Multi-scale Modeling of Composite Material Damage: An Overview

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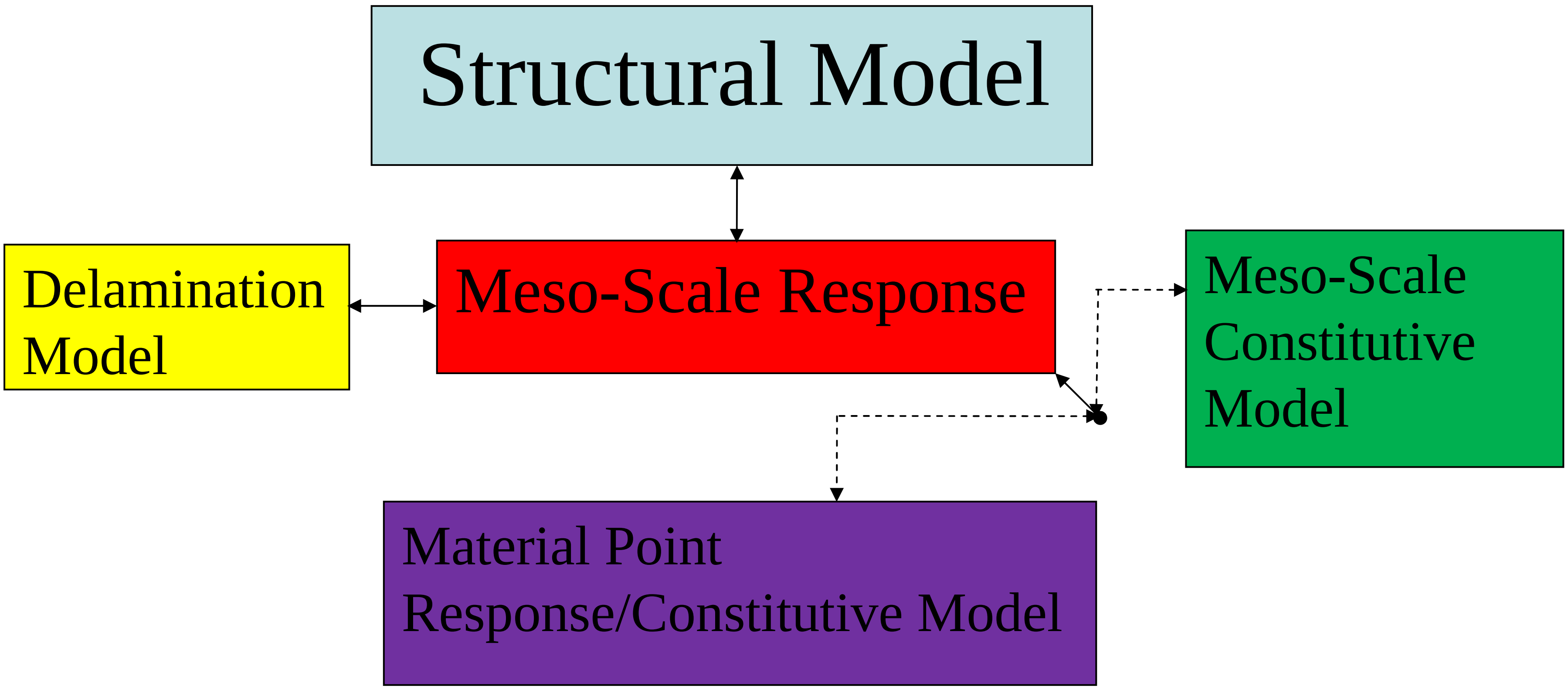
Scope of Talk

- Give an overview of damage modeling approaches at the different pertinent length scales for laminate structures
  - Structural models : O(m) , structural thickness
  - Meso-scale models, O(mm) , lamina thickness
    - Delamination modeling
    - Meso-scale constitutive models
  - Material point models, O(μm – sub mm)
    - Continuum (constitutive & failure surface) models
    - Micromechanical models
      - Deterministics
      - Stochastic
- Strengths/weaknesses/validation & other considerations

