Multiscale Modeling of Interfaces

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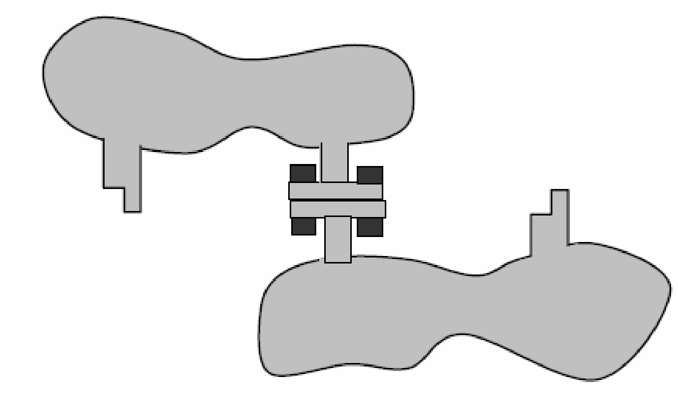
Outline

1. Conclusions from NSF-Sandia Workshop, October 2006
   - Merging the top-down and bottom-up approaches
2. Issues involved in the Modeling of Joint Interfaces
3. Modeling of Multiscale Structural Response
4. Merging CG and DG Methods for Joint Interfaces
5. Error Estimation

Merging the Top-Down and Bottom-Up Approaches (NSF-Sandia Conf. Oct 2006)



Segalman *et al. Sandia Report*

1. Consider the interface as an entity that can be represented at various scales through different types of "constitutive relations".

2. Multiscale Material Modeling: Hierarchical models that have micro / nano information built in.

3. Multiscale Variational Frameworks: Sub-scale modeling concepts.

Technical Issues involved in Multiscale Modeling of Joints

Material models with inherent scale effects

Geometric modeling of joint interfaces induce scale effects, both linear and nonlinear

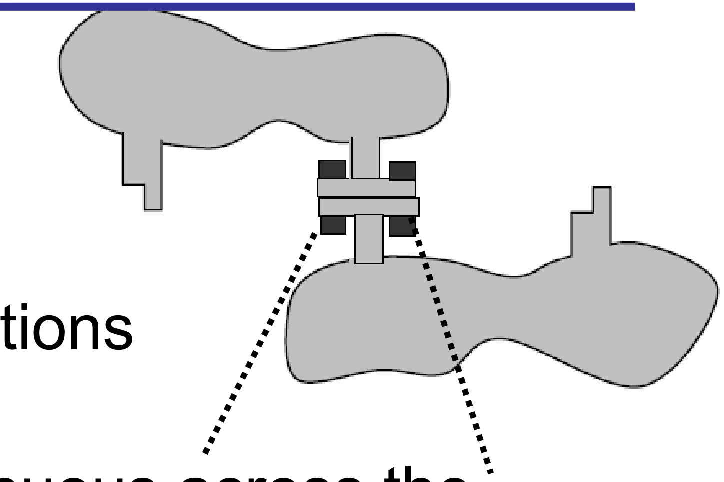
Response functions with embedded scale effects

Sensitivity with respect to the variation in the values of the parameters

Predictive capability for the modeling of multiscale effects requires multiscale error estimators

Heterogeneous multiscale phenomena with different PDE’s appearing at different scales

Geometric Description of the Joint Interface



Consider the body as one domain

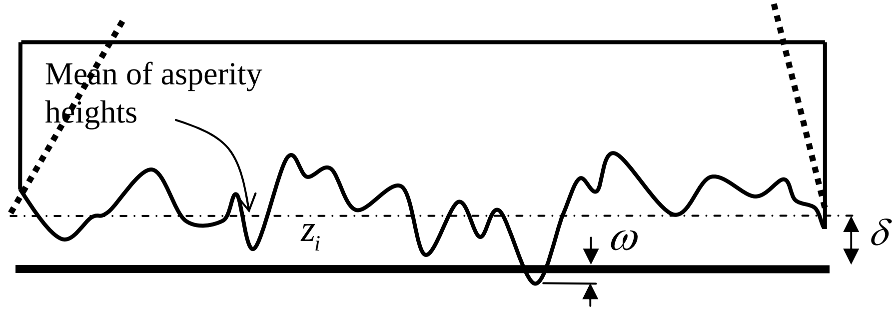
Employ DG ideas ⇨ discontinuous functions

