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

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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 $\mathbb{R}^3$:

$$0 \rightarrow \Omega^0(\mathbb{R}^3)/\mathbb{R} \overset{\mathrm{grad}}{\rightarrow} \Omega^1(\mathbb{R}^3) \overset{\mathrm{curl}}{\rightarrow} \Omega^2(\mathbb{R}^3) \overset{\mathrm{div}}{\rightarrow} \Omega^3(\mathbb{R}^3)/\mathbb{R} \rightarrow 0$$

- Differential complex property:

$$\mathrm{curl} \circ \mathrm{grad} = 0$$

$$\mathrm{div} \circ \mathrm{curl} = 0$$

- Integral identities (Stokes' theorem):

$$\int_V \mathrm{div}\, \alpha \, dV = \int_{\partial V} \alpha \cdot \nu \, dS$$

$$\int_S \mathrm{curl}\, \beta \, dS = \oint_{\partial S} \beta \cdot dx$$

Geometric mechanics

- Helmholtz-Hodge decomposition:

$$\Omega^1(\mathbb{R}^3) \ni \beta = \text{grad}\phi + \text{curl}A + \gamma, \qquad \Delta\gamma = 0$$

and decomposition L^2-orthogonal.

- de Rham cohomology:

$$\left.\begin{aligned} H^1(\mathbb{R}^3) &= \ker(\text{grad}) \\ H^2(\mathbb{R}^3) &= \ker(\text{curl})/\text{im}(\text{grad}) \\ H^3(\mathbb{R}^3) &= \ker(\text{div})/\text{im}(\text{curl}) \end{aligned}\right\}$$

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:

$$\left.\begin{aligned} \mathrm{div}(\varepsilon\, E) &= \rho \\ \mathrm{div}(\mu\, H) &= 0 \\ \mathrm{curl} E &= -\partial_t(\mu\, H) \\ \mathrm{curl} H &= J + \partial_t(\varepsilon\, E) \end{aligned}\right\} \quad \begin{aligned} &\text{(Gauss law)} \\ &\text{(Gauss law for magnetism)} \\ &\text{(Faraday's law of induction)} \\ &\text{(Ampère's law)} \end{aligned}$$

$E \equiv$ electric field,

$\rho \equiv$ charge density,

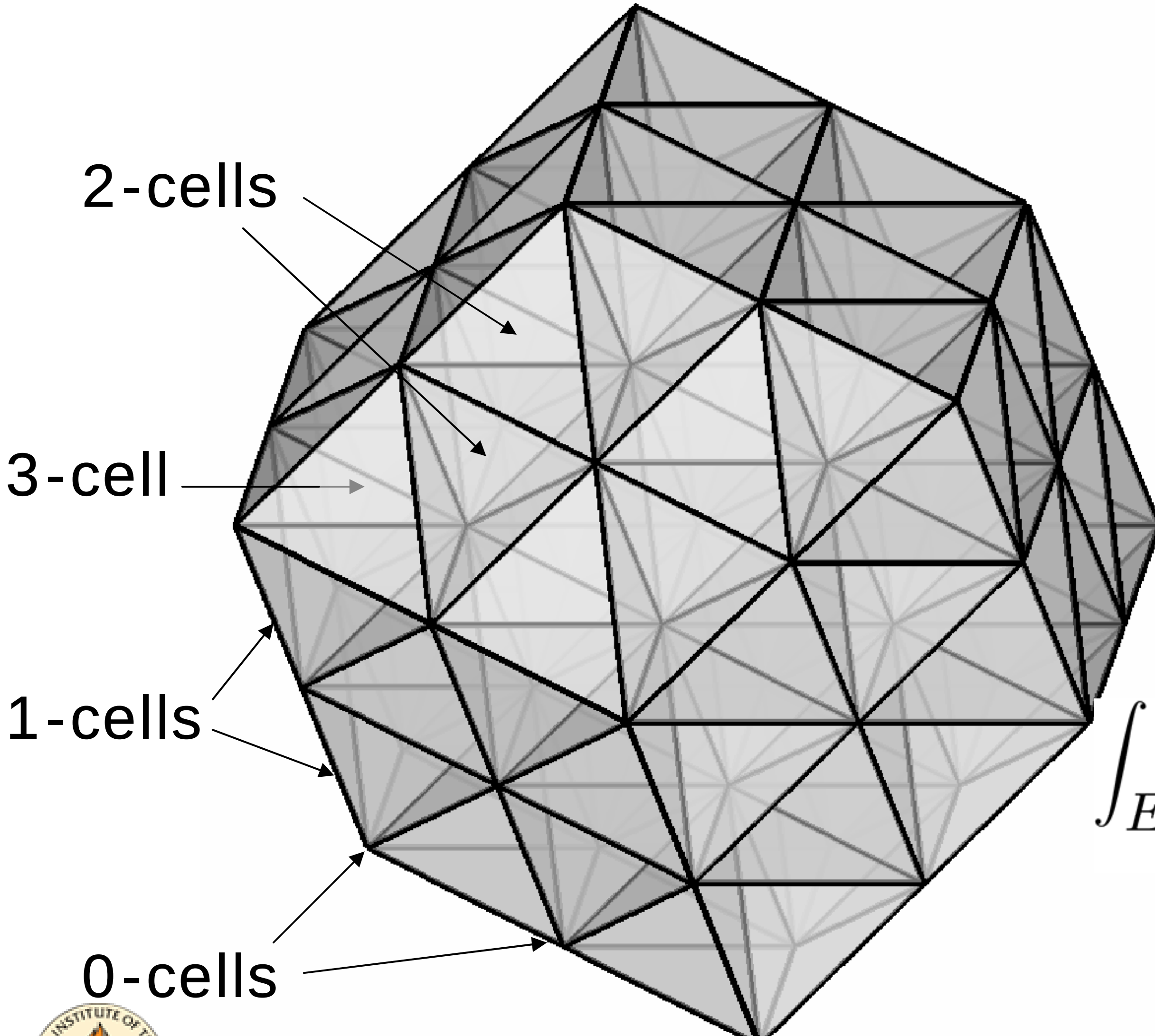
$\varepsilon \equiv$ electrical permitivity,

$H \equiv$ magnetic field,

$J \equiv$ current density.

