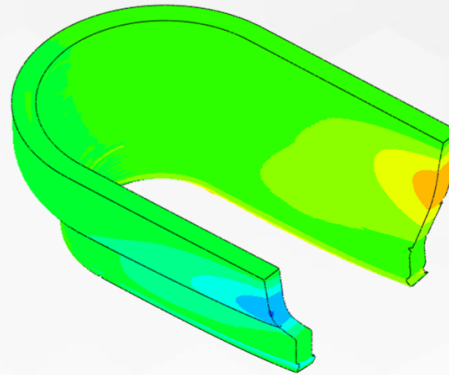
Nominal Geometry



Process Simulation  
ADDITIVE3D™

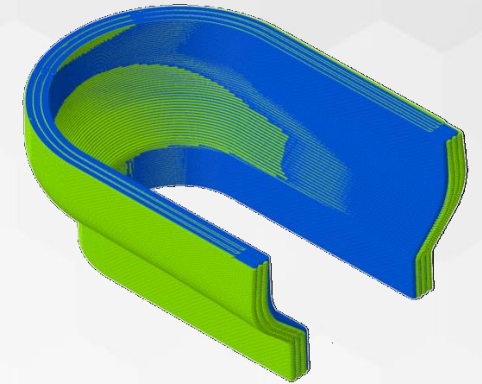


Post-Printing Geometry

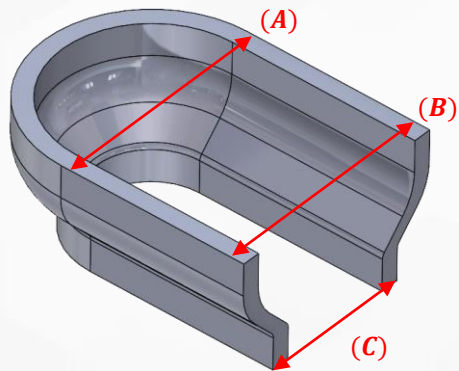


Shape Compensation

Compensated Geometry



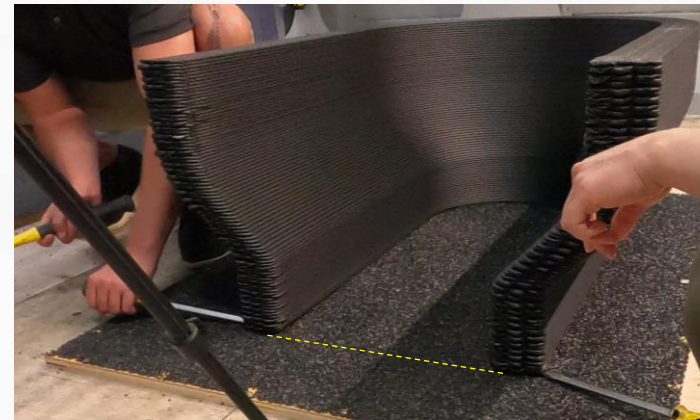
Printed vs Nominal Geometry



Location	Nominal vs Printed Geometry (mm)
A	0.71
B	1.01
C	0.89

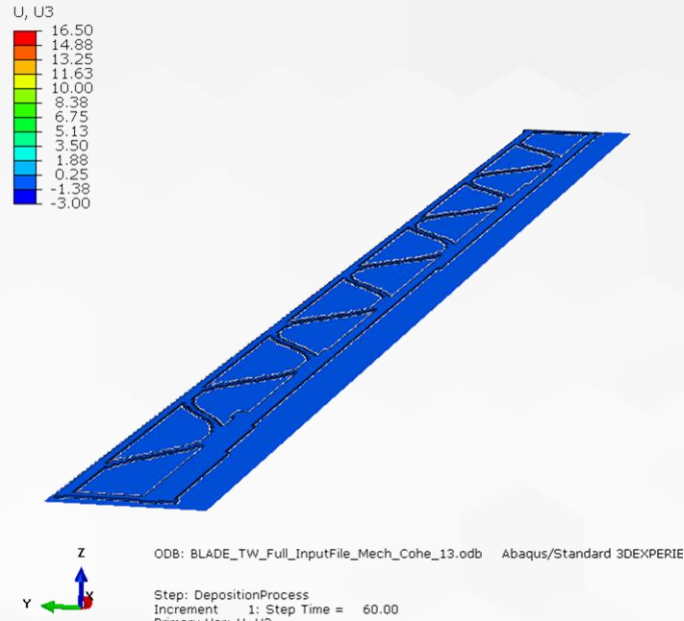
Validation

Removal of Printed Geometry



Printing

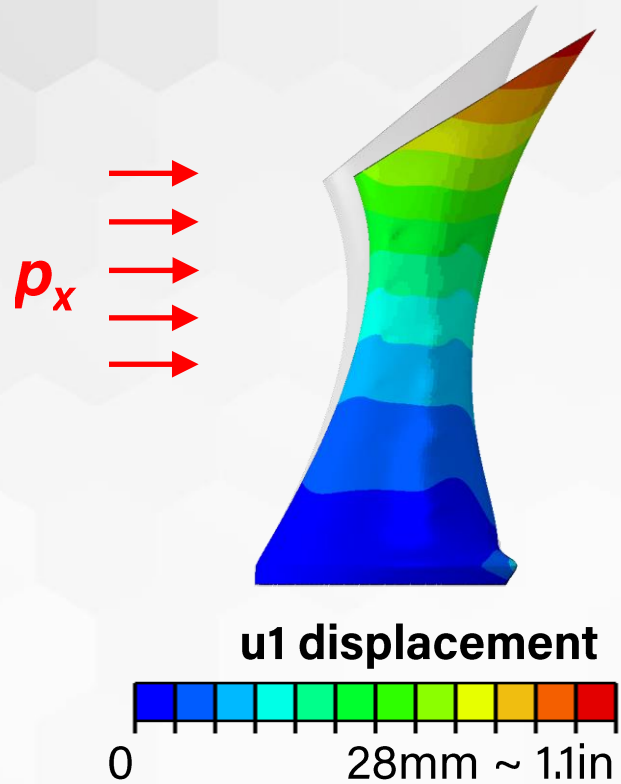
# Reduction of Part Deformation Driven by Analysis



- ◆ Autoclave tool made from Techmer PM Electrafil® PESU 1810 3DP
- ◆ Three failed print iterations utilizing ~1,500lb each -> ~75% savings.
- ◆ ADDITIVE3D simulations utilized after multiple failures to drive success on the final print.

