Finite Element Mapping for Spring Network Representations of the Mechanics of Solids

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• Spring network method
  – Atomistic & mesoscopic models
• Finite element mapping procedure for defining spring network models
  – Regular grids and unstructured networks
  – Piecewise homogeneous composite media
• Structural parts from short fiber reinforced polymers
  – Properties of local fiber orientational states
• Phase separated block copolymers
  – Problems with constitutive equations
• Conclusions and perspectives
Atomic Lattice Models

- **Elasticity and lattice dynamics of crystals**
  - Born & von Kármán (1910), Born (1912), Born & Huang (1954)

Simple Cubic Lattice

Diamond Crystal Structure

- **Vibration of long chain molecules**
  - Kirkwood (1939)

\[
U = \frac{1}{2} \alpha \sum (\Delta l)^2 + \frac{1}{2} \beta \sum (\Delta \varphi)^2
\]

- **Forcefield for molecular level simulations**
2D Spring Network Models

- **Isotropic systems**
  - Bond length & bond angle terms
  \[ U = \frac{1}{2} \alpha \sum_{\text{bonds}} (\Delta l)^2 + \frac{1}{2} \beta \sum_{\text{angles}} (\Delta \varphi)^2 \]
  - A limited range of \(-1 \leq \nu \leq \frac{1}{3}\)

- **Anisotropic systems**
  \[ U = \frac{1}{2} \sum_{\text{bonds}} \alpha (\Delta l)^2 + \frac{1}{2} \sum_{\text{angles}} \beta (\Delta \varphi)^2 \]
  - No systematic framework

- **Frequently used for fracture simulation**
  - e.g., power law acoustic emission
  - Numerically efficient
  - Sequential bond removal

\[ \{\alpha, \beta\} \Rightarrow \mathbf{C} \]
3D Spring Network Models

• Isotropic materials
  – Bond length & bond angle terms
    \[ U = \frac{1}{2} \sum_{\text{bonds}} \alpha (\Delta l)^2 + \frac{1}{2} \sum_{\text{angles}} \beta (\Delta \varphi)^2 \]
  – Nearest neighbor simple cubic lattice
    Poisson’s ratio \( v = 0 \)
  – Including next nearest neighbors
    still problems with rotational invariance

• Anisotropic materials
  – In general, 21 independent \( C_{ik} \) constants
  – No systematic framework

• Concerns regarding physical significance
Finite Element Approach

- **Dividing continuum in small discrete elements**
  - Courant (1943)
  - Nodal displacements \( \mathbf{d}^T = \{u_1, \ldots, u_N\} \)
  - System strain energy \( U = \frac{1}{2} \mathbf{d}^T \mathbf{K} \mathbf{d} \)

- **Systematic approach**
  - Turner, Clough, Martin, and Topp (1956)
  - Later became known as the Finite Element Method

- **Element formulation**
  - Displacement vector \( \mathbf{d}^e_T = \{u_1, \ldots, u_M\} \)
  - Strain energy \( U^e = \frac{1}{2} \mathbf{d}^e_T \mathbf{K}^e \mathbf{d}^e \)

- **Assembly**
  - From \( U = \Sigma U^e \), one obtains \( \mathbf{K} = \Sigma \mathbf{K}^e \)
Element Level

- **Element stiffness matrix $K^e$**
  - Symmetric dense 8x8 matrix
  - Geometry: shape & size
  - Material: elastic constants $C$
- **Consistency**
  - For any uniform strain $\varepsilon$
    \[ U^e = \frac{1}{2} V \varepsilon C \varepsilon \]
  - Define as $u_a = \varepsilon r_a$
  - Compose $d^e = \{u_1, u_2, u_3, u_4\}$
  - The identity
    \[
    \frac{1}{2} V \varepsilon C \varepsilon \equiv \frac{1}{2} d^e \mathbf{K}^e d^e
    \]
    always holds
Assembly Level

• Assembled stiffness matrix $K$
  – Symmetric sparse 18x18 matrix
  – Consists of 2x2 blocks $K_{ab}$
  – $K_{ab} = 0$ if $a$ & $b$ doesn’t interact
  – All $K_{5b}$ & $K_{a5}$ are fully assembled

• Total strain energy
  – $U = \frac{1}{2} d^T K d$
  – where $d^T = \{u_1, \ldots, u_9\}$

• Translational invariance
  – For any row (or column)
    $$K_{aa} = - \sum_{a \neq b} K_{ab}$$
Spring Network Representation

