

Multiscale Computational Methodology for the Mechanical Response of Nano- and Micro-Fiber Reinforced Cementitious Composites

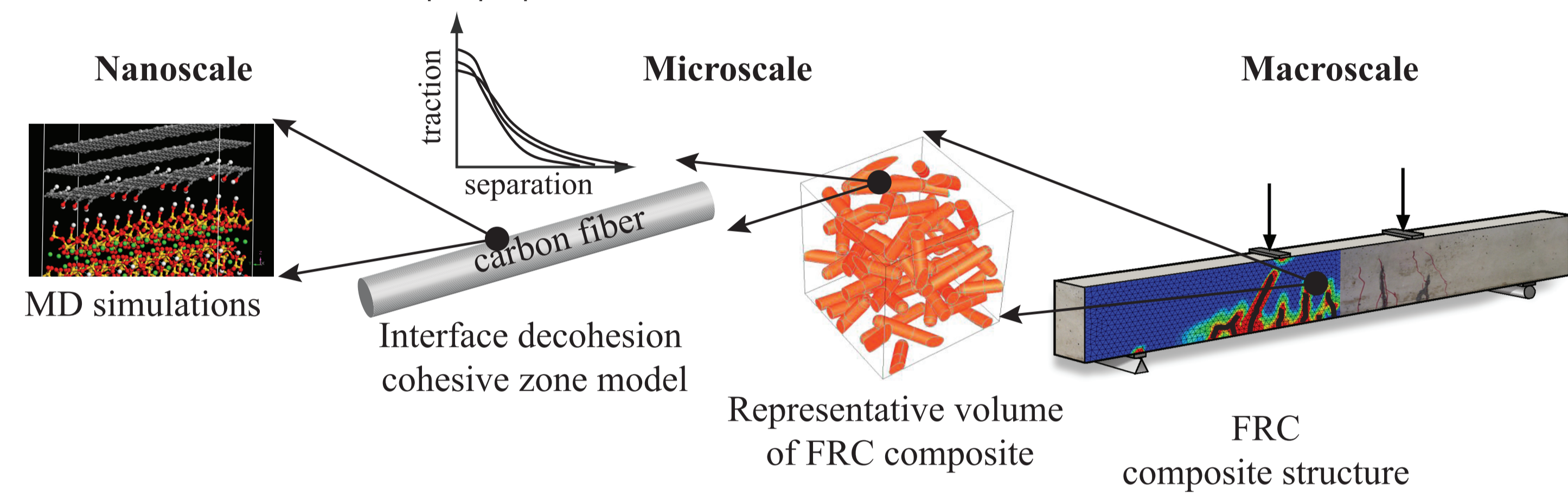