Physical fields may or may not be continuous across the strong discontinuity ⇨ relative slip is permitted

Flux terms weakly enforce the continuity of the fields

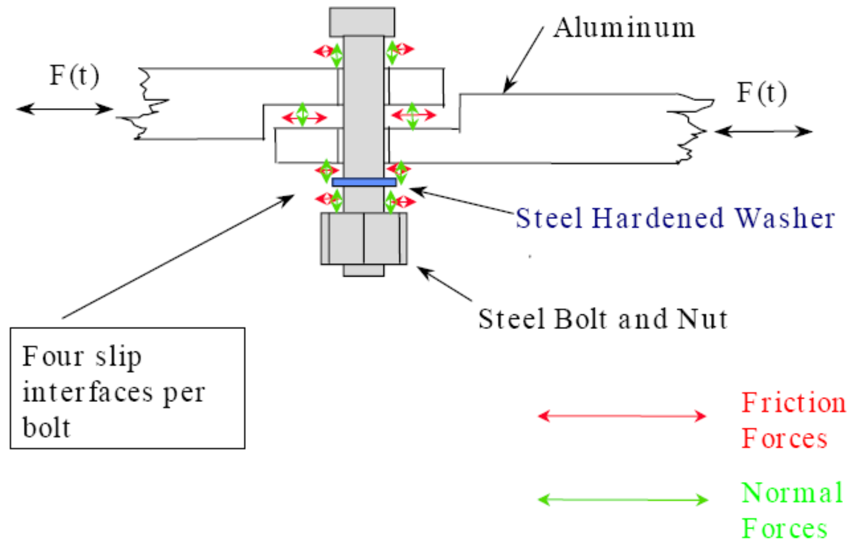
Flux terms provide a mechanism to embed friction models

Schematic diagram of interface:
Can be defined at various levels



Asperities of a rough surface on a nominally flat surface.

Modeling of Multiscale Structural Response



- Model Problem

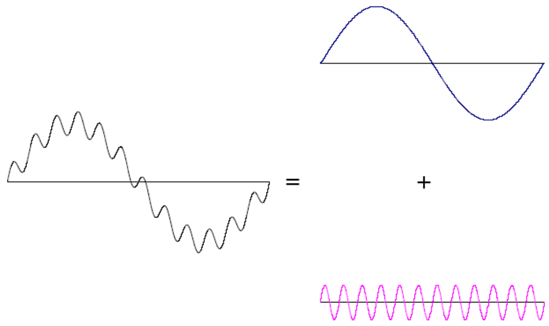
$$\mathcal{L}\boldsymbol{u} = \boldsymbol{f}$$

- Weak Form

$$(\boldsymbol{w}, \mathcal{L}\,\boldsymbol{u}) = (\boldsymbol{w}, \boldsymbol{f})$$

- Scale Decomposition

$$\boldsymbol{u} = \bar{\boldsymbol{u}} + \boldsymbol{u}' \qquad \boldsymbol{w} = \bar{\boldsymbol{w}} + \boldsymbol{w}'$$



- Multiscale Weak Form

$$(\bar{\boldsymbol{w}} + \boldsymbol{w}', \mathcal{L}(\bar{\boldsymbol{u}} + \boldsymbol{u}')) = (\bar{\boldsymbol{w}} + \boldsymbol{w}', \boldsymbol{f})$$

Multiscale Structural Response (cont'd)

- Coarse Scale Problem

$$(\bar{\boldsymbol{w}}, \mathcal{L}(\bar{\boldsymbol{u}} + \boldsymbol{u}')) = (\bar{\boldsymbol{w}}, \boldsymbol{f})$$