• **Spring stiffness matrix**
  – Displacement vector $d^s T = \{u_1, u_2\}$
  – Elastic energy $U^s = \frac{1}{2} d^s T K^s d^s$
  – Spring stiffness matrix
    $$K^s = \begin{bmatrix}
    \kappa^s & -\kappa^s \\
    -\kappa^s & \kappa^s
    \end{bmatrix}$$
  – where $\kappa^s$ is a 2x2 matrix

• **Assembly**
  – From $U = \Sigma U^s$, one has $K = \Sigma K^s$
  – Translational invariance
Finite Element Mapping

• Parent serendipity family rectangular elements
  – A 2x2 assembly
  – Node 5 interacts with all 9 nodes
  – 2x2 blocks $K_{5a}$ are fully assembled
    • will never receive further contributions
    • are thus representative for larger assemblies

• General mapping procedure
  – Use off-diagonal $K_{5a}$ to define spring matrices $\kappa^s$
    $$\kappa^s_{5a} \equiv K_{5a}$$

• For infinite systems
  assembled FE & spring $K$ will always be the same
2D isotropic triangular LSM

- Imposed plain strain material behavior
  - with two Lame constants $\lambda$ & $\mu$
  - A single distinct spring with $\kappa^s$
  - which is common to 2 triangles
- An assembly of 2 adjacent triangles
  - A total of 8 degrees of freedom
  - An 8x8 assembled matrix $K$
  - By using the mapping procedure, we extract

$$
\kappa' = \frac{1}{2\sqrt{3}} \begin{pmatrix}
3\lambda + 5\mu & 0 \\
0 & \mu - \lambda
\end{pmatrix}
$$

- For a special case of solids with $\lambda = \mu$
  - Classical scalar LSM, derived by Hrennikoff (1941), Ashurst & Hoover (1976)
Serendipity Family Linear Brick Elements

- **81x81 assembled stiffness matrix \( K \)**
  - Central node \( a \) interacts with all nodes
  - 3x3 blocks \( K_{ab} \) are fully assembled
  - Use them to define spring matrices \( \kappa \)

- **Isotropic solids**
  - Cubic bricks, Lame constants \( \lambda \) & \( \mu \)
  - There are 3 distinct, basic springs

\[
\begin{array}{c|c|c|c}
\hline
\kappa_1 & \frac{4}{9}(\lambda + \mu) & \frac{1}{18}(5\lambda + 8\mu) & \frac{1}{36}(4\lambda + 7\mu) \\
\kappa_2 = \kappa_3 & -\frac{2}{9}(\lambda + \mu) & -\frac{1}{18}(\lambda - 2\mu) & -\frac{1}{72}(\lambda - 5\mu) \\
\end{array}
\]
Composite Media

• Composite finite elements
  – On the basis of the integral definition
    \[ K^e \equiv \int (B^T DB) dV \Rightarrow fK^e_{\text{inc}} + (1 - f)K^e_{\text{mat}} \]
  – \( B^e \) is geometrical, strain-displacement matrix
  – \( D^e \) is material, stress-strain matrix
  – Exact for linear elements (\( B^e = \text{const} \))

• Composite springs
  – On the basis of the series connection premise
    \[ \frac{1}{\kappa^s_{\alpha}} = \frac{f}{\kappa_{\alpha}^{\text{inc}}} + \frac{1-f}{\kappa_{\alpha}^{\text{mat}}} \]
Piecewise Homogeneous Media with Spherical and Cylindrical Inclusions

- **Cubic unit cells**
  - Inclusion fraction $f = 0.5$

- **Periodic cubic grids**
  - Matrix: $E = 3$ GPa, $\nu = 0.35$
  - Inclusions: $E = 70$ GPa, $\nu = 0.2$
  - Serendipity linear bricks
  - $N \times N \times N$ grids, $N$ from 4 to 161
Conclusions and Perspectives

- **Finite element mapping procedure** *(AAG, Phys. Rev. Lett. 034302)*
  - Isotropic and anisotropic media
  - Regular and unstructured networks
  - Exact mapping for any discrete system
  - Appealing opportunities for composite media
    - No meshing
    - Physically motivated local constitutive equations
- **Mixed form formulations, viscoelasticity, plasticity** *(tangent $K_T$), etc.*
- **Nano-structured materials**
  - Complex morphology block copolymers, cell membranes, etc.
  - Linking atomic & mesoscopic scales