Model Connectivity



Setting the Stage

- Advanced structural applications – increasingly operate in regimes dominated by history-dependent phenomena
  - Increasing use of laminated composite structures to meet demands
- To accurately model damage/history-dependent behavior over multiple scales must:
  - Explicitly couple behaviors across the different scales
  - Consider mesoscale directly rather than in smeared sense
  - Deal with complex material models
  - Have accurate fields representations – Nonlinear evolution
  - Not introduce restrictive assumptions about constitutive behavior/models and types of damage states

Setting the Stage

- To model damage/failure traverse all realms of behavior:
  - Elastic
    - Viscoelastic/viscoplastic
      - Damage initiation – Types of damage?
        - » Damage growth – More types of damage?
        - » Failure

- Interactions of different mechanisms at each & over all the different length scales can result in non-intuitive behaviors

- Complex loading states

- Strain rate : Static, Intermediate, Dynamic
  - Shock : Wave propagation, strong field gradients

Structural Modeling

- What is full range of structural response characteristics expected, i.e. what need to be incorporated in the structural theory?
  - Static vs. Dynamic behavior
  - Vibration modes
  - Bending/extension
  - Degree of deformation
    - Small rotation/small strain – Geometric linearity
    - Moderate rotation/small strain – Von Karman assumption
    - Large rotation/small strain
    - Finite deformations (large rotations/large deformations/large strains)
  - Buckling
- What are the structural boundary conditions?
  - Dirichlet, Neumann, Robin (mixed) B.C.s
    - Simply supported, clamped, etc

Structural Modeling

- Traditional (3D) Finite Elements
  - Strengths
    - *Flexible set up/solution of problem – Available tools for meshing/analysis*
    - *Well proven – Extensive application to many problems*
    - Can handle complex constitutive models
    - Delamination can be handled using various types of cracking analyses - Cohesive zone models, VCCT, etc.
  - Weaknesses
    - Typically uses lower order elements in practice – Use more elements?
    - *Locking/Element aspect ratio*
      - *Lower order elements*
      - *Computational efficiency for many lamina*
    - *Most current practical forms have discontinuous fields at interfaces*
      - *Implications for evolution of history-dependent effects*
    - Cracking only between elements

Structural Modeling

- Plate/Shell Theories
  - Smeared/Equivalent Single Layer
    - Strengths
      - Global responses ok for large plate aspect ratios (> 20)
        - » Vibration modes
        - » Bending/extension
      - *Computationally efficient*
    - Weaknesses
      - *Can't provide accurate representations of local fields – Inaccurate estimates for evolution of history-dependent effects/damage/failure in general loading situations*
      - *Can't incorporate delamination effects*
      - Some versions don't go to correct limits (thick/thin plate limits)
      - Discontinuous tractions at interfaces
      - Often limited types of boundary conditions on top/bottom surfaces

Structural Modeling

- Plate/Shell Theories (cont'd)
  - Discrete layer/Zig-Zag
    - Strengths
      - *Can provide very accurate estimates for local fields*
      - Can handle complex constitutive theories (not Zig-Zag theories)
      - Can incorporate delamination thru CZM, VCCT, etc
      - *Approach satisfaction of interfacial continuity as order increases*
    - Weaknesses
      - *Accurate solutions - Computationally demanding*

Structural Modeling

- Plate/shell theories
  - Multiscale theories – Global/Local fields
    - Strengths
      - *Can provide very accurate estimates for local fields*
      - Can handle complex constitutive theories (not Zig-Zag theories)
      - Can incorporate delamination thru CZM, VCCT, etc
      - *Potentially more computationally efficient than discrete layer theories*
        - » *Mix global orders and local orders to obtain optimal efficiency*
      - Can satisfy interfacial constraints exactly (GMSST)
      - Framework from which to obtain ESL, DL, as well as global/local
      - *Transition from multiscale to global only analysis w/in surface of plate/shell*
        - » *Obtain accurate results in critical regions and less accurate results in regions far away*
        - » *Enhanced computational efficiency for entire solution*
    - Weaknesses
      - *More computationally demanding that smeared theories*