- Fine Scale Problem

$$(\boldsymbol{w}', \mathcal{L}(\bar{\boldsymbol{u}} + \boldsymbol{u}')) = (\boldsymbol{w}', \boldsymbol{f})$$

- Fine Scale Solution

$$\boldsymbol{u}' = -\boldsymbol{\tau}\boldsymbol{r} \qquad \text{where} \qquad \boldsymbol{r} = \mathcal{L}\,\bar{\boldsymbol{u}} - \boldsymbol{f}$$

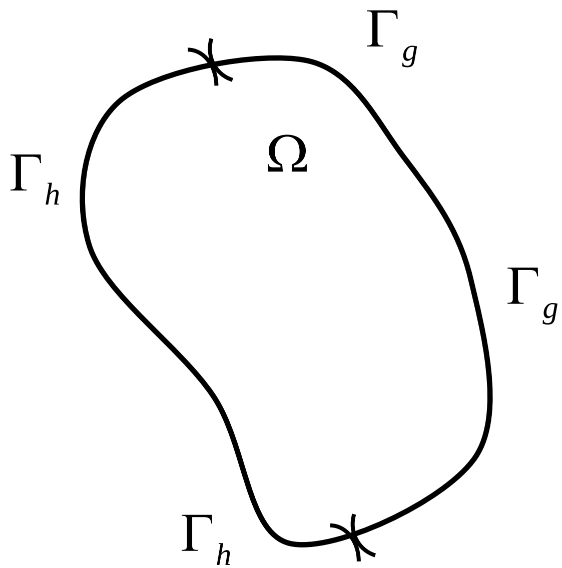
- Modified Coarse Problem

$$(\bar{\boldsymbol{w}}, \mathcal{L}\,\bar{\boldsymbol{u}}) + (\mathcal{L}^{*}\bar{\boldsymbol{w}}, \boldsymbol{\tau}\,\mathcal{L}\bar{\boldsymbol{u}}) = (\bar{\boldsymbol{w}}, \boldsymbol{f}) + (\mathcal{L}^{*}\bar{\boldsymbol{w}}, \boldsymbol{\tau}\,\boldsymbol{f})$$

Continuous and Discontinuous Galerkin Methods

- Standard "Continuous" Weak From

$$\int_{\Omega} \left[\operatorname{div} \boldsymbol{\sigma} + \boldsymbol{f} \right] \cdot \boldsymbol{w} \, d\Omega + \int_{\Gamma_h} \left[\boldsymbol{h} - \boldsymbol{\sigma n} \right] \cdot \boldsymbol{w} \, d\Gamma = 0$$



$$\sum_e \int_{\Omega^e} \left[-\boldsymbol{\sigma} \cdot \nabla \boldsymbol{w}^h + \boldsymbol{f} \cdot \boldsymbol{w}^h \right] d\Omega + \sum_e \int_{\Gamma_e} \boldsymbol{\sigma n} \cdot \boldsymbol{w}^h d\Gamma$$

$$+ \sum_e \int_{\Gamma_h \cap \Gamma_e} \left[\boldsymbol{h} - \boldsymbol{\sigma n} \right] \cdot \boldsymbol{w}^h d\Gamma = 0$$

Continuous and Discontinuous Galerkin Methods

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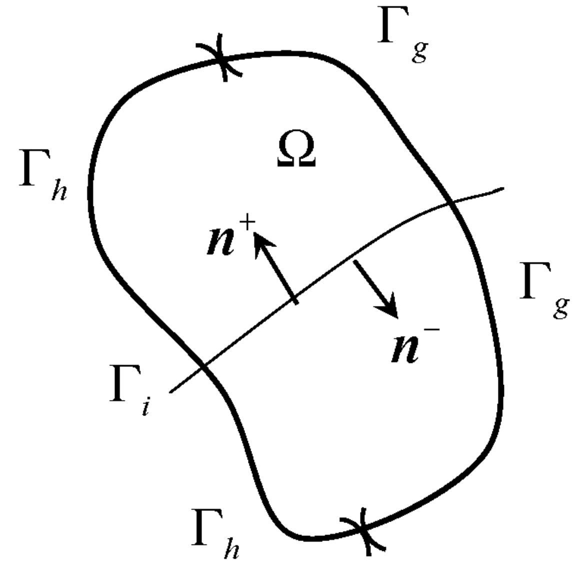


