Emergent properties in interface mechanical problems: A paradigm of organized complexity

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Outline

1. Organized complexity & emergent properties in interface problems
2. An example in contact mechanics
3. An example in fracture mechanics
4. A multiphysics application: photovoltaics
5. Ongoing research topics
Acknowledgements

AvH Fellowship in Hannover 2010-2011

Vigoni 2010

FIRB Future in Research 2010

ERC Starting Grant IDEAS 2011
Emergent properties in ordered complexity

Classical examples of complex systems:

- Earthquakes
- Climate systems
- Living systems
- Social systems
- Economical systems

Organized complexity resides in the non-random, or correlated, nonlinear interaction between the parts of a system.

Coordinated systems exhibit emergent properties not easily predictable from the properties of their constituents.
Organized complexity in interface problems

Contact mechanics
- Scaling of contact properties (friction coefficient, adhesion, thermal contact conductance)

Fracture mechanics & fatigue
- Scaling of strength and toughness

Metamaterials
- Scaling of optical and electromagnetic properties

Common features:
Nonlinear relations; multiple scales; fractality / hierarchy
Two examples of emergent properties

(1) Interface thermal resistance due to roughness

(2) Flaw-tolerance of hierarchical polycrystalline materials

**Aim:** study of the emergence of macro-properties from micro-properties (bottom-up approach)

**Methods:** nonlinear mechanics, computational methods, optimization
Interface contact conductance

Self-affinity

5−2D

1/Δ

1/δ

ω (m⁻¹)
Fractality

• Self-affinity (even of a random nature)
• Non integer dimension

Examples:

<table>
<thead>
<tr>
<th>dim. $1 \div 2$</th>
<th>dim. $2 \div 3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>- mountains profiles</td>
<td>- sponge-cloths</td>
</tr>
<tr>
<td>- clouds profiles</td>
<td>- foams</td>
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<tr>
<td>- coastlines profiles</td>
<td>- brain folds</td>
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<td>- river patterns</td>
<td>- universe mass</td>
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<td>- diffusion fronts</td>
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<td>- moon craters</td>
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<td>- arterial systems</td>
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</table>
The contact conductance is proportional to the contact stiffness (Barber, PRS 2003; Paggi and Barber, IJHMT 2011):

\[ C = -\frac{2}{\rho E} \frac{dp}{dd} \]

\[ \tilde{C} \equiv C \rho \Delta \]

\[ \tilde{d} = \frac{d}{\sqrt{m_0}} \]

\[ \tilde{p} = \frac{p \Delta}{E \sqrt{m_0}} \]

\[ \tilde{C} = \tilde{p}^\beta \Phi_2 \left( \frac{\delta}{\Delta}, \frac{L}{\Delta}, D \right) \]

\[ \tilde{p} = A (\tilde{d}_0 - \tilde{d})^{\frac{1}{1-\beta}} \]
**Inverse problem**

**Problem:** extract the interface contact conductance (nonlinear mesoscopic property) from global stiffness data (emergent macroscopic property)

**Macroscopic curvature effects**

**Finite size effects** (boundary effects)
Global stiffness by varying the punch size $L$

Rough punch composed of $n \times n$ RMD patches

$n=4$

$n \sim L/\Delta$
Proposed solution strategy

1. Solve the contact problem between the rough punch and the half-plane (global solution)

2. Imagine the surface as a collection of nonlinear punches whose constitutive equation is:

   \[ \tilde{p} = A(\tilde{d}_0 - \tilde{d})^{1-\beta} \]

3. Solve the contact problem and find the optimal values of the 3 free parameters to match the global solution
Result of the optimization problem
Optimal solution independent of BCs (model-independent interface contact conductance):

\[ \tilde{d}_0 = 4.83 \]
\[ \beta = 0.80 \]
\[ \Phi_2 = 13 \]

\[ \tilde{C} = 13 \tilde{\rho}^{0.8} \]
\[ \tilde{\rho} = 0.01(4.83 - \tilde{d})^5 \]
Hierarchical polycrystalline materials

How do the strength depend on the interaction between interfaces at different scales?

Is there any emergence of an optimal configuration to tolerate defects (flaw tolerance)?