Structual Modeling

- FE application of plate/shell theories
  - *Easier mesh generation than 3D Finite Elements*
  - *Computationally more efficient than 3D FE due to separation of inplane and through thickness integration*
  - Locking/Aspect ratio issues still present (inplane)
    - Some FE implementations of plate theory do not go to the correct limits (Classical FE/FSDT locks for thin plates, unlike FE/CLT)
- Can implement plate/shell theories in other types of numerical strategies
  - Particle Methods
  - Etc.

Structural Modeling – V&V Issues

- Can carry out initial V&V w/in context of exact solutions for boundary value problems (BVPs)
  - Use of exact solutions eliminates uncertainty issues
  - What BVPs most appropriate/most demanding?
    - Types of B.C.s – Cylindrical bending, etc
    - Types of layups – Monolithic, Cross ply, angle ply, general layup
    - Types of material behavior (currently almost exclusively elastic material behavior)
      - Need to incorporate inelastic effects
    - Loading states (currently mostly static BVPs)
      - Need BVPs for dynamic effects
- Comparison w/other analysis techniques for some problem set

Structural Modeling – V&V Issues

- Comparison w/experimental data for structural response
  - Introduces the need to quantify uncertainty in material behavior/constitutive theories
    - Material consistency/uniformity
    - Identification of constitutive model parameters : Extra work/money
- Appropriate combination of the above comparisons?
- Statistical issues
  - Variability of material properties
    - Fiber alignments
    - Gaps between tows
  - Variability of lamina thickness
  - Variability of interlaminar regions

Meso-Scale Modeling

- Types of failure mechanisms
  - Ply cracking/splitting
  - Delamination
  - Sublaminate buckling
  - Crushing
  - Kink band formation
  - Localization of failure
  - Interactions between mechanisms

Meso-Scale Modeling

- Models for delamination
  - Cohesive zone models (CZMs) - Relates interfacial tractions to displacement discontinuities
    - Strengths
      - *Can predict initiation and growth w/o a priori assumptions about cracks*
      - Can formulate using internal state variable formalism
        Variety of (coupled) history-dependent effects
      - *Can be implemented into many types of numerical strategies*
        - » *Applicable to complex structures subjected to complex loading states*
      - Direct connection to fracture mechanics
    - Weaknesses
      - Currently accurate assessments tied to element size in FE
        - » Computational efficiency (unpublished work at LANL shows how to eliminate this constraint)
      - Actual shape of the CZM may not be important – Uniqueness?
      - *Characterization data can be hard to obtain*

Meso-Scale Modeling

- Models for delamination
  - Fracture Mechanics based analyses : LEFM, VCCT, etc.
    - General Strengths
      - *Large body of work*
      - *Different types of growth criteria : SIF, SERR, etc.*
      - Some versions of these techniques can handle complex constitutive models for material behavior
    - General weaknesses
      - *Assumptions about cracks*
        - » *Number of cracks*
        - » *Location of crack(s)*
        - » *Size of crack(s)*
        - » *Can be difficult to determine direction of growth/mode separation*
      - *Potential length scale issues in composites (process zone size)*
      - *Application to complex structures subjected to complex loading states can be difficult*
      - Characterization data can be hard to obtain