$$\sum_e\int_{\Omega^e}\left[-\boldsymbol{\sigma}\cdot\nabla\boldsymbol{w}^h+\boldsymbol{f}\cdot\boldsymbol{w}^h\right]d\Omega+\sum_e\int_{\Gamma_e}\boldsymbol{\sigma}\boldsymbol{n}\cdot\boldsymbol{w}^h d\Gamma$$

$$+\sum_e\int_{\Gamma_h\cap\Gamma_e}\left[\boldsymbol{h}-\boldsymbol{\sigma}\boldsymbol{n}\right]\cdot\boldsymbol{w}^h d\Gamma=0$$

$$\Gamma_{eh}=\Gamma_e\cap\Gamma_h$$

$$\Gamma_{ei}=\Gamma_e\cap\Gamma_i$$

$$\Gamma_{eh}\cap\Gamma_{ei}=\phi$$

- "Discontinuous at Interface" ⇨ Jump Terms

$$-\sum_e\int_{\Omega^e}\boldsymbol{\sigma}\cdot\nabla\boldsymbol{w}^h\,d\Omega+\sum_e\int_{\Omega^e}\boldsymbol{f}\cdot\boldsymbol{w}^h\,d\Omega+\sum_e\int_{\Gamma_{eh}}\boldsymbol{h}\cdot\boldsymbol{w}^h d\Gamma$$

$$+\sum_e\int_{\Gamma_{ei}}\boldsymbol{\sigma}\boldsymbol{n}\cdot\boldsymbol{w}^h d\Gamma=0\qquad\forall\ \boldsymbol{w}^h\in V^h$$

Interface Stabilization

$$-\sum_e \int_{\Omega^e} \boldsymbol{\sigma} \cdot \nabla \boldsymbol{w}^h \, d\Omega + \sum_e \int_{\Omega^e} \boldsymbol{f} \cdot \boldsymbol{w}^h \, d\Omega + \sum_e \int_{\Gamma_{eh}} \boldsymbol{h} \cdot \boldsymbol{w}^h d\Gamma$$

$$+ \sum_e \int_{\Gamma_i} \boldsymbol{\sigma n} \cdot \boldsymbol{w}^h d\Gamma - \sum_i \int_{\Gamma_i} \left[\boldsymbol{\sigma n}^+ + \boldsymbol{\sigma n}^- \right] \cdot \overline{\boldsymbol{w}}^{h-} d\Gamma \; = \; 0$$

- $\sum_e \int_{\Gamma_{ei}} \boldsymbol{\sigma n} \cdot \boldsymbol{w}^h d\Gamma = \sum_i \int_{\Gamma_i^+} \boldsymbol{\sigma n}^+ \cdot \boldsymbol{w}^{h+} d\Gamma + \sum_i \int_{\Gamma_i^-} \boldsymbol{\sigma n}^- \cdot \boldsymbol{w}^{h-} d\Gamma \equiv$ jump term
- $\overline{\boldsymbol{w}}^h \equiv \left(\boldsymbol{w}^{h+} + \boldsymbol{w}^{h-} \right) / 2 \equiv$ average of variational displacement along Γ_i

Interface Stabilized Form

$$-\sum_e \int_{\Omega^e} \boldsymbol{\sigma} \cdot \nabla \boldsymbol{w}^h \, d\Omega + \sum_e \int_{\Omega^e} \boldsymbol{f} \cdot \boldsymbol{w}^h \, d\Omega + \sum_e \int_{\Gamma_{et}} \boldsymbol{h} \cdot \boldsymbol{w}^h d\Gamma$$

$$+ \frac{1}{2} \sum_i \int_{\Gamma_i^+} \boldsymbol{\sigma n}^+ \cdot \left[\boldsymbol{w}^{h+} - \boldsymbol{w}^{h-} \right] d\Gamma + \frac{1}{2} \sum_i \int_{\Gamma_i^-} \boldsymbol{\sigma n}^- \cdot \left[\boldsymbol{w}^{h-} - \boldsymbol{w}^{h+} \right] d\Gamma = 0$$