$\mu \equiv$ magnetic permeability.

Discrete mechanics − Cell complexes



- Cell complex:
  $C \equiv \{\text{cells}\}$
- $E_p \equiv \{p - \text{cells}\}$
- p-forms: $\Omega^p(C) \equiv \{\omega : E_p \to \mathbb{R}^n\}$
- Integration:

$$\int_{E_p} \omega \equiv \sum_{e_p \in E_p} \omega(e_p)|e_p|$$

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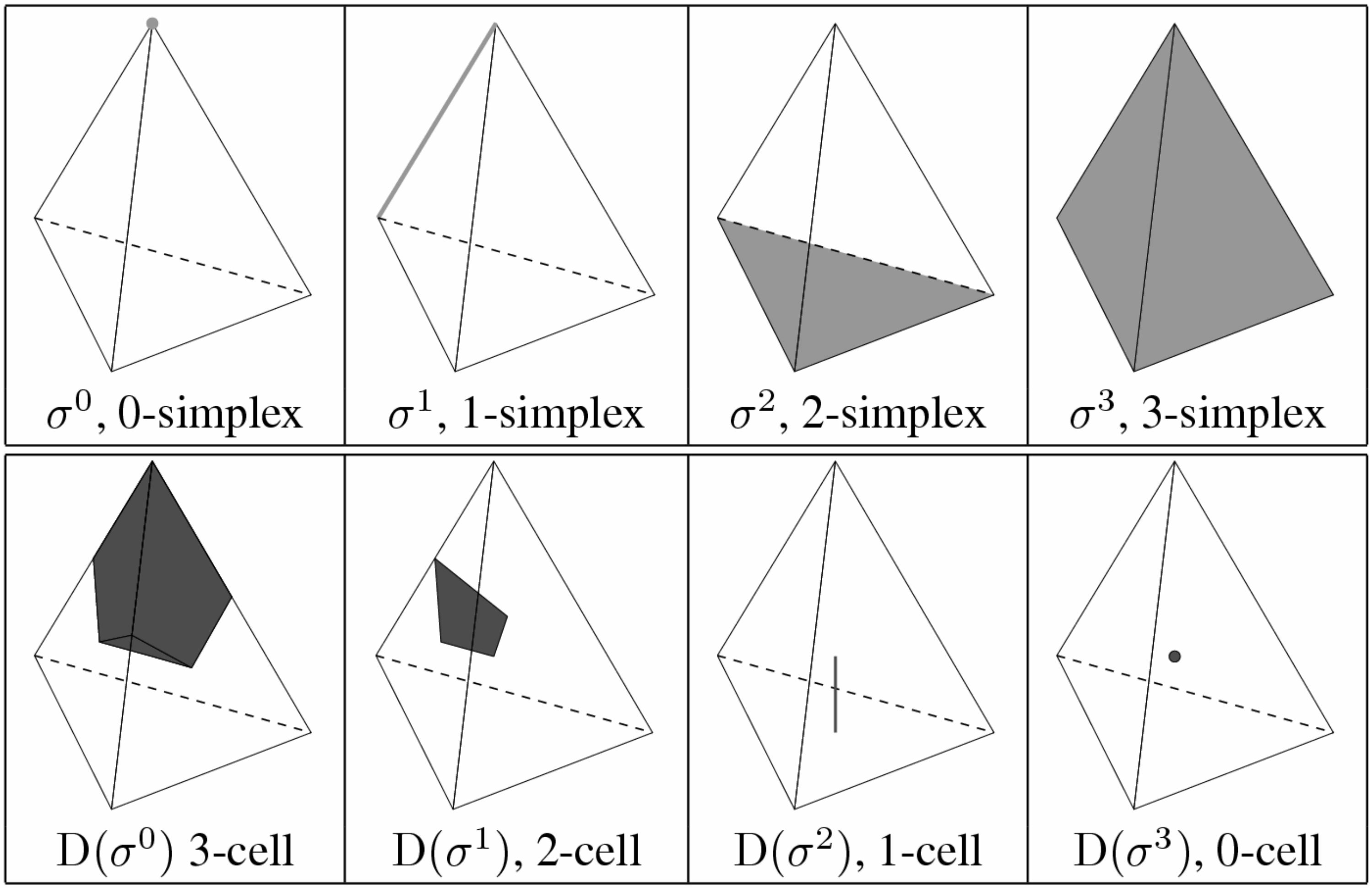
Cell complexes – Dual cell complex



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

Discrete differential complexes

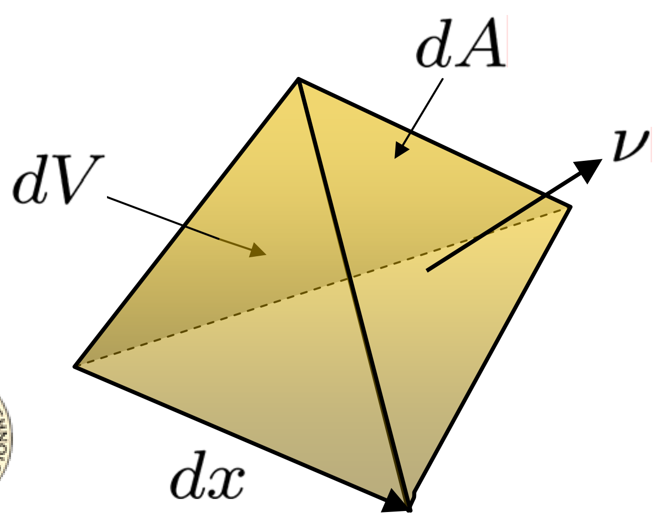
- Discrete de-Rham differential complex: Sequence

$$0 \rightarrow \Omega^0(C)/\mathbb{R} \xrightarrow{\text{grad}} \Omega^1(C) \xrightarrow{\text{curl}} \Omega^2(C) \xrightarrow{\text{div}} \Omega^3(C)/\mathbb{R} \rightarrow 0$$