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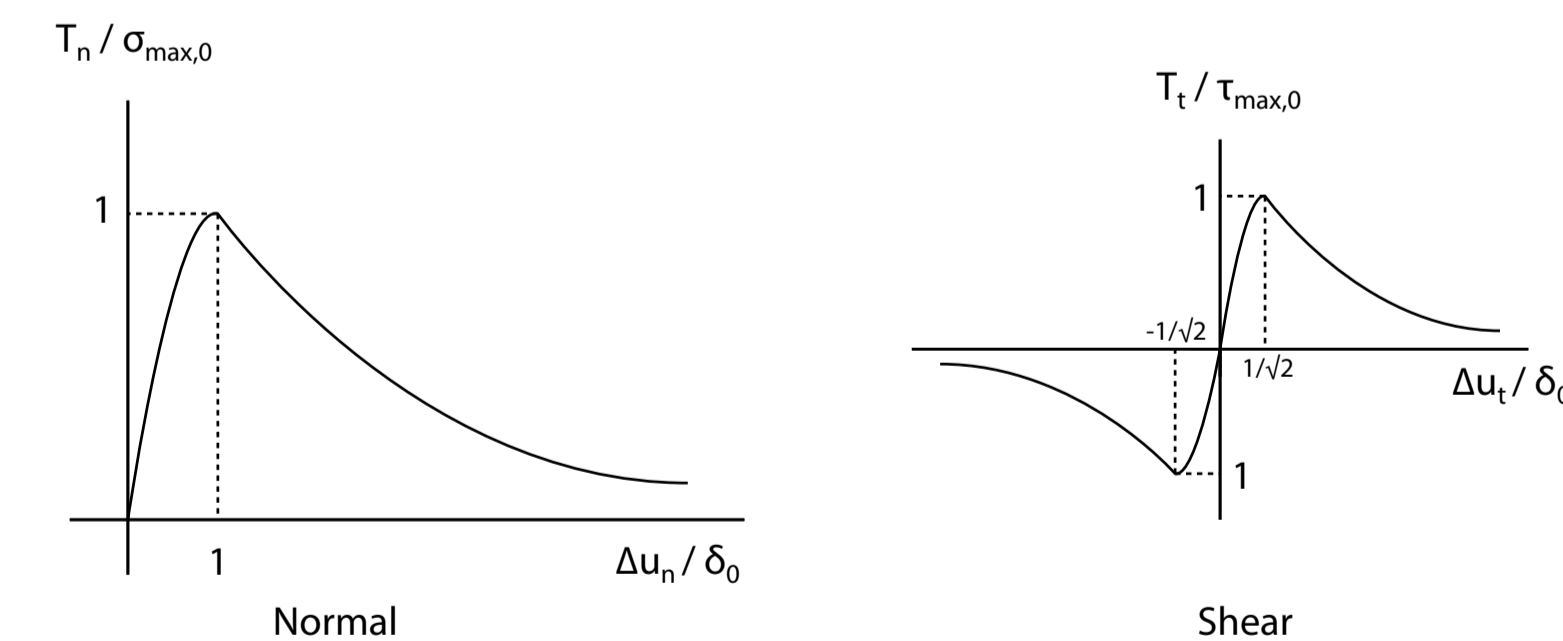
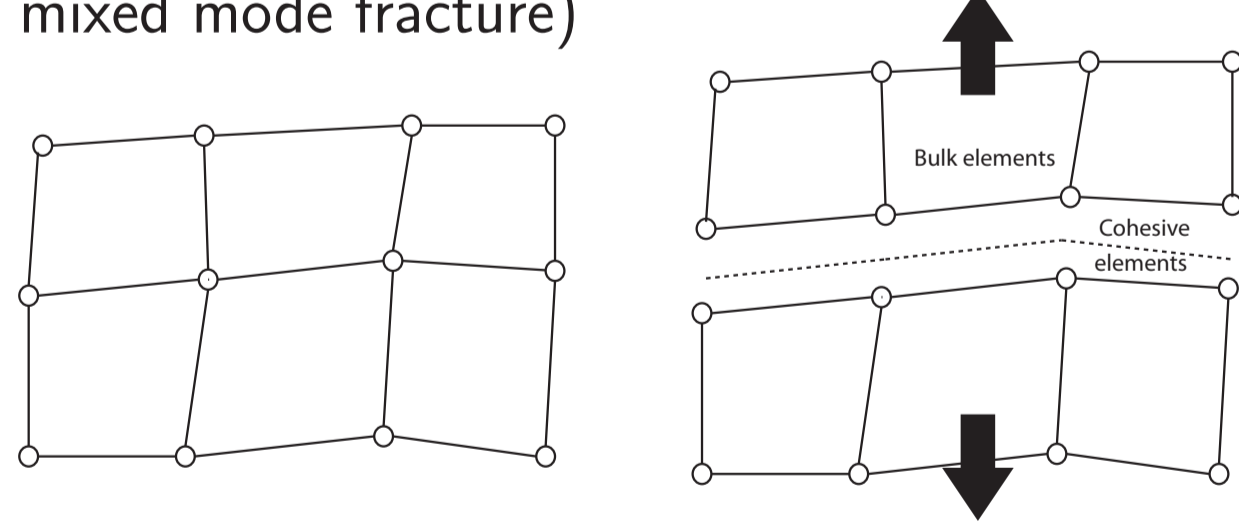
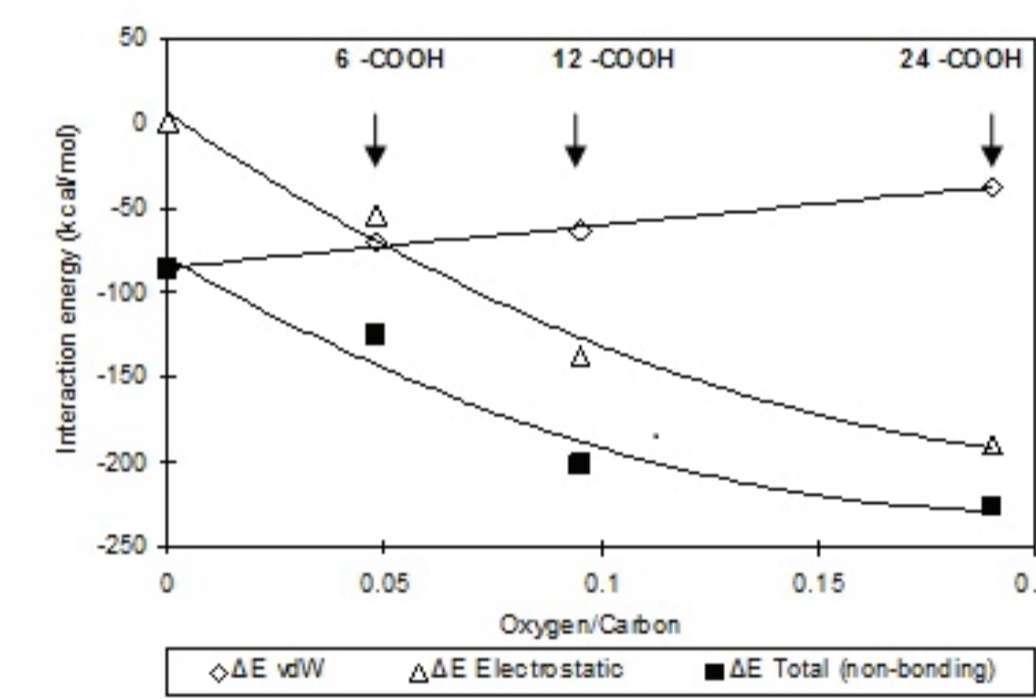
Introduction