Error Estimation

- Explicit Error Estimation

Fine Scale Solution: $\boldsymbol{u}' = -\boldsymbol{\tau}\boldsymbol{r} = -\boldsymbol{\tau}[\mathcal{L}\bar{\boldsymbol{u}} - \boldsymbol{f}]$ $\quad (*)$

Solve coarse problem ⇨ Substitute the nodal values for $\bar{\boldsymbol{u}}$ in $(*)$

- Implicit Error Estimation

Fine Scale Problem: $(\boldsymbol{w}', \mathcal{L}(\boldsymbol{u}')) = (\boldsymbol{w}', \boldsymbol{f} - \mathcal{L}(\bar{\boldsymbol{u}}))$ $\quad (**)$

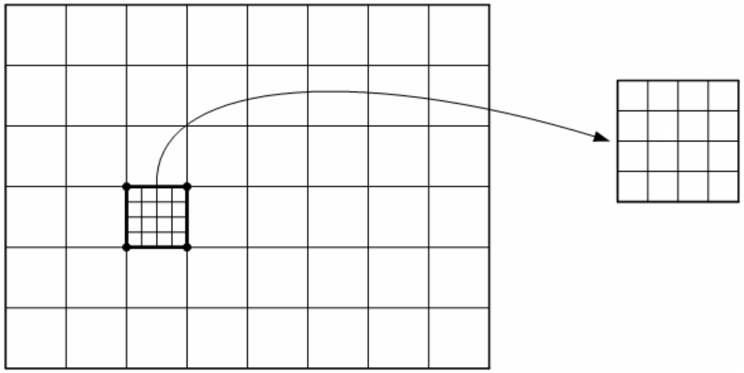
Substitute the nodal values for $\bar{\boldsymbol{u}}$ in $(**)$ and solve it.

Construct patches to solve local / element level problems

- Element based approach
- Node based approach

Error Estimation (cont'd)

Element Based Approach



$$(\psi w', \mathcal{L}(u')) = (\psi w', f - \mathcal{L}(\bar{u}))$$

- Need flux boundary conditions

$\psi = 1$ for given element e; $\psi = 0$ outside e

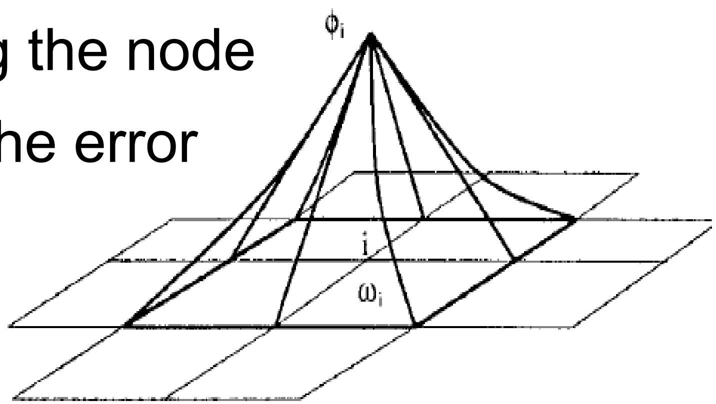
Node Based Approach

$$(\psi w', \mathcal{L}(u')) = (\psi w', f - \mathcal{L}(\bar{u}))$$

- Need to determine size of patch feeding the node
  - ⇨ Elements within the radius feed into the error associated with node