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

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

- Example: C simplicial,



$$\left.\begin{aligned} \text{grad}u &\equiv \frac{du \otimes dx}{|dx|^2} \\ \text{curl}\beta &\equiv \frac{d(\beta \cdot dx)}{dA}\nu \\ \text{div}\alpha &\equiv \frac{d(\alpha \cdot \nu dA)}{dV} \end{aligned}\right\}$$

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Discrete Maxwell's equations

- Continuum (in $\mathbb{R}^3$):

$$\left.\begin{aligned} \text{div}(\varepsilon\, E) &= \rho \\ \text{div}(\mu\, H) &= 0 \\ \text{curl} E &= -\partial_t(\mu\, H) \\ \text{curl} H &= J + \partial_t(\varepsilon\, E) \end{aligned}\right\}$$

- Discrete (on C):

$$\left.\begin{aligned} \text{div}(\varepsilon\, E) &= \rho \\ \text{div}(\mu\, H) &= 0 \\ \text{curl} E &= -\partial_t(\mu\, H) \\ \text{curl} H &= J + \partial_t(\varepsilon\, E) \end{aligned}\right\}$$

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

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

$$\varepsilon : \Omega^1(C) \to \Omega^2(C^*), \quad \mu : \Omega^1(C^*) \to \Omega^2(C).$$

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

- The Kröner differential complex:

$$0 \rightarrow \Omega^0(\mathbb{R}^3)/\mathrm{RM} \xrightarrow{\mathrm{Def}} \Omega^3(\mathrm{sym}\,\mathbb{R}^{3\times3}) \xrightarrow{\mathrm{Inc}} \Omega^3(\mathrm{sym}\,\mathbb{R}^{3\times3}) \xrightarrow{\mathrm{Div}} \Omega^0(\mathbb{R}^3)/\mathrm{RM} \longrightarrow 0$$

Domain and range	'nabla' expression	Coordinate expression
$\mathrm{Def}: \Omega^0(\mathbb{R}^3) \rightarrow \Omega^3(\mathrm{sym}\,\mathbb{R}^{3\times3})$	$\nabla^S \equiv (\nabla + \nabla^T)/2$	$(\mathrm{Def}\,u)_{ij} = (u_{i,j} + u_{j,i})/2$
$\mathrm{Inc}: \Omega^3(\mathrm{sym}\,\mathbb{R}^{3\times3}) \rightarrow \Omega^3(\mathrm{sym}\,\mathbb{R}^{3\times3})$	$\nabla \times (\bullet \times \nabla)$	$(\mathrm{Inc}\,\epsilon)_{ij} = \epsilon_{kl,mn} e_{kmi} e_{lnj}$
$\mathrm{Div}: \Omega^3(\mathrm{sym}\,\mathbb{R}^{3\times3}) \rightarrow \Omega^0(\mathbb{R}^3)$	$\nabla \cdot$	$(\mathrm{Div}\,\sigma)_i = \sigma_{ij,j}$

- $\mathrm{Inc} \circ \mathrm{Def} = 0, \qquad \mathrm{Div} \circ \mathrm{Inc} = 0$

- The isotropic differential complex:

$$\Omega^0(\mathbb{R}^3) \xrightarrow{\mathrm{div}} \Omega^3(\mathbb{R}) \xrightarrow{0} \Omega^3(\mathbb{R}) \xrightarrow{\mathrm{grad}} \Omega^0(\mathbb{R}^3)$$

$$\mathrm{grad}\,\mathrm{p} = \mathrm{Div}\,(\mathrm{p}\,\mathrm{g}^\sharp), \qquad \mathrm{div} \mathrm{u} = \mathrm{g}^\sharp \cdot \mathrm{Def}\,\mathrm{u}$$

Geometric linear elasticity

- Compressible linear elasticity:

$$-\mathrm{Div}\,(2\mu\,\mathrm{Def}\,\mathrm{u}) - \mathrm{div}\,(\lambda\,\mathrm{grad}\,\mathrm{u}) = \mathrm{f} + \mathrm{t}, \quad \text{in } \Omega \cup \Gamma_N$$

$$\mathrm{u} = 0, \qquad \text{on } \Gamma_D$$

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

$$-\mathrm{Div}\,(2\mu\,\mathrm{Def}\,\mathrm{u}) - \mathrm{grad}\,\mathrm{p} = \mathrm{f} + \mathrm{t}, \quad \text{in } \Omega \cup \Gamma_N$$

$$\mathrm{div}\,\mathrm{u} = 0, \qquad \text{in } \Omega$$

$$\mathrm{u} = 0, \qquad \text{on } \Gamma_D$$

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

- $C = \mathcal{S}_h \equiv$ simplicial complex of size h.
- Discrete Kröner differential complex:

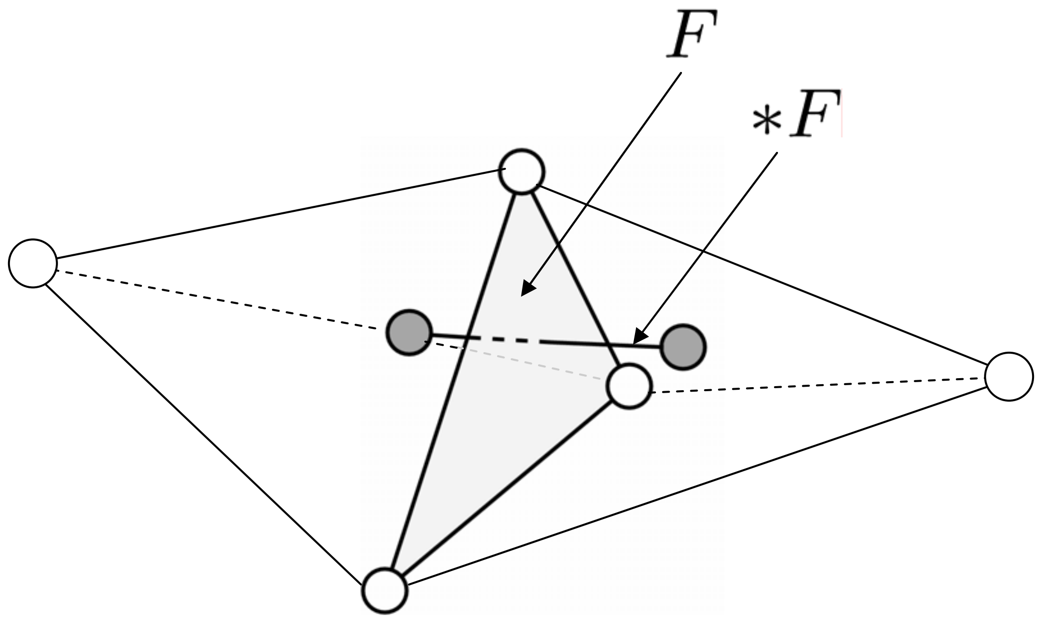
Domain and range	Definition
$\mathsf{Def} : \Omega^0(\mathcal{S}_h; \mathbb{R}^3) \to \Omega^3(\mathcal{S}_h; \mathsf{sym}\, \mathbb{R}^{3\times 3})$	$(\mathsf{Def}\, \mathsf{u})(T) = \frac{1}{2\,\|T\|} \sum_{F \prec T} \|F\| \left(\langle \mathsf{u} \rangle \otimes \mathsf{n} + \langle \mathsf{u} \rangle \otimes \mathsf{n}\right)$
$\mathsf{Inc} : \Omega^3(\mathcal{S}_h; \mathsf{sym}\, \mathbb{R}^{3\times 3}) \to \Omega^3(\mathcal{S}_h; \mathsf{sym}\, \mathbb{R}^{3\times 3})$	$(\mathsf{Inc}\, \epsilon)(T) = \frac{1}{\|T\|} \sum_{F \prec T,\ F \not\subset \partial\Omega} (\mathsf{n} \times [\![\epsilon]\!]) \times \mathsf{n}$
$\mathsf{Div} : \Omega^3(\mathcal{S}_h; \mathsf{sym}\, \mathbb{R}^{3\times 3}) \to (\mathcal{S}_h; \Omega^0 \mathbb{R}^3)$	$(\mathsf{Div}\, \sigma)(N) = \frac{1}{3} \sum_{F \succ N} \|F\|\ [\![\sigma]\!] \cdot \mathsf{n}$

- Verify: $\mathsf{Inc} \circ \mathsf{Def} = 0, \qquad \mathsf{Div} \circ \mathsf{Inc} = 0$
- The isotropic differential complex:

Domain and range	Definition
$\mathsf{grad} : \Omega^3(\mathcal{S}_h; \mathbb{R}) \to \Omega^0(\mathcal{S}_h; \mathbb{R}^3)$	$(\mathsf{grad}\, \mathsf{u})(T) = \frac{1}{\|T\|} \sum_{F \prec T} \|F\|\ \langle \mathsf{u} \rangle \cdot \mathsf{n}$
$\mathsf{div} : \Omega^0(\mathcal{S}_h; \mathbb{R}^3) \to \Omega^3(\mathcal{S}_h; \mathbb{R})$	$(\mathsf{div}\, \sigma)(N) = \frac{1}{3} \sum_{F \succ N} \|F\|\ [\![\sigma]\!] \cdot \mathsf{n}$

- Simplicial interpolation! Locking!

Counterexample II



- $\mathsf{Grad} : \Omega^0(\mathcal{S}_h, \mathbb{R}^3) \times \Omega^0(\mathcal{S}_h^*, \mathbb{R}^3) \to \Omega^2(\mathcal{S}_h, \mathbb{R}^{3\times 3})$: Two columns of Grad computed from F; third column of Grad computed from $*F$.
- Can complete differential complex Def $\to$ Inc $\to$ Div such that $\mathsf{Inc} \circ \mathsf{Def} = 0$ and $\mathsf{Div} \circ \mathsf{Inc} = 0$.