- ▶ **Goals**
 - ▷ To gain a fundamental understanding of the nanoscopic chemo-mechanical interactions at the fiber-matrix interface in carbon nano- and micro-fiber reinforced cement composites
 - ▷ To evaluate the effects of the chemical structure of the interface on the macroscopic mechanical failure properties
- ▶ **Computational design of carbon nano- and micro-fiber reinforced cementitious composites**
 - ▷ Controlling and optimizing the mechanical and failure response through molecular scale engineering
 - ▷ The interfacial interaction between the matrix and the reinforcement has significant effect on the overall response of the composite structure
 - ▷ Molecular scale engineering to control the chemical structure of the interface (e.g., functionalization, number and area density of the functional groups)
 - ▷ Characterization of interfaces solely based on experimentation is costly and difficult
- ▶ **Proposed multiscale computational framework**
 - ▷ Nanoscale investigations and nanoscopically informed cohesive zone model
 - ▷ Modeling the microscale: representing volumes by extended finite element method (XFEM)
 - ▷ Bridging micro and macroscales for macroscopic properties



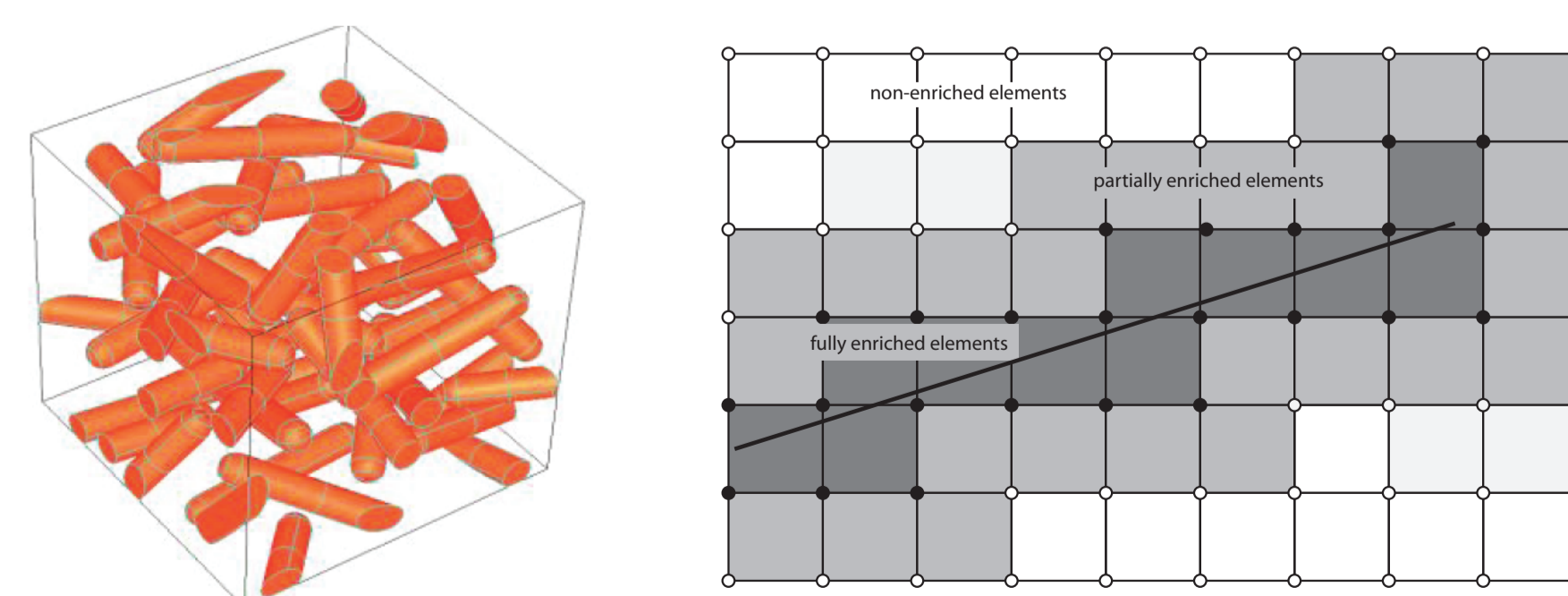
Nanoscopically Informed Interface Cohesive Zone Model

