Diamonds: Finite Element/Discrete Mechanics schemes with guaranteed optimal convergence

M. Ortiz
California Institute of Technology
In collaboration with: P. Hauret and E. Kuhl

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Outline

• Overview of discrete mechanics for vector problems
• Discrete mechanics in the context of tensor problems
• Diamonds: Finite element/discrete mechanics approximation schemes with guaranteed optimal convergence
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Discrete mechanics

• Aka: Discrete Exterior Calculus (DEC)…
• Reformulation of the field equations of mechanics in which space (and possibly time) are discrete *ab initio*
• The field equations of mechanics retain their form, but:
  – *Are defined on a discrete geometrical space (cell complex)*
  – *Are expressed in terms of discrete differential and integral operators*
• Discrete mechanics enjoys a long tradition in problems of the ‘vector type’, e.g.:
  – *Bossavit (electromagnetism)*
  – *Hipmair (electromagnetism)*
  – *Arnold (also 2d tensor problems such as elasticity)*
  – *Desbrun, Hirani, Kanso, Leok, Marsden, Schröder…*
Geometric mechanics

- The de-Rham differential complex in $\mathbb{R}^3$:

\[ 0 \rightarrow \Omega^0(\mathbb{R}^3)/\mathbb{R} \rightarrow \Omega^1(\mathbb{R}^3) \rightarrow \Omega^2(\mathbb{R}^3) \rightarrow \Omega^3(\mathbb{R}^3)/\mathbb{R} \rightarrow 0 \]

- Differential complex property:

\[ \text{curl} \circ \text{grad} = 0 \]

\[ \text{div} \circ \text{curl} = 0 \]

- Integral identities (Stokes’ theorem):

\[ \int_V \text{div} \alpha \, dV = \int_{\partial V} \alpha \cdot \nu \, dS \]

\[ \int_S \text{curl} \beta \, dS = \int_{\partial S} \beta \cdot dx \]
Geometric mechanics

- Helmholtz-Hodge decomposition:
  \[ \Omega^1(\mathbb{R}^3) \ni \beta = \text{grad} \phi + \text{curl} A + \gamma, \quad \Delta \gamma = 0 \]
  and decomposition \( L^2 \)-orthogonal.

- de Rham cohomology:
  \[
  \begin{align*}
  H^1(\mathbb{R}^3) &= \ker(\text{grad}) \\
  H^2(\mathbb{R}^3) &= \ker(\text{curl}) / \text{im}(\text{grad}) \\
  H^3(\mathbb{R}^3) &= \ker(\text{div}) / \text{im}(\text{curl})
  \end{align*}
  \]

Lemma. (Poincaré) \( H^p(\mathbb{R}^3) = 0 \).

Lemma. \( \{ \gamma, \Delta \gamma = 0 \} \) isomorphic with \( H^3(\mathbb{R}^3) \).

Corollary. \( \Omega^1(\mathbb{R}^3) \ni \beta = \text{grad} \phi + \text{curl} A \).
Model problem – Maxwell’s equations

- Maxwell’s equations for linear materials:

\[ \text{div}(\varepsilon \, E) = \rho \quad \text{(Gauss law)} \]
\[ \text{div}(\mu \, H) = 0 \quad \text{(Gauss law for magnetism)} \]
\[ \text{curl} \, E = -\partial_t (\mu \, H) \quad \text{(Faraday’s law of induction)} \]
\[ \text{curl} \, H = J + \partial_t (\varepsilon \, E) \quad \text{(Ampère’s law)} \]

\[ E \equiv \text{electric field}, \quad H \equiv \text{magnetic field}, \]
\[ \rho \equiv \text{charge density}, \quad J \equiv \text{current density}. \]
\[ \varepsilon \equiv \text{electrical permittivity}, \quad \mu \equiv \text{magnetic permeability}. \]
Discrete mechanics – Cell complexes

- Cell complex:
  \[ C \equiv \{ \text{cells} \} \]
- \( p \)-forms: \( \Omega^p(C) \equiv \{ \omega : E_p \to \mathbb{R}^n \} \)
- Integration:
  \[ \int_{E_p} \omega \equiv \sum_{e_p \in E_p} \omega(e_p)|e_p| \]
Cell complexes – Dual cell complex