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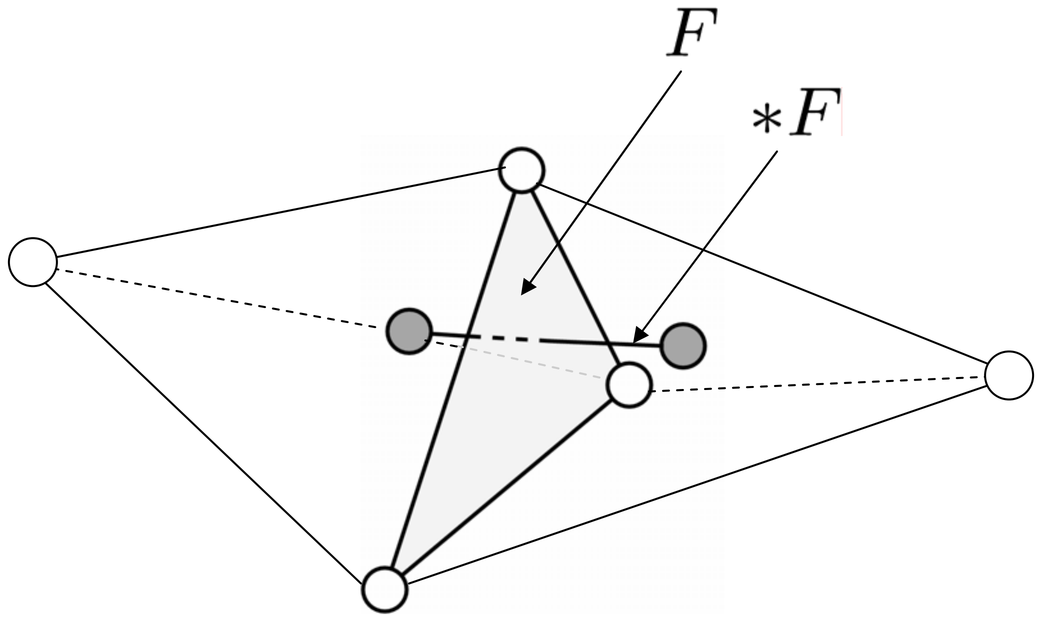
Counterexample II



- 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 $\mathbb{Q}_1/\mathbb{P}_0$: 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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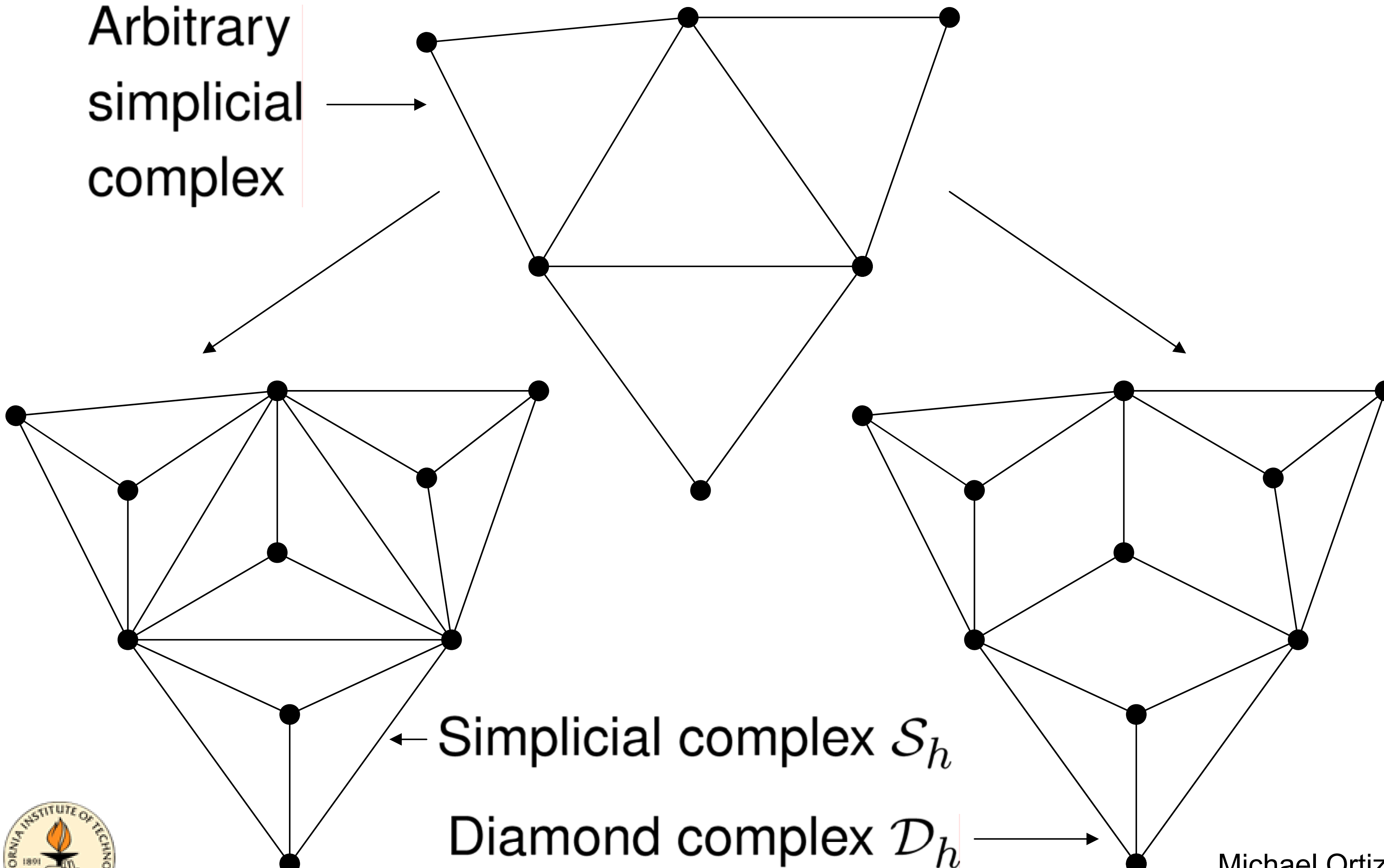
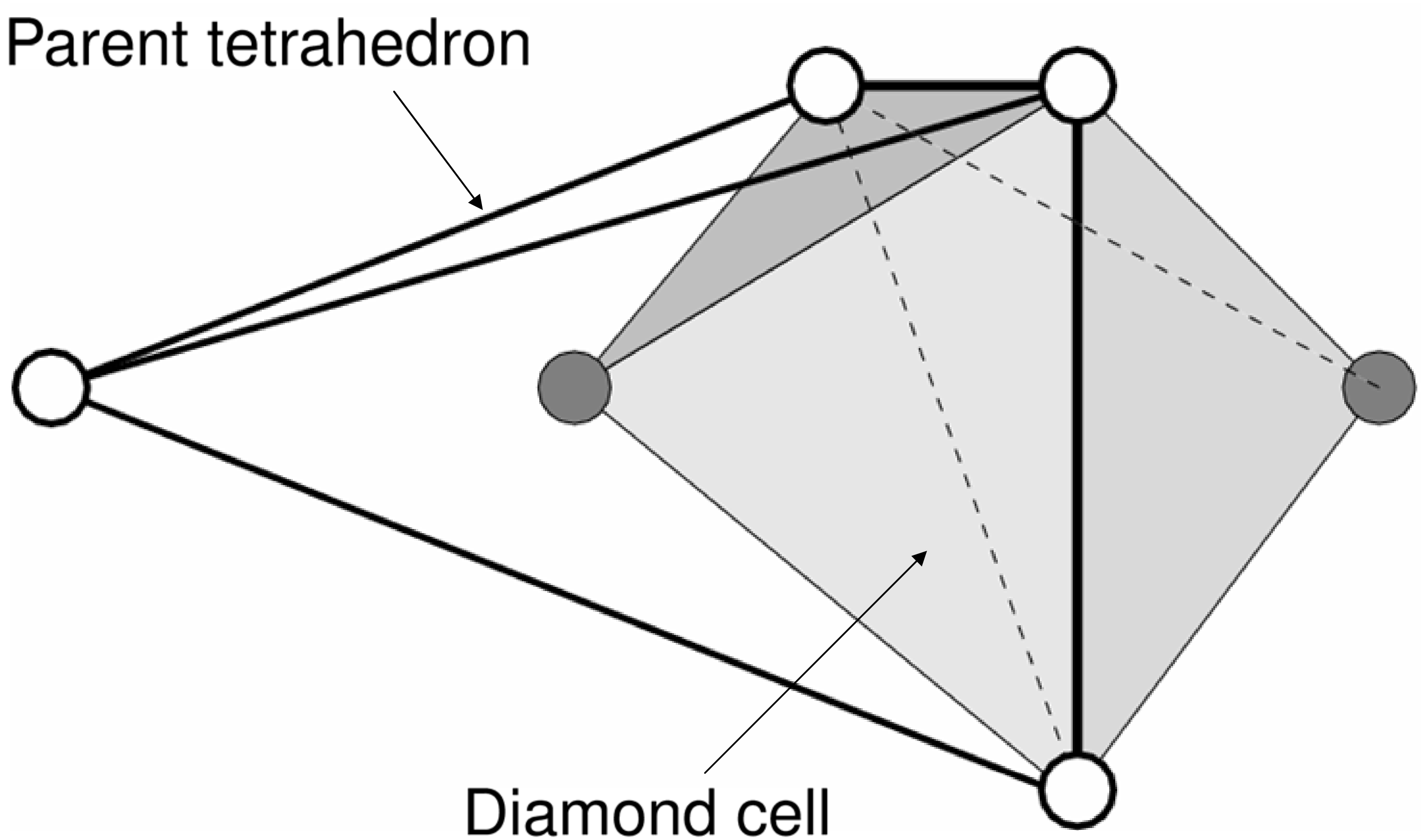
Diamonds