Mimicking nature: interfaces at different scales

Hard Tissues:
- Trabecular bone
- Cortical bone
- Woven bone
- Cementum
- Dentin
- Enamel

Constituents:
- COLLAGEN
- APATITE
- WATER

Characterisation:
- ultrasound
- micro-mechanical testing
- SAM
- AFM

Characterisation scales:
- nm
- μm
- mm

Microstructural levels:
- nanostructure
- submicrostructure
- microstructure
- macrostructure

Imaging techniques:
- SEM
- AFM
- X-ray μCT
- IMAGING
The Cohesive Zone Model

Open issues:
(1) How to relate the shape of the CZM to physics?
(2) How to take into account the finite thickness of real interfaces?
A nonlocal CZM for finite thickness interfaces

\[ \sigma = \frac{E_2}{l_2} \frac{1 - D^\alpha}{D^\alpha} g_N \]


Shape of the CZM by varying \( \alpha \)  
Damage evolution

**Copper (fcc crystal)**

\[2l_2 + l_1 = 43.38 \text{ Å}, \ E_1 = E_2 = 110 \text{ GPa}\]

\[\delta_e = 0.2 \text{ Å}, \ \delta_c = 8.0 \text{ Å}, \ \alpha = 0.9\]

**Shape of the CZM**

**Comparison with MD**
Weak form

\[ \int (\nabla \delta \mathbf{u})^T \boldsymbol{\sigma} \, dV = \int \delta \mathbf{u}^T \mathbf{f} \, dS + \int \delta \mathbf{g}^T \mathbf{t} \, dS \]

\[ \int q \, \nabla \delta T \, dV = \int \rho c_V \dot{T} \delta T \, dV + \int q_n \delta T \, dS + \int q_s \delta T \, dS \]

\[ G_{\text{int}} = \int_{S} (\delta g_T, \delta g_N, \delta \Delta T) \begin{pmatrix} \tau \\ \sigma \\ q_s \end{pmatrix} \, dS \]

\[ \Delta G_{\text{int}} = \int_{S} (\delta g_T, \delta g_N, \delta \Delta T) \mathbf{C} \begin{pmatrix} g_T \\ g_N \\ \Delta T \end{pmatrix} \, dS \]

\[ \mathbf{C} = \begin{bmatrix} \frac{\partial \tau}{\partial g_T} & \frac{\partial \tau}{\partial g_N} & 0 \\ \frac{\partial \sigma}{\partial g_T} & \frac{\partial \sigma}{\partial g_N} & 0 \\ \frac{\partial q_s}{\partial g_T} & \frac{\partial q_s}{\partial g_N} & \frac{\partial q_s}{\partial \Delta T} \end{bmatrix} \]
Finite element implementation in FEAP

Application to polycrystalline materials

Grain size

Fracture energy

Interface thickness
3D Virtual tensile test

Effect of hierarchy on anisotropy
Effect of hierarchy on strength

$$\frac{\sigma}{\sigma_{\text{max}}}$$

level 1

level 2

$$\frac{g_N}{g_{N_c}}$$

Fictitious crack tip

Real crack tip

$\gamma_{\text{CZM}}$
Effect of hierarchy on strength

\[ \frac{\sigma N}{\sigma N_c^{\text{level 1}}} \]

\[ \sigma_p^{\text{level 1}} / G_c^{\text{level 2}} \]

\[ l_{\text{CZM}} = \text{process zone size for the grain boundaries of the level 2} \]

\[ d^{\text{level 1}} = \text{diameter of the rods (level 1)} \]
Interfaces in multiphysics

Thermal field
Elastic field
Electric field
Thermo-electric field
Electro-elastic field
Thermo-elastic field
Electro-thermo-elastic field
A multiscale solution strategy

Macro-model:
Multi-layered plate (homogeneous cells)

Micro-model:
Polycrystalline Si cells with grain boundaries

M. Paggi, M. Corrado, M.A. Rodriguez (2013)
Composite Structures, 95:630-638.
Micro-crack pattern in Silicon cells

Simply supported plate subjected to a pressure of 5400 Pa
Electrically inactive areas

Simply supported plate subjected to a pressure of 5400 Pa
Centre for Risk Analysis and Durability of Structures

3D confocal-interferometric profilometer (LEICA, DCM 3D)

SEM (ZEISS, EVO MA15)

Testing stage (DEBEN, 5000S)

Thermocamera (FLIR, T640bx)

Photocamera for EL tests (PCO, 1300 Solar)

Testing machine & thermostatic chamber (Zwick/Roell, Z010TH)

Server HP Proliant DL585R07
Ongoing research topics

Determination of interface properties via inverse analysis of microstructure evolution of polycrystals during a tensile tests

(with Dr. M. Schaper, Lebniz University Hannover)

SEM image with superimposed digital image correlation of the strain field
Ongoing research topics

Quantitative analysis of EL images via fractal concepts and spectral methods

(with Ing. I. Berardone & ISFH)

EL image of a microcracked Silicon cell
Ongoing research topics

Thermoelastic cohesive zone models (with Dr. A. Sapora)
Ongoing research topics

Nonlinear crack propagation in dynamics
(with Dr. M. Corrado)

\( v = 2 \text{ m/s} \)