Meso-Scale Modeling

- Meso-scale (lamina scale) continuum damage modeling
  - *Assumes uniform stress/strain states within lamina*
  - Thermodynamically derived constitutive relations for lamina behavior : Internal state variable (ISV) formalism
  - Strengths
    - *Computationally efficient since no field variation through thickness*
    - History-dependent behavior predicted :
      - Can incorporate many types of (smeared) effects: Viscoplasticity, Cracking, Etc.
  - Weaknesses
    - *Accuracy of smeared assumption*
      - *Variation from mean fields*
      - *Static vs. Dyn. loading states : Dyn. – Potentially strong grad. w/in lamina*
    - *Characterization/interpretations of model parameters*

Meso-Scale Modeling – V&V Issues

- How to uniquely validate a given meso-scale fracture model since typically have material effects influencing behavior
  - Multiple phenomena interacting at lower length scales
  - Complex, 3D constitutive models
- Statistical issues
  - Sensitivity of the predictions to variations in the model parameters
    - Variations in model parameters : Variability in experimental data/material behavior: Elastic properties, damage location/localization, strength, etc.

Material Point Modeling

- (Some) General requirements for Material Models
  - Processing effects
  - *Changing strain rates (static to dynamic)*
  - *Changing load paths (monotonic vs cyclic vs complex)*
  - Changing temperatures rates and paths
  - Coupling between mechanical, thermal, and moisture (and chemical and electrical?) effects
  - Aging
  - *Influence of microstructure : Interactions between the constituents/interfaces*
  - *Types and evolution of damage : Appropriate underlying physics – Many types at once*
  - *Interactions between the different effects*
- Pick some?

Material Point Modeling

- Large number of damage mechanisms
  - *Debonding of constituents*
  - Micro-buckling/kinking of constituents
  - *History-dependent deformations within constituents*
  - Void initial/growth/coalescence
  - Fiber bridging
  - *Fiber or matrix damage/cracking*
  - Others?

Material Point Modeling

- Two types of theories : Continuum & Micromechanical
  - Continuum level theories :
    - Consider material behavior at macroscopic level as function of current state
    - Thermodynamically based OR Empirically postulated
    - Many types : LEFM, Weibull Strength of brittle materials, Phenomenological failure theories, Phenomenological constitutive theories
  - Micromechanical theories :
    - Directly consider the material microstructure and the phase behaviors to predict both macroscopic and microscopic responses
      - Homogenization based theories
        Deterministic vs stochastic
      - Direct micromechanical analyzes
  - Both types of models assume scale separation

Material Point Modeling – Continuum Theories

- Failure surface models
  - Many types – Max. strain/stress, Tsai-Hill, Polynomial Tensor, etc.
    - Range from simple to fairly complex
  - World-wide failure exercise discusses formulations and capabilities of many leading theories of this type
  - Strengths
    - *Computationally efficient*
    - Easily implemented in various types of numerical strategies
    - Useful for examining trends in many possibilities
  - Weaknesses
    - *Independent of material constitutive behavior – Not history-dependent*
    - *Phenomenological/Empirical*
    - Predictions : Initial damage state vs final damage state?
    - Validity in coupled loading states
    - Identification of model parameters

Material Point Modeling – Continuum Theories

- Macroscopic constitutive theories
  - Material behavior determined by current state
  - Basis (often) rests on thermo-dynamic constraints/relations although have empirical developments as well
    - 1st and 2nd law
    - Thermo-dynamic potentials
  - *Postulates types/evolution/interactions of history-dependent effects – Internal State Variables (ISV)*
    - *Only two observable external state variables : Strain and Temperature*
    - *ISVs inferred/postulated : Attempt to account for changes in internal state/structure*
  - Gives macroscopic response only
  - Examples – Viscoelastic theories, Incremental plasticity, Bodner-Partom viscoplastic theory, Continuum Damage Mechanics (scalar and tensor forms), etc.