Arbitrary simplicial complex
Simplicial complex $\mathcal{S}_h$
Diamond complex $\mathcal{D}_h$

Diamonds



Diamonds

- Discrete Kröner differential complex:

Domain and range	Definition
$\mathsf{Def} : \Omega^0(\mathcal{S}_h;\mathbb{R}^3) \to \Omega^3(\mathcal{S}_h;\mathsf{sym}\,\mathbb{R}^{3\times 3})$	$(\mathsf{Def}\,\mathsf{u})(T) = \frac{1}{2\lvert T\rvert}\sum_{F\prec T}\lvert F\rvert\,(\langle \mathsf{u}\rangle\otimes\mathsf{n} + \langle\mathsf{u}\rangle\otimes\mathsf{n})$
$\mathsf{Inc} : \Omega^3(\mathcal{S}_h;\mathsf{sym}\,\mathbb{R}^{3\times 3}) \to \Omega^3(\mathcal{S}_h;\mathsf{sym}\,\mathbb{R}^{3\times 3})$	$(\mathsf{Inc}\,\epsilon)(T) = \frac{1}{\lvert T\rvert}\sum_{F\prec T,\ F\not\subset\partial\Omega}(\mathsf{n}\times[\![\epsilon]\!])\times\mathsf{n}$
$\mathsf{Div} : \Omega^3(\mathcal{S}_h;\mathsf{sym}\,\mathbb{R}^{3\times 3}) \to (\mathcal{S}_h;\Omega^0\mathbb{R}^3)$	$(\mathsf{Div}\,\sigma)(N) = \frac{1}{3}\sum_{F\succ N}\lvert F\rvert\,[\![\sigma]\!]\cdot\mathsf{n}$