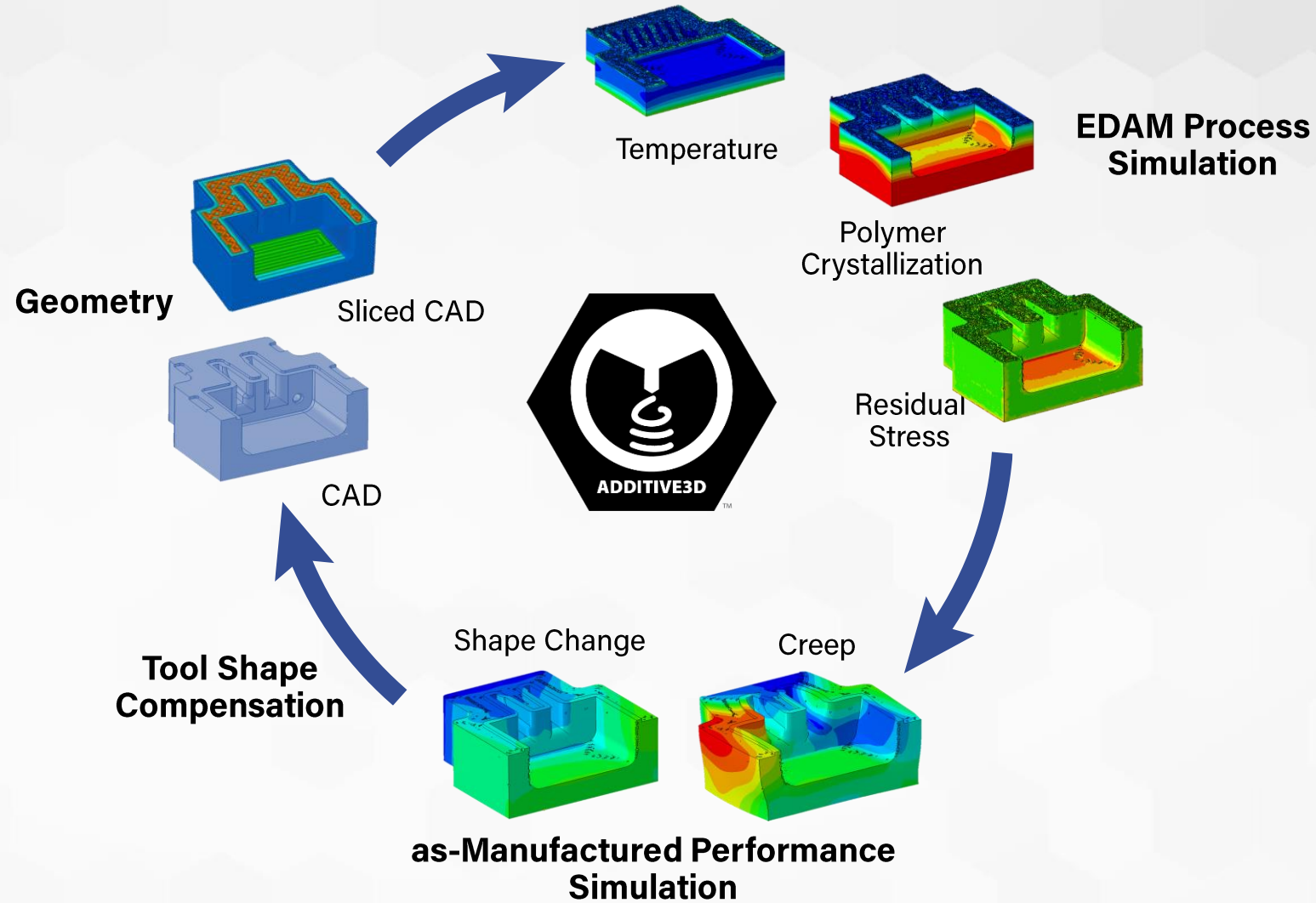


# Structural Analysis of Printed Torch



- ◆ Structural analysis to quantify displacement under load
- ◆ Risk assessment to ensure structural integrity

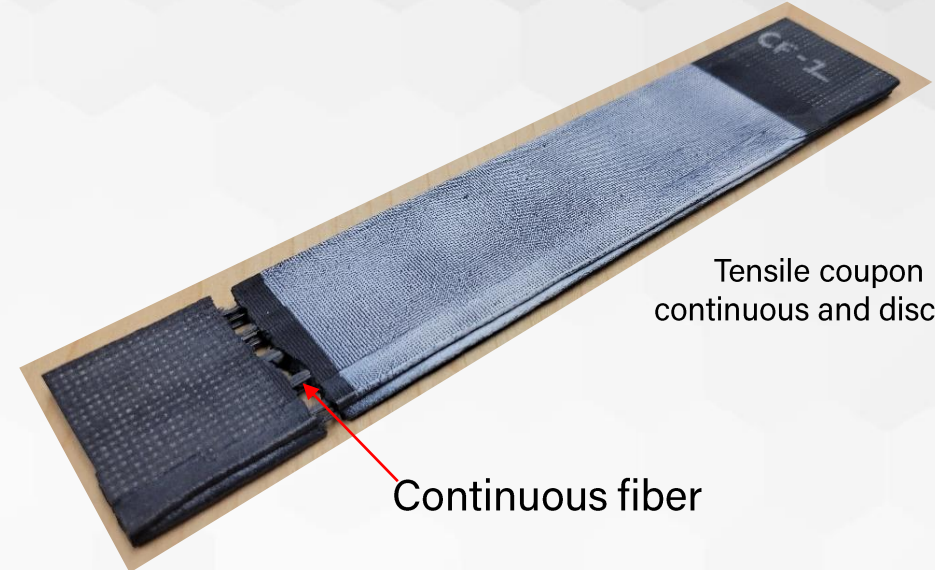
# ADDITIVE3D for "First time right printing"



# **Horizons and Opportunities in Composites Additive Manufacturing**

# Printing of Hybrid Continuous and Discontinuous Fiber Systems

- ◆ Opportunity
  - ◆ Elevate the large-scale additive manufacturing process to produce semi-structural components
  - ◆ Printing rates similar to large scale additive manufacturing with short fiber reinforced polymers are possible
  - ◆ Selective printing of continuous and discontinuous fibers
  - ◆ Integration of sensors and services (heating) in continuous fibers
- ◆ Process demonstrated in the CAMRI system at Purdue with continuous fiber filament impregnated in house (AS4 – PPS)



Tensile coupon printed with continuous and discontinuous fibers

Continuous fiber



US011214006B2

(12) **United States Patent**  
Barocio et al.