Three-dimensional dual complex (A. Hirani, 2003)
Discrete differential complexes

- Discrete de-Rham differential complex: Sequence

\[ 0 \to \Omega^0(C)/\mathbb{R} \to \Omega^1(C) \to \Omega^2(C) \to \Omega^3(C)/\mathbb{R} \to 0 \]

such that: \(\text{curl} \circ \text{grad} = 0, \text{div} \circ \text{curl} = 0\).

\[ \int_V \text{div} \alpha \, dV = \int_{\partial V} \alpha \cdot \nu \, dS, \quad \int_S \text{curl} \beta \, dS = \int_{\partial S} \beta \cdot dx \]

- Example: \(C\) simplicial,

\[
\begin{align*}
\text{grad}u & \equiv \frac{du \otimes dx}{|dx|^2} \\
\text{curl} \beta & \equiv \frac{d(\beta \cdot dx)}{dA} \nu \\
\text{div} \alpha & \equiv \frac{d(\alpha \cdot \nu dA)}{dV} 
\end{align*}
\]
Discrete Maxwell’s equations

- **Continuum (in \( \mathbb{R}^3 \)):**
  \[
  \begin{align*}
  \text{div}(\varepsilon \, E) &= \rho \\
  \text{div}(\mu \, H) &= 0 \\
  \text{curl} \, E &= -\partial_t(\mu \, H) \\
  \text{curl} \, H &= J + \partial_t(\varepsilon \, E)
  \end{align*}
  \]

- **Discrete (on \( C' \)):**
  \[
  \begin{align*}
  \text{div}(\varepsilon \, E) &= \rho \\
  \text{div}(\mu \, H) &= 0 \\
  \text{curl} \, E &= -\partial_t(\mu \, H) \\
  \text{curl} \, H &= J + \partial_t(\varepsilon \, E)
  \end{align*}
  \]

\[
E \in \Omega^1(C'), \quad (\varepsilon \, E) \in \Omega^2(C^*), \quad \rho \in \Omega^3(C^*),
\]

\[
H \in \Omega^1(C^*), \quad (\mu H) \in \Omega^2(C), \quad J \in \Omega^2(C^*),
\]

\[
\varepsilon : \Omega^1(C) \to \Omega^2(C^*), \quad \mu : \Omega^1(C^*) \to \Omega^2(C).
\]
Discrete mechanics – Vector problems

- Continuum and discrete mechanics are identical, with the discrete field equations expressed on cell complexes in terms of discrete differential operators
- Discrete mechanics works with the field equations directly, bypasses the usual variational detour
- Discrete mechanics schemes satisfy conservation laws exactly (Stokes’ theorem), possess a Helmholtz-Hodge decomposition
- Discrete mechanics schemes have been successfully applied to vector problems such as electromagnetism
- Are discrete mechanics schemes inherently superior?
- Do they work for solid mechanics (tensor problems)?
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Geometric linear elasticity

\[ 0 \rightarrow \Omega^0(\mathbb{R}^3)/\text{RM} \rightarrow \Omega^3(\text{sym } \mathbb{R}^{3 \times 3}) \rightarrow \Omega^3(\text{sym } \mathbb{R}^{3 \times 3}) \rightarrow \Omega^0(\mathbb{R}^3)/\text{RM} \rightarrow 0 \]

- **The Kröner differential complex:**

<table>
<thead>
<tr>
<th>Domain and range</th>
<th>'nabla' expression</th>
<th>Coordinate expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>Def : ( \Omega^0(\mathbb{R}^3) \rightarrow \Omega^3(\text{sym } \mathbb{R}^{3 \times 3}) )</td>
<td>( \nabla^S \equiv (\nabla + \nabla^T)/2 )</td>
<td>( (\text{Def } u)<em>{ij} = (u</em>{i,j} + u_{j,i})/2 )</td>
</tr>
<tr>
<td>Inc : ( \Omega^3(\text{sym } \mathbb{R}^{3 \times 3}) \rightarrow \Omega^3(\text{sym } \mathbb{R}^{3 \times 3}) )</td>
<td>( \nabla \times (\cdot \times \nabla) )</td>
<td>( (\text{Inc } \epsilon)<em>{ij} = \epsilon</em>{kl, mn} \epsilon_{km} \epsilon_{ln} j )</td>
</tr>
<tr>
<td>Div : ( \Omega^3(\text{sym } \mathbb{R}^{3 \times 3}) \rightarrow \Omega^0(\mathbb{R}^3) )</td>
<td>( \nabla \cdot )</td>
<td>( (\text{Div } \sigma)<em>i = \sigma</em>{ij,j} )</td>
</tr>
</tbody>
</table>