- Verify: $\mathsf{Inc}\circ\mathsf{Def} = 0, \qquad \mathsf{Div}\circ\mathsf{Inc} = 0$
- Discrete metric: $\mathsf{g}^\sharp \equiv$ piecewise constant on $\mathcal{D}_h$
- The isotropic differential complex:

$$\Omega^0_*(\mathcal{D}_h;\mathbb{R}^3) \xrightarrow{\mathsf{div}} \Omega^3_*(\mathcal{D}_h;\mathbb{R}) \xrightarrow{0} \Omega^3_*(\mathcal{D}_h;\mathbb{R}) \xrightarrow{\mathsf{grad}} \Omega^0_*(\mathcal{D}_h;\mathbb{R}^3),$$

$$\mathsf{grad}\,\mathsf{p} = \mathsf{Div}(\mathsf{p}\,\mathsf{g}^\sharp), \quad \mathsf{div}\,\mathsf{u} = \mathsf{g}^\sharp\cdot\mathsf{Def}\,\mathsf{u}$$

(constant pressure over diamond cells)

Diamonds – Convergence analysis

- Express discrete problem in variational form:

$$\mathsf{V}_h = \{u_h, \text{ piecewise affine on } \mathcal{S}_h\}$$

$$\mathsf{P}_h = \{u_h, \text{ piecewise constant on } \mathcal{D}_h\}$$

$$\begin{cases} a(u_h, v_h) + b(v_h, p_h) = f(v_h), & \forall v_h \in \mathsf{V}_h \\ b(u_h, q_h) = 0, & \forall q_h \in \mathsf{P}_h \end{cases}$$

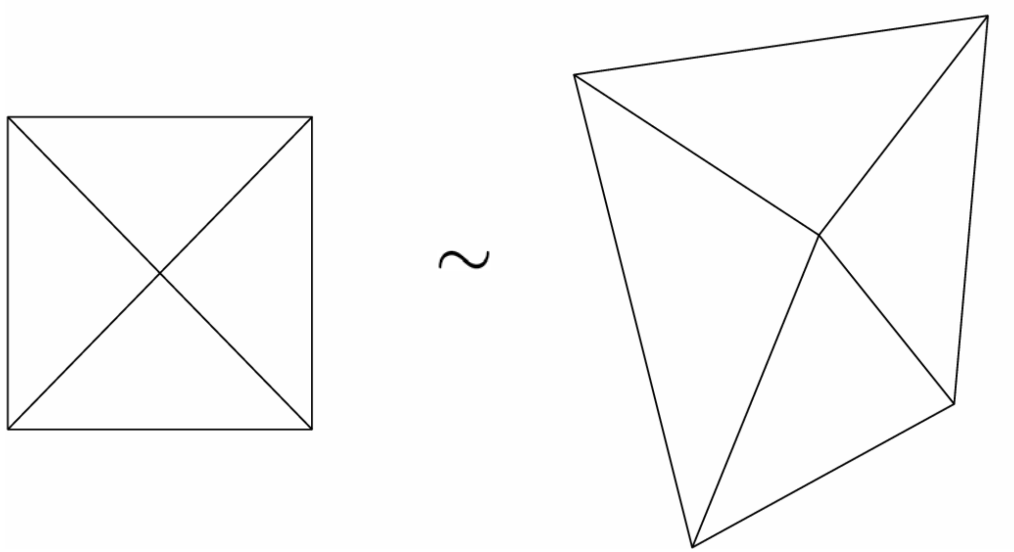
Proposition *For any initial simplicial mesh,* $\exists \beta > 0$ *independent of* h *such that the* inf-sup *condition*

$$\inf_{q_h \in \mathsf{P}_h \setminus \{0\}} \sup_{v_h \in \mathsf{V}_h \setminus \{0\}} \frac{b(v_h, q_h)}{\|q_h\|_{0,\Omega} \, \|v_h\|_{1,\Omega}} \geq \beta_h > 0$$

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.



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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) $\forall M \in \mathcal{E}_i, i = 1, 2, .., q, q_h \in \mathsf{P}_h(M)$,

$$\int_M q_h \, \mathrm{div} v_h = 0 \quad \forall v_h \in \mathsf{V}_h^0(M) \Rightarrow q_h = \mathrm{const.}$$

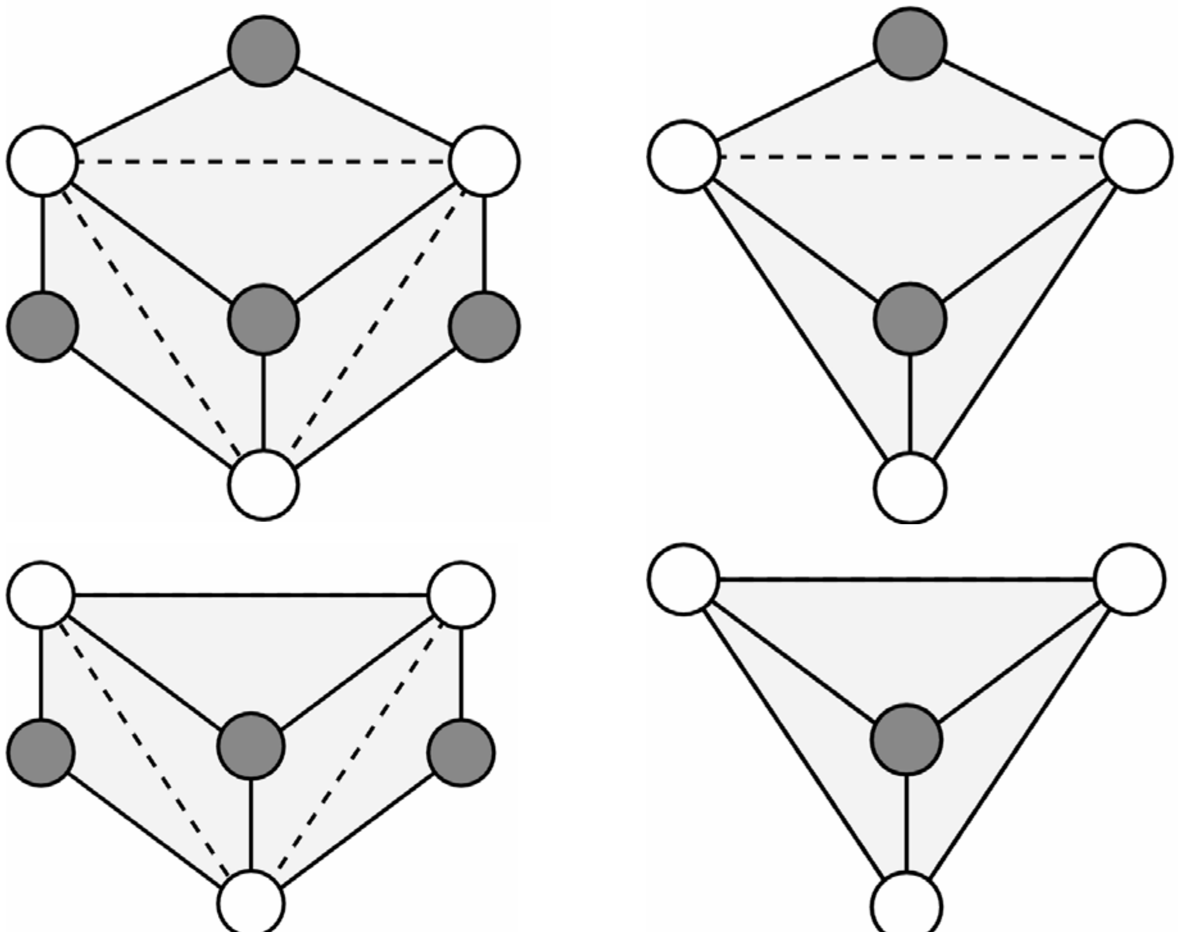
ii) Each $M \in \mathcal{M}_h$ *belongs to one of the classes* $\mathcal{E}_i$.