\+ Better accuracy

− Computationally expensive



$\psi = 1$ for node n; $\psi = 0$ at distance $\geq r$

Explicit Error Estimation for Elasticity

Standard L2 error norm

$$L_2 \boldsymbol{e} = \left[\int_\Omega \left(u^h - u^{\text{exact}} \right)^{\mathrm{T}} \left(u^h - u^{\text{exact}} \right) d\Omega \right]^{1/2}$$

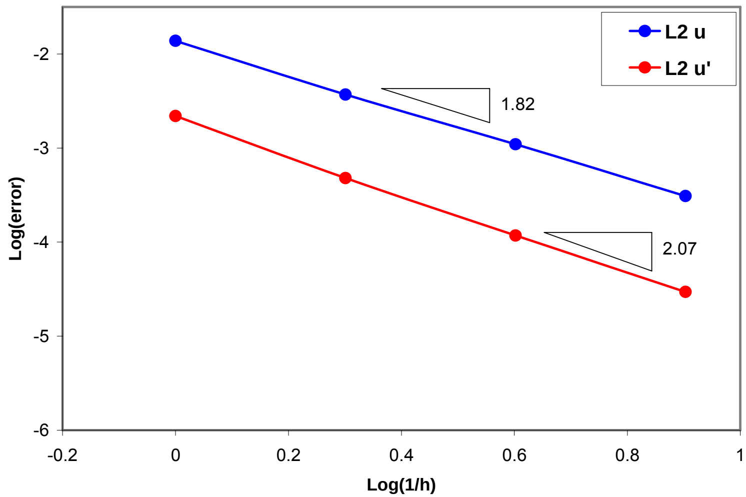
L2 error norm from fine-scales

$$\boldsymbol{e} \cong \boldsymbol{u}' = -\tau \left[\boldsymbol{f} - \mathcal{L}\, \overline{\boldsymbol{u}} \left(\boldsymbol{u}' \right) \right]$$

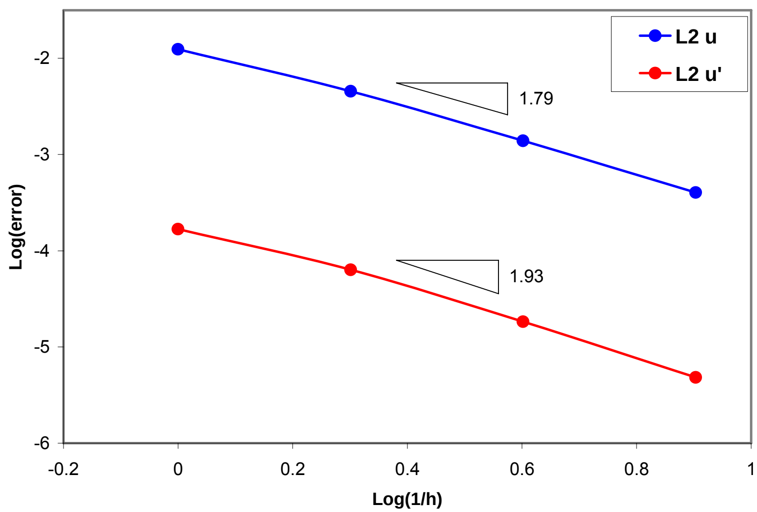
$$L_2 \boldsymbol{e} = \frac{1}{2} \sqrt{\left(\boldsymbol{e} \cdot \boldsymbol{e} \right)}$$

$$H^1 \boldsymbol{e} = \frac{1}{2} \sqrt{\left(\nabla \boldsymbol{e} \cdot \nabla \boldsymbol{e} \right)}$$

4-node quads



3-node triangles



Concluding Remarks

The meso-to-micro scale response of the interface is mathematically nested into the meso-to-macro scale response of the system.

A-posteriori error estimator is naturally built into the framework.

Modeling interface as a discontinuity blends ideas from CG and DG methods ⇨ provides a variationally consistent method for embedding interface models.

Points for Discussion:

Significance of the "Interface" Nonlinear Dynamic Effects.

Should Verification and Validation be an integral part of the analysis strategy?

Do we have the right mathematical framework for the analysis of systems that are multiphysics and multiscale in nature?