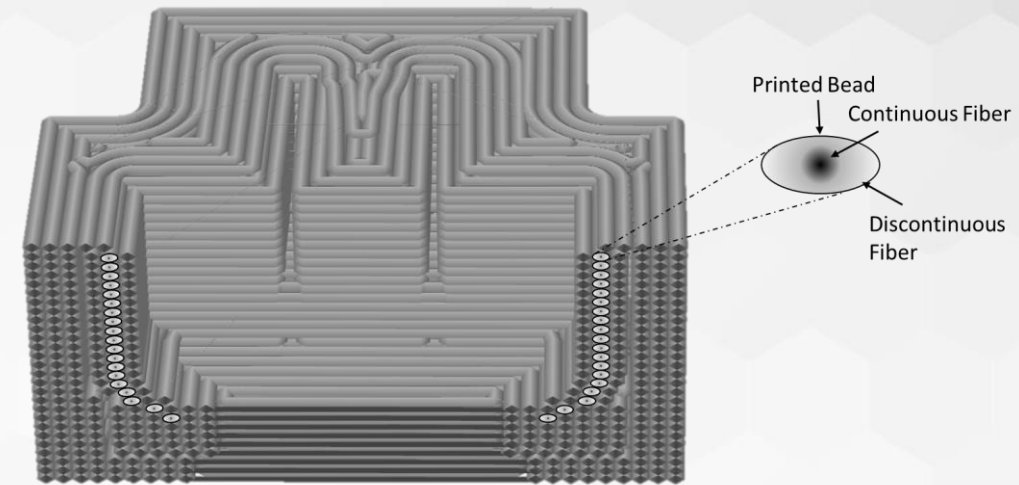
(10) **Patent No.:** US 11,214,006 B2  
(45) **Date of Patent:** Jan. 4, 2022

(54) METHODS AND APPARATUS FOR ADDITIVE MANUFACTURING UTILIZING MULTIFUNCTIONAL COMPOSITE MATERIALS, AND ARTICLES MADE THEREFROM

(58) **Field of Classification Search**  
CPC ... B29C 64/336; B29C 64/118; B29C 64/209; B33Y 10/00; B33Y 30/00; B33Y 40/00; B33Y 70/00  
See application file for complete search history.


# Printing of Continuous and Discontinuous Fibers

- ◆ Fundamental problems to investigate:
  - Concurrent flow of continuous and discontinuous fibers from nozzle to deposition
  - Adhesion between continuous and discontinuous fiber systems
  - Optimal microstructures for load transfer
  - Strength characteristics of hybrid printed materials
  - Design for printing with hybrid continuous and discontinuous fibers

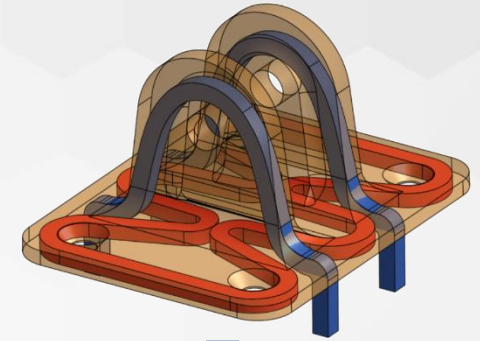


Compression molding tool concept printed with continuous and discontinuous fibers

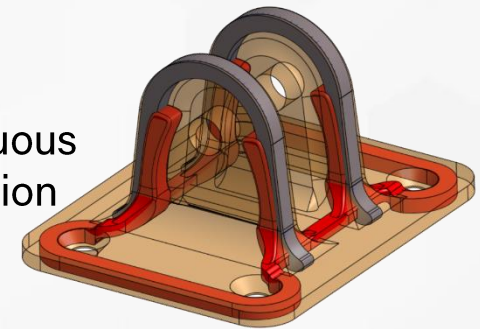
# Compression Molding of SMC and Printed Continuous Fiber Preforms

- ◆ Opportunity
  - ◆ Increase strength characteristics of compression molded components
  - ◆ Reduce variability in strength characteristics which elevates design allowables for this class of material systems
  - ◆ Elevate value of recycled material (upcycle) with the addition of a small fraction of continuous fiber printed preforms
- ◆ Initial demonstration of the potential for this technology through a pin bracket geometry in collaboration with  9T LABS

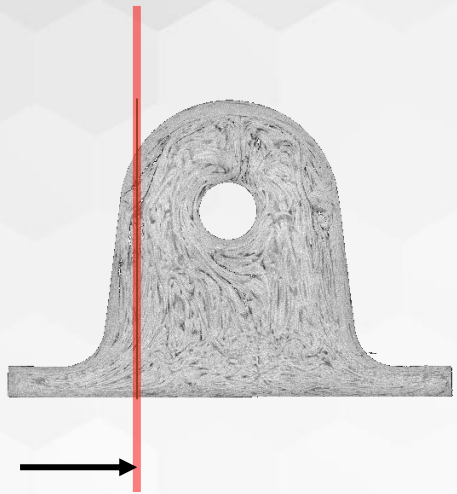
Initial Continuous  
Fiber Preform  
Configuration