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:



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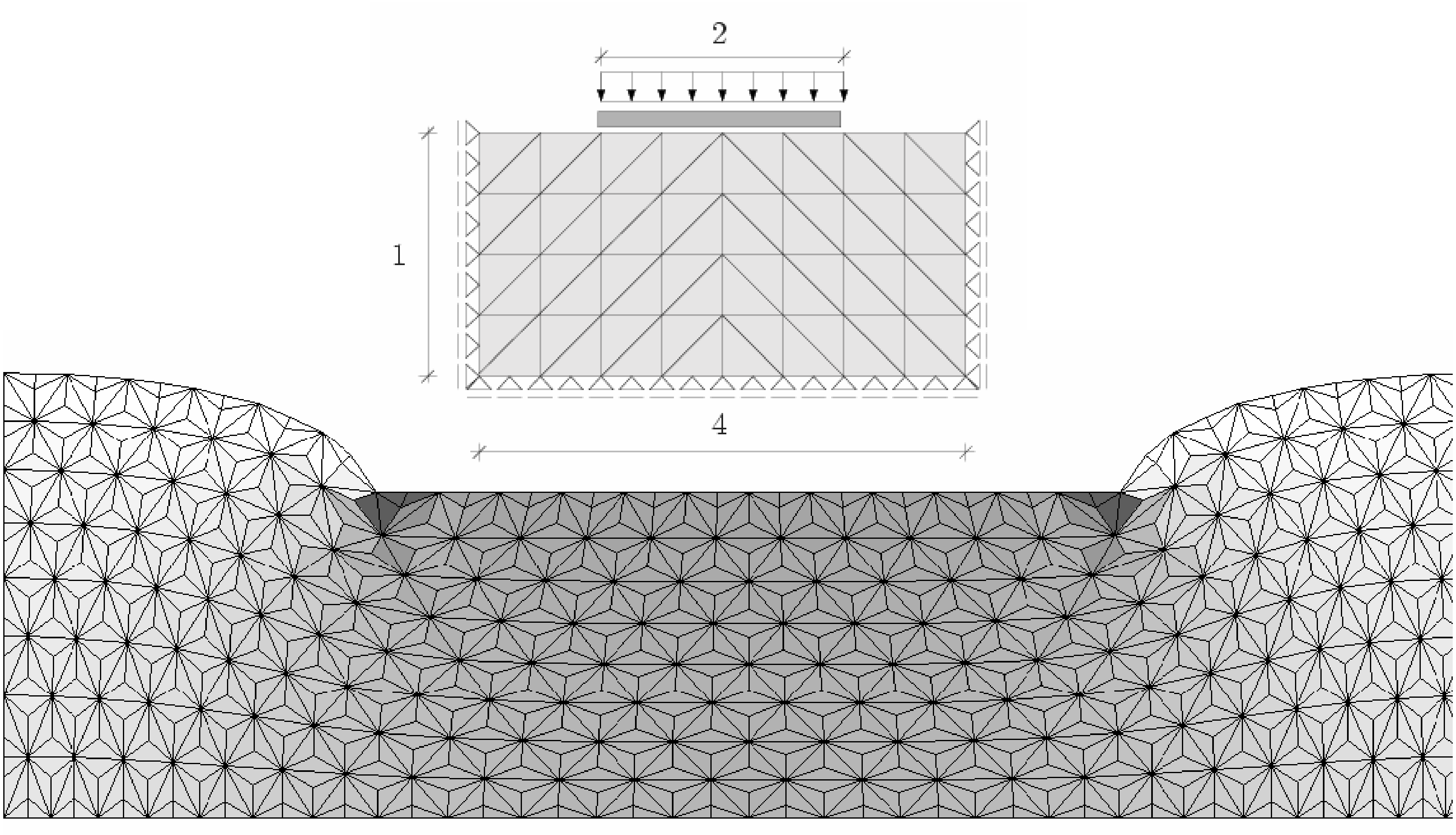