- ▶ **Link between the chemical structure and mechanical properties of the fiber-matrix interface**
 - ▷ Based on molecular dynamics simulations
- ▶ **Energy-based cohesive zone model**
 - ▷ Constitutive relationship between the cohesive tractions and the displacement jumps along the reinforcement-cement interface
 - ▷ Function of the molecular structure of the interface
 - ▷ Separation resisted by cohesive tractions, represented as interfacial potential energy
 - ▷ Zero thickness elements between standard finite elements, viewed as cohesive forces
- ▶ **Reinforcement-cement interface energies and potential-based traction-separation law**
 - ▷ Molecular dynamics simulations between surface functionalized graphitic structures and calcium-silicate-hydrate (C-S-H)
 - ▷ Incremental deformations and successive energy minimizations
 - ▷ Interaction energies and molecular structure of the interface for different loading configurations (tensile, shear and intermediate direction for mode I, II, and mixed mode fracture)



Modeling Short Rigid Fiber Reinforced Composites Using XFEM

- ▶ **Representative volume element (RVE)**
 - ▷ Constitutive response of the cohesive zone model for interdependent damage plasticity-modeling of the cement phase
 - ▷ Random short-fiber reinforced matrix idealization
 - ▷ XFEM framework to evaluate the response of the RVE
- ▶ **Extended finite element method (XFEM)**
 - ▷ Fibers accounted for by using additional enrichment functions
 - ▷ Enrichment of the finite element approximation by additional functions that model the internal boundaries
 - ▷ Complex finite element discretizations eliminated