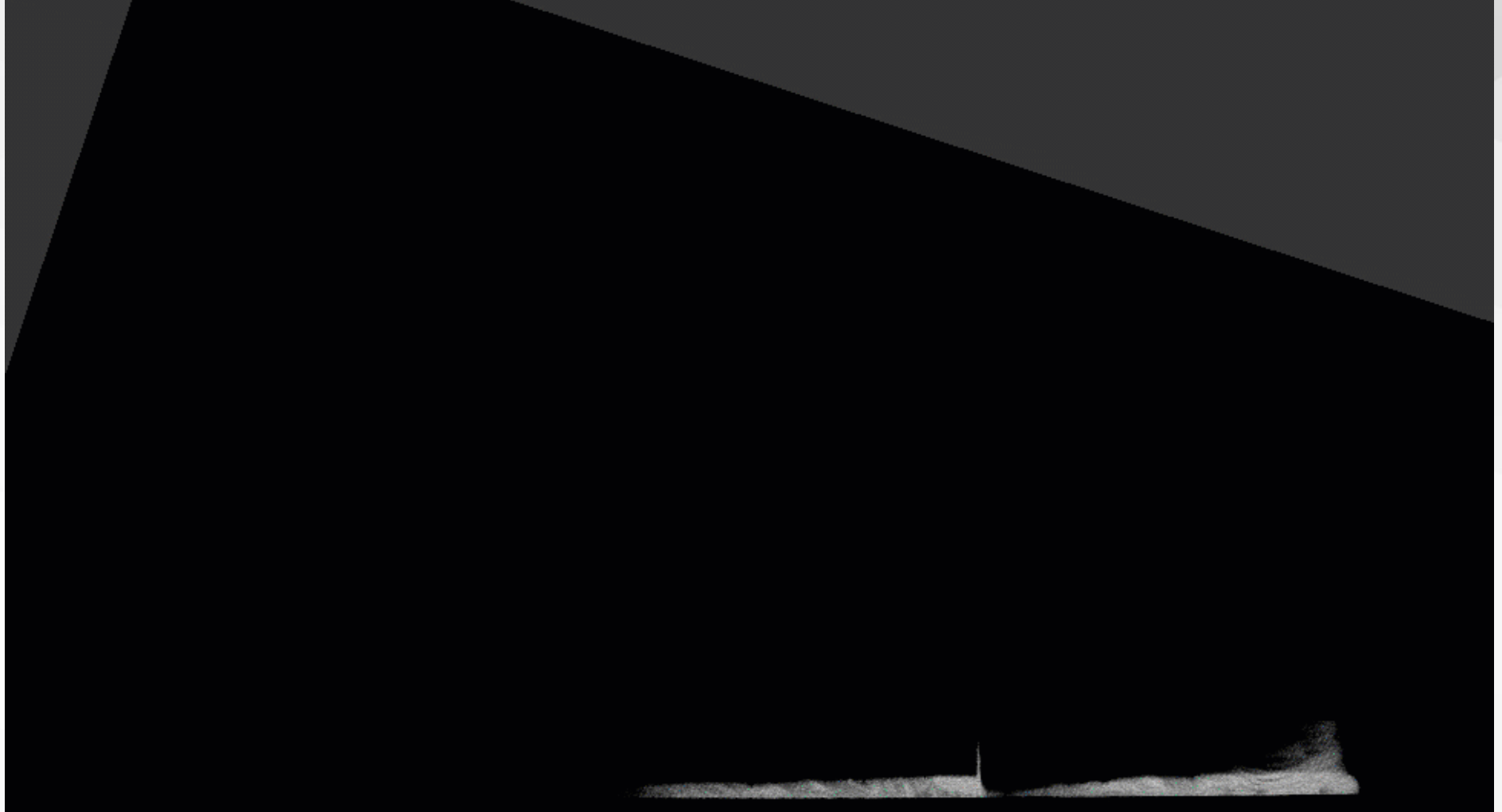
Expected Continuous  
Fiber Configuration  
after Flow



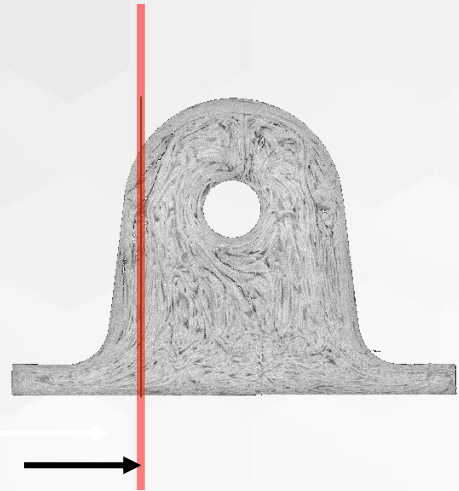
# CT-Scan of Bracket Molded with Hybrid Material System