- Inc \( \circ \) Def = 0, \( \text{Div} \circ \text{Inc} = 0 \)

- **The isotropic differential complex:**

\[ \begin{align*}
\Omega^0(\mathbb{R}^3) & \rightarrow \Omega^3(\mathbb{R}) \\
\Omega^3(\mathbb{R}) & \rightarrow \Omega^3(\mathbb{R}) \\
\Omega^0(\mathbb{R}^3) & \rightarrow \Omega^0(\mathbb{R}^3)
\end{align*} \]

\[ \text{grad } p = \text{Div } (p \, g^\#), \quad \text{div } u = g^\# \cdot \text{Def } u \]
Geometric linear elasticity

- Compressible linear elasticity:

\[- \text{Div } (2\mu \text{Def } u) - \text{div } (\lambda \text{grad } u) = f + t, \quad \text{in } \Omega \cup \Gamma_N\]
\[u = 0, \quad \text{on } \Gamma_D\]

- Incompressible linear elasticity ($\lambda \uparrow +\infty)$:

\[- \text{Div } (2\mu \text{Def } u) - \text{grad } p = f + t, \quad \text{in } \Omega \cup \Gamma_N\]
\[\text{div } u = 0, \quad \text{in } \Omega\]
\[u = 0, \quad \text{on } \Gamma_D\]
Discrete linear elasticity

- Discrete linear elasticity schemes can be obtained by defining discrete counterparts to the continuum Kröner and isotropic differential complexes, keeping the field equations unchanged.
- Does discrete mechanics guarantee superior numerical schemes?
- Two counterexamples!
Counterexample I

- $C = S_h \equiv$ simplicial complex of size $h$.
- Discrete Kröner differential complex:

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<td>$(\text{Div } \sigma)(N) = \frac{1}{3} \sum_{F \supset N}</td>
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- Verify: $\text{Inc} \circ \text{Def} = 0$, $\text{Div} \circ \text{Inc} = 0$
- The isotropic differential complex:

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<td>$\text{grad} : \Omega^3(S_h; \mathbb{R}) \rightarrow \Omega^0(S_h; \mathbb{R}^3)$</td>
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- Simplicial interpolation! Locking!
Counterexample II

- $\text{Grad} : \Omega^0(\mathcal{S}_h, \mathbb{R}^3) \times \Omega^0(\mathcal{S}_h^*, \mathbb{R}^3) \rightarrow \Omega^2(\mathcal{S}_h, \mathbb{R}^{3 \times 3})$: Two columns of $\text{Grad}$ computed from $F$; third column of $\text{Grad}$ computed from $*F$.

- Can complete differential complex $\text{Def} \rightarrow \text{Inc} \rightarrow \text{Div}$ such that $\text{Inc} \circ \text{Def} = 0$ and $\text{Div} \circ \text{Inc} = 0$. 
Counterexample II

• However: \((\text{Grad } u)([F, *F]) = \int_{[F, *F]} \nabla u_h \, dx\),
  where \(u_h \equiv\) interpolant of \(u\) linear on faces of \([F, *F]\).

• Same situation as \(Q_1/P_0\): checkerboard modes!
Discrete linear elasticity

• Discrete mechanics is no guarantee of superior performance in tensor problems

• Examples of non-convergent discrete linear elasticity schemes:
  – Simplicial interpolation can be expressed as discrete elasticity scheme, locks in incompressible limit
  – Certain discrete differential complexes result in checkerboard modes

• These difficulties (locking, checkerboarding) are typical of tensor problems and do not arise in vector problems
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Diamonds

Arbitrary simplicial complex

Simplicial complex $S_h$

Diamond complex $D_h$
Diamonds

Parent tetrahedron

Diamond cell
Diamonds

- Discrete Kröner differential complex:

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- Verify: $\text{Inc} \circ \text{Def} = 0, \quad \text{Div} \circ \text{Inc} = 0$