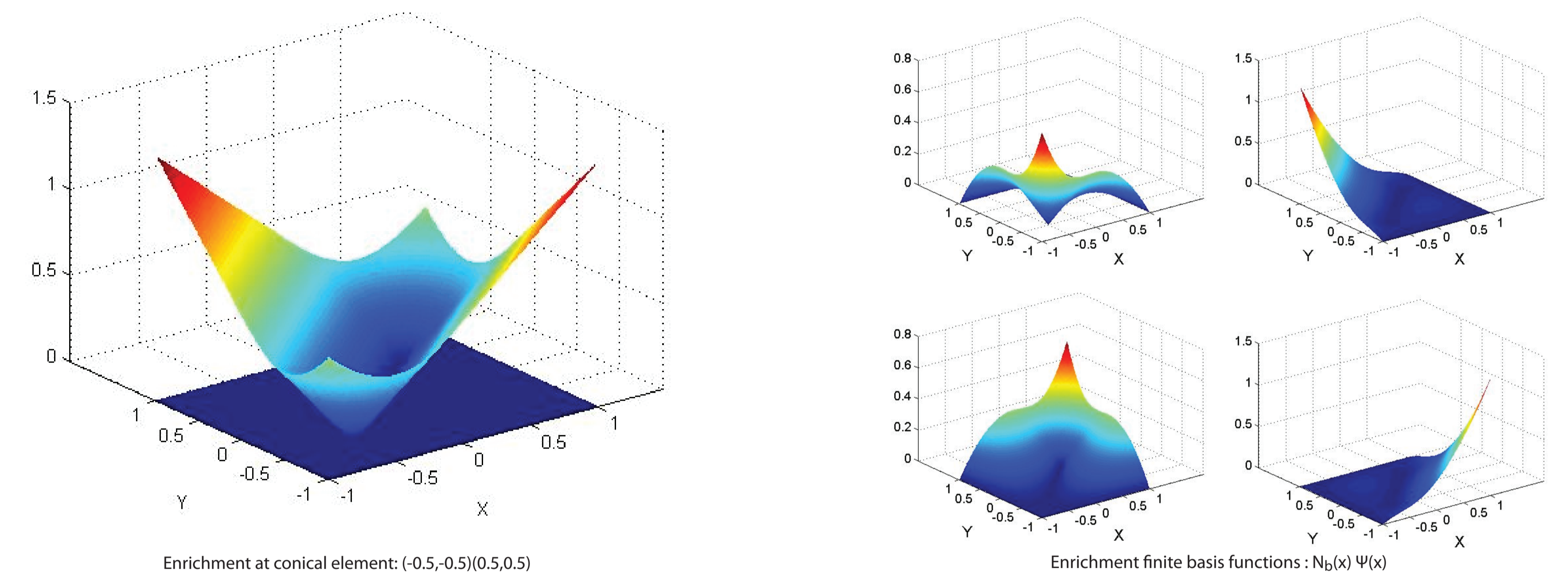
$$\mathbf{u}(\mathbf{x}) = \sum_{a \in \alpha} N_a(\mathbf{x}) \hat{\mathbf{U}}_a + \sum_{b \in \beta} N_b(\mathbf{x}) \Psi(\mathbf{x}) \hat{\mathbf{C}}_b$$

▷ $N(\mathbf{x})$: nodal shape function, $\hat{\mathbf{U}}$: nodal value, $\Psi(\mathbf{x})$: enrichment function, $\hat{\mathbf{C}}$: additional degree of freedom nodal value