Material Point Modeling – Continuum Theories

- Macroscopic constitutive theories
  - Strengths
    - *Computationally efficient*
    - Large historical body of work
    - Flexible formulational framework
    - *Can couple many types of physical mechanisms interactively*
    - Can be/have been implemented into many numerical schemes
    - Characterization of model parameters can be simpler than for micromechanical models (no interface parameters needed)

Material Point Modeling – Continuum Theories

- Macroscopic constitutive theories
  - Weaknesses
    - No direct account of microstructure
    - No direct account of fundamental response mechanisms/interactions
    - *Postulates types/evolution/interactions of history-dependent effects*
      - *Only two observable state variables : Strain and Temperature*
      - *Internal state variables inferred/postulated*
      - *No generally accepted set of ISVs for given class of materials*
        - *Some art in chosing set of ISVs, the thermodynamic potentials, and the evolution equations for ISVs*
      - *Need to reformulate if postulated physics changes*
    - Complex models – Large numbers of ISVs
      - More difficult to integrate due to many time scales
      - More difficult to characterize model parameters
      - More difficult to interpret meaning of different parameters
      - More sensitive to changes in the data?
    - Development for anisotropic materials more complex than for isotropic materials

Material Point Modeling – Micromech. Theories

- Micromechanical theories
  - General Strengths
    - *Direct insight into microstructural effects*
    - *Direct insight into fundamental response mechanisms and their relative importance*
    - Gives both micro and macro responses
    - Can incorporate physics as necessary
    - Handles anisotropy naturally

Material Point Modeling – Micromech. Theories

- Micromechanical theories
  - General Weaknesses
    - *How much microstructural info is enough?*
      - *Definition of appropriate microstructure (RVE/Unit Cell)*
      - *Mean fields vs. detailed microstructural info*
    - Type of physics incorporated influences predictions
    - More characterization info req'd than continuum constitutive theories
      - Phase properties,
      - Interface properties (Often very difficult to obtain accurately)
    - Accurate simulations
      - *More computational state variables to carry in analysis*
        - » *More memory intensive*
        - » *More computationally demanding (than most continuum level theories)*

Material Point Modeling – V&V Issues

- Interpretation of Exp. Data – What is the appropriate underlying physics?
- Material characterization –
  - Simple tests – Sufficiency/uniqueness?
  - Elimination of structural size effects to obtain pure material behavior
  - Nonlinear, multivariable optimization for advanced continuum level models
    - Sensitivities of the models to variation in the parameters
    - Influence of experimental data variability
- Satisfaction of the scale separation assumption?
  - Under strong dynamic loading assumption may not be satisfied.

Summary/Final Considerations

- Many required component models required to analyze multiscale BVPs
  - Non-intuitive interactions between different physics and different component models can occur
- Questions that need to be addressed within the context of a given modeling framework:
  - Accuracy
    - How is this judged?
    - What is good enough?: Trends/Engineering analyses vs. accurate predictive analyses? Probably require both to ensure safety.
  - Accuracy vs. computational efficiency vs. modeling framework/ complexity vs. computational resources – Trade offs
  - Where's the uncertainty and how is it propagating thru analysis?

Not so Bleak – Dedicated to Frank Addessio

- Outlined many problems but is the picture so bleak? NO.
  - Any approach is a optimization of different considerations : Must balance needs/capabilities
    - Identify size of critical regions in structure?
    - Is computational efficiency more important than accuracy or vice versa or is this even a necessary questions?
      - Can different techniques be combined to enhance both accuracy and OVERALL computational efficiency?
        - » Use meso-scale constitutive models away from critical area while use continuum or micromechanical constitutive models in critical area?
      - Can new techniques be introduced?
        - » Multiscale analysis with global/local to global only transitions can enhance comp. efficiency.
      - Are trends good enough or do you need predictive capabilities?
        - » A lot of experimental data vs. little experimental data?
    - Computational resources are getting more capable all the time.
    - How much time to you have to do the implementations?

Not so Bleak

- Additional considerations
  - Computational resources are getting more capable all the time.
    - Parallel processing makes some things more feasible.
  - How much time to you have to do the implementations?
  - How much expertise required to do the implementations?
    - Modeling is getting more complex → Team efforts becoming more important