- Discrete metric: $g^\# \equiv$ piecewise constant on $\mathcal{D}_h$

- The isotropic differential complex:

\[
\begin{align*}
\Omega^0_*(\mathcal{D}_h; \mathbb{R}^3) & \to \Omega^3_*(\mathcal{D}_h; \mathbb{R}) & \to \Omega^3_*(\mathcal{D}_h; \mathbb{R}) & \to \Omega^0_*(\mathcal{D}_h; \mathbb{R}^3), \\
\text{grad } p & = \text{Div}(p \ g^\#), & \text{div } u & = g^\# \cdot \text{Def } u \\
(\text{constant pressure over diamond cells})
\end{align*}
\]
Diamonds – Convergence analysis

- Express discrete problem in variational form:

\[ V_h = \{ u_h, \text{ piecewise affine on } S_h \} \]
\[ P_h = \{ u_h, \text{ piecewise constant on } D_h \} \]

\[
\begin{align*}
  a(u_h, v_h) + b(v_h, p_h) &= f(v_h), \quad \forall v_h \in V_h \\
  b(u_h, q_h) &= 0, \quad \forall q_h \in P_h
\end{align*}
\]

**Proposition** For any initial simplicial mesh, \( \exists \beta > 0 \) independent of \( h \) such that the inf-sup condition

\[
\inf_{q_h \in P_h \setminus \{0\}} \sup_{v_h \in V_h \setminus \{0\}} \frac{b(v_h, q_h)}{\|q_h\|_0,\Omega \|v_h\|_1,\Omega} \geq \beta_h > 0
\]

is satisfied with \( \beta_h \geq \beta \) for all \( h > 0 \).
Diamonds – Convergence analysis

- Proof based on Stenberg’s *macroelement* method.
- A *macroelement* is a cell complex.
- Two simplicial macroelements are *equivalent* if they can be mapped into each other by a continuous mapping that is affine on every simplex.
Diamonds – Convergence analysis

**Theorem** [Stenberg] Suppose that there exist macroelement equivalence classes \( \{ \mathcal{E}_i, i = 1, 2, ..., q \} \) and a finite cover \( \mathcal{M}_h \) of macroelements such that:

i) \( \forall M \in \mathcal{E}_i, i = 1, 2, ..., q, q_h \in P_h(M), \)

\[
\int_M q_h \, \text{div} \nu_h = 0 \quad \forall \nu_h \in V^0_h(M) \Rightarrow q_h = \text{const.}
\]

ii) Each \( M \in \mathcal{M}_h \) belongs to one of the classes \( \mathcal{E}_i \).

iii) Each face \( F \) is contained in the interior of macroelements \( M \in \mathcal{M}_h \).

Then, the inf-sup condition is satisfied.
Diamonds – Convergence analysis

- Diamonds satisfy conditions of Stenberg theorem with the choice of macroelements:
Diamonds – Numerical tests

Two-dimensional flat punch test
Diamonds – Numerical tests

Three-dimensional flat punch test
Inf-sup condition and topology

• Stenberg’s analysis shows that the inf-sup condition is topological in nature: If one mesh satisfies the inf-sup condition, any continuous deformation of the mesh also satisfies the inf-sup condition

• The inf-sup condition can be verified based on the mesh connectivity (topology) only, without reference to nodal coordinates

• Connection between inf-sup condition and topological invariants?
Inf-sup condition and topology

- Recall: Isotropic differential complex:

\[ \Omega^0_*(\mathbb{R}^3) \rightarrow \Omega^3_*(\mathbb{R}) \rightarrow \Omega^3_*(\mathbb{R}) \rightarrow \Omega^0_*(\mathbb{R}^3), \]

- Isotropic complex cohomology:

\[
\begin{align*}
H^2 &= \Omega^3_*(\mathbb{R})/\text{im}(\text{div}) \\
H^3 &= \ker(\text{grad})
\end{align*}
\]

Proposition. The following statements are equivalent:

i) \( H^2 = \{0\}, \)

ii) \( H^3 = \{0\}, \)

iii) the inf-sup condition is satisfied.
Concluding remarks

• There is a vast difference between vector and tensor problems where discrete mechanics is concerned.
• In applications to tensor problems, geometrical considerations must be carefully balanced against analysis considerations (e.g., convergence).
• Diamonds:
  – *Are a discrete mechanics approximation scheme (exact satisfaction of conservation laws, Helmholtz-Hodge)*
  – *Automatically satisfy the inf-sup condition (convergence)*
  – *Make possible incompressible elasticity, plasticity, analysis on arbitrary simplicial meshes (advantageous in applications to contact, explicit dynamics, mesh adaption)*
• Uniqueness? Extension to finite kinematics?...