Nodal Enrichment to Describe fiber response

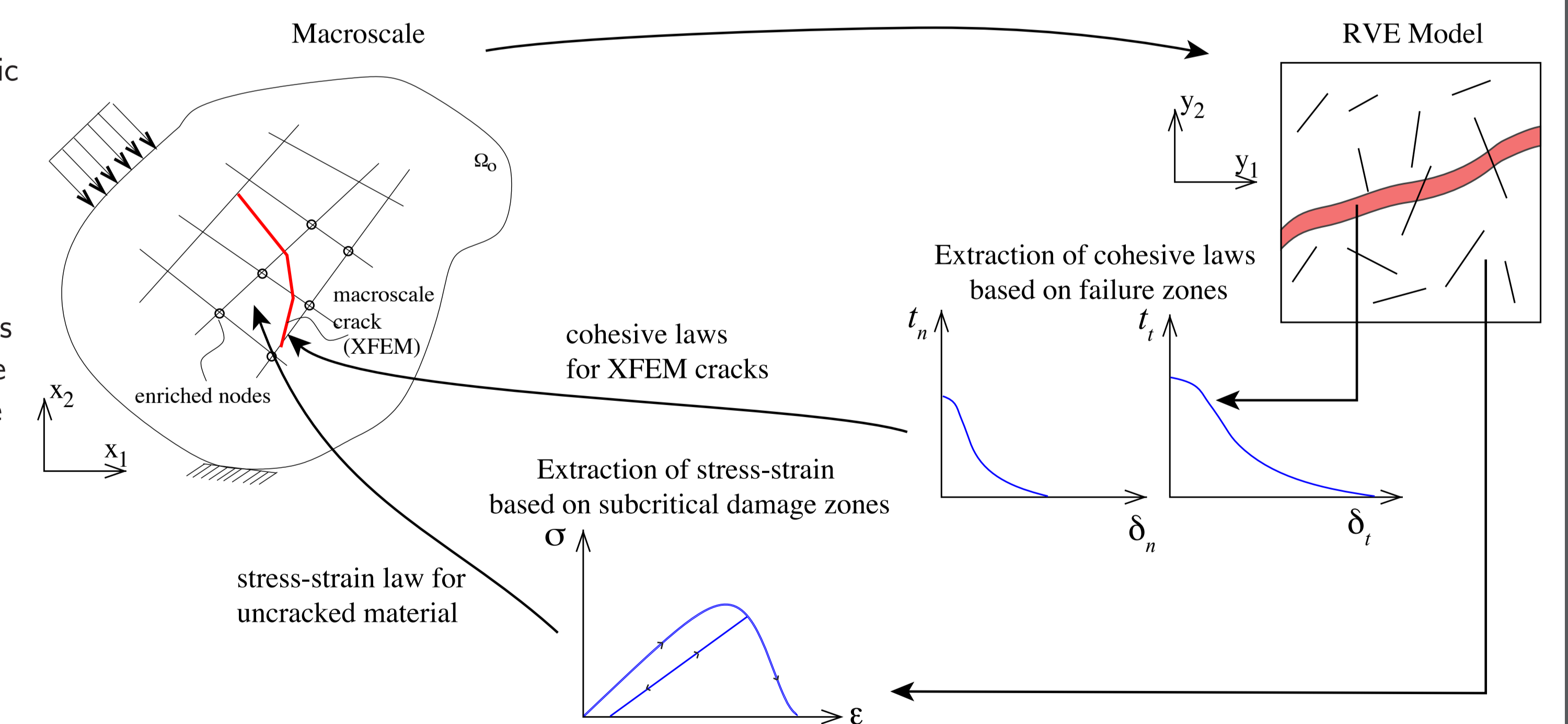
- ▶ **Enrichment of rigid fiber**

$$\Psi(\mathbf{x}) = \left(\prod_{i=1}^2 H_i(-\phi_i) \right) \phi_c(\mathbf{x}) + \sum_{i=1}^2 H_i(\phi_i) d_i, \quad \text{note: } H(\cdot): \text{ heavyside function}$$
 - ▷ $\phi_i(\mathbf{x}, t) = (\mathbf{x} - \mathbf{x}_i) \cdot \hat{\mathbf{t}}$: level set function at fiber tip - tracks the motion of the fiber tip
 - ▷ $\phi_c(\mathbf{x}, t) = \min \|\mathbf{x} - \mathbf{x}_r\|$: level set function at interface - tracks the motion of the fiber interface
- ▶ **Rigid body constraint**
 - ▷ Each fiber moves as a rigid body
 - ▷ Interfacial elements move with fibers
 - ▷ Penalty constraints to enforce rigid motion of fibers



Bridging the Scales for Macroscopic Properties

- ▶ **Computational homogenization method (CHM)**
 - ▷ Failure processes within the RVE at the microscale is propagated to the macroscale
 - ▷ Original response fields are expressed in terms of two (or more) spatial position vectors (e.g., $\mathbf{u}^c(\mathbf{x}) = \mathbf{u}(\mathbf{x}, \mathbf{y}(\mathbf{x}))$), \mathbf{y} and \mathbf{x} indicate the position within the microscale and the macroscale, respectively
 - ▷ Response fields are decomposed into macroscale and microscale components based on asymptotic expansions and asymptotic matching is employed to formulate boundary value problems: $\mathbf{u}^c(\mathbf{x}) = \mathbf{u}^0 + \zeta \mathbf{u}^1(\mathbf{x}, \mathbf{y}(\mathbf{x})) + \dots$
- ▶ **Multiscale crack enrichment**
 - ▷ Crack enrichment to eliminate mesh dependency and spurious localizations
 - ▷ Macroscopic cracks due to the failure processes occurring at the microscale incorporated using XFEM
 - ▷ Detection of zero eigenvalues and eigenvectors of the acoustic tensors at a macroscale integration point



Summary

- ▶ **Multiscale computational framework for modeling the mechanical response of nano- and micro-fiber reinforced cementitious composites**
 - ▷ Semi concurrent multiscale procedure (non concurrent: nano to microscale, concurrent: micro to macroscale)
 - ▷ Chemo-mechanical characteristics of reinforcement-matrix interfaces elements based on MD simulations
 - ▷ Nanoscale response with the nanoscopically informed interface cohesive zone model
 - ▷ Micro and the macroscale response are evaluated in a fully coupled manner using CHM
 - ▷ An efficient XFEM approach is proposed to evaluate the RVE response
- ▶ **Future potential**
 - ▷ Pathway to achieve simulation based molecular scale engineering of cementitious composite
 - ▷ Aid in the composite material design process