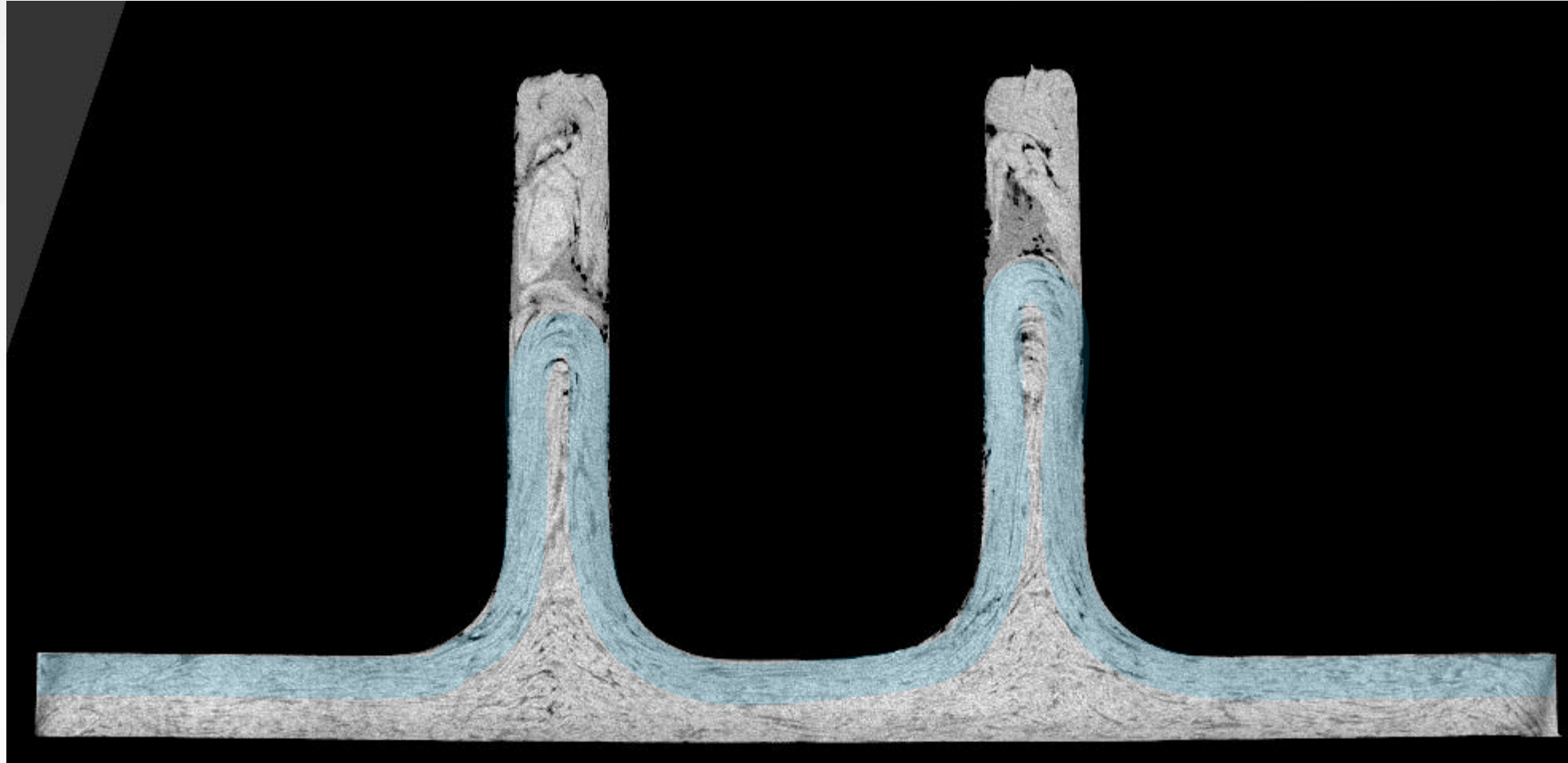
Hybrid Platelet  
+  
CF Preform



# CT-Scan of Bracket Molded with Hybrid Material System



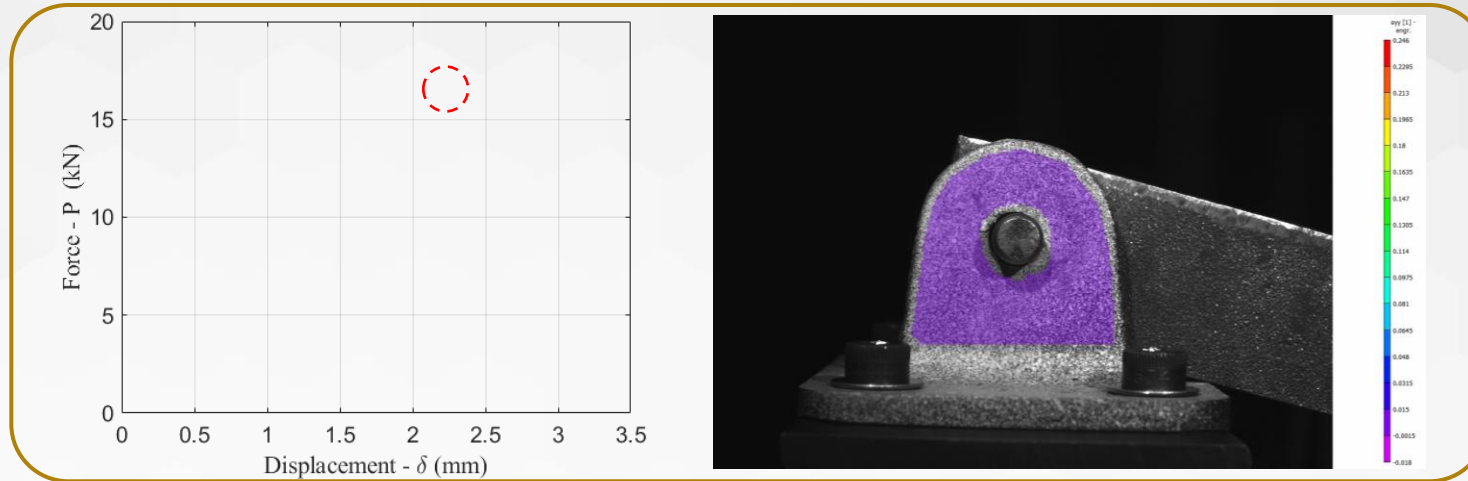
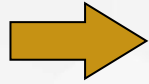
Hybrid Platelet  
+  
CF Preform



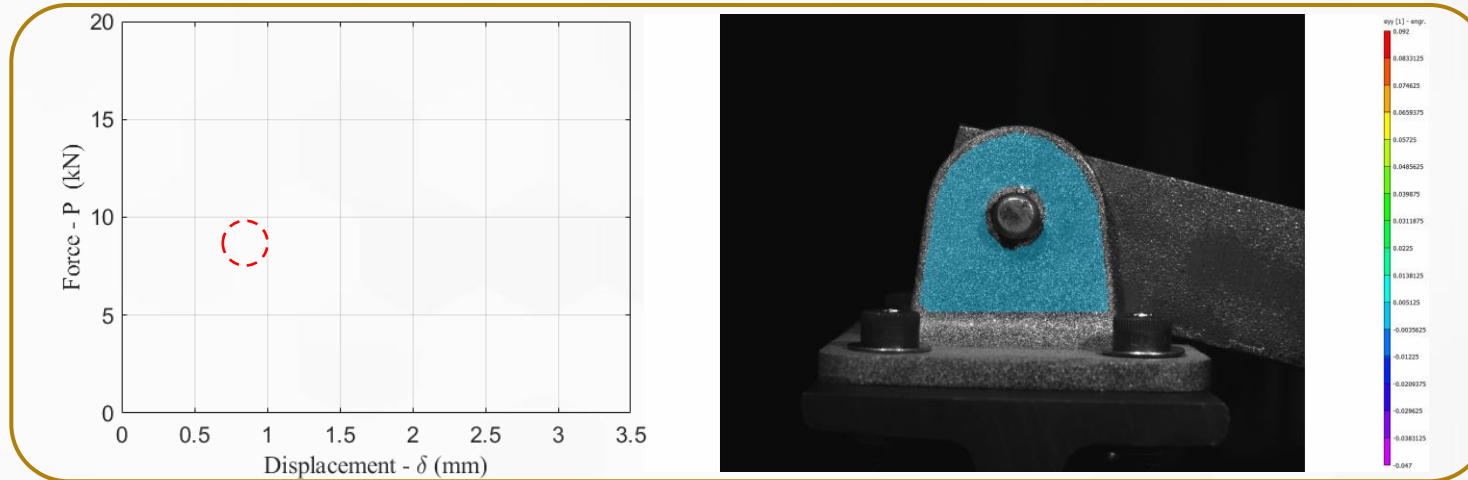
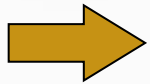


# Structural Performance of Hybrid Material System

Hybrid  
SMC  
+  
CF  
Preform



SMC



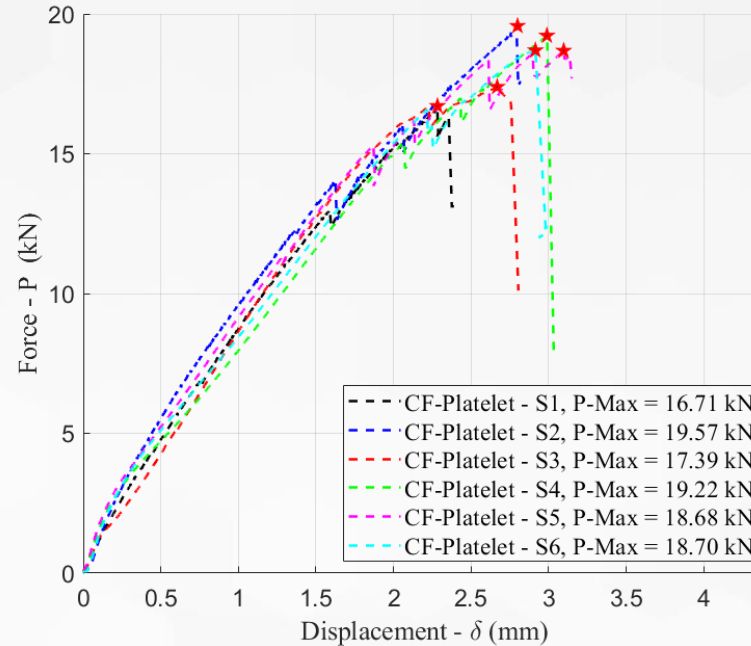
Barocio E, Eichenhofer M, Kalman J, Fjeld LM, Kirchoff J, Kim G, et al. Compression Molding of Hybrid Continuous and Discontinuous Fiber Reinforced Thermoplastics for Enhancing Strength Characteristics. SAMPE Conf., Seattle, WA: SAMPE; 2023.

# Compression Molding of Continuous and Discontinuous Fibers

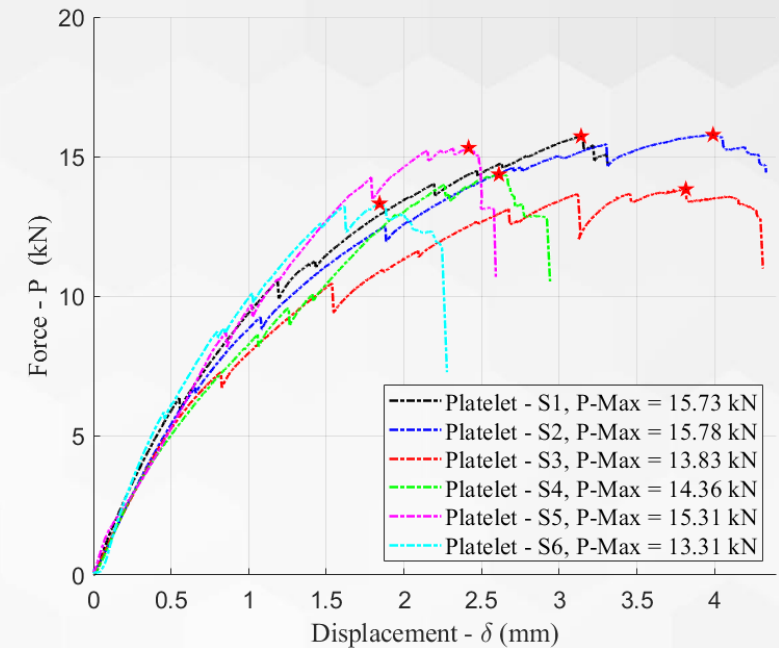


Test  
Fixture

Brackets Reinforced with Continuous  
Fiber Printed Preform



SMC Only



Pin Bracket Type	Average	Standard Deviation	Coefficient of Variance
<b>Load - P (kN) @ Onset of Failure</b>			
SMC	7.67	1.40	18.19%
CF & SMC	15.32	1.50	9.81%
<b>Load - P (kN) @ Ultimate Failure</b>			
SMC	14.72	1.04	7.05%
CF & SMC	18.38	1.10	6.01%

# Acknowledgements

## Composites Additive Manufacturing Group



## Research Sponsors / Partners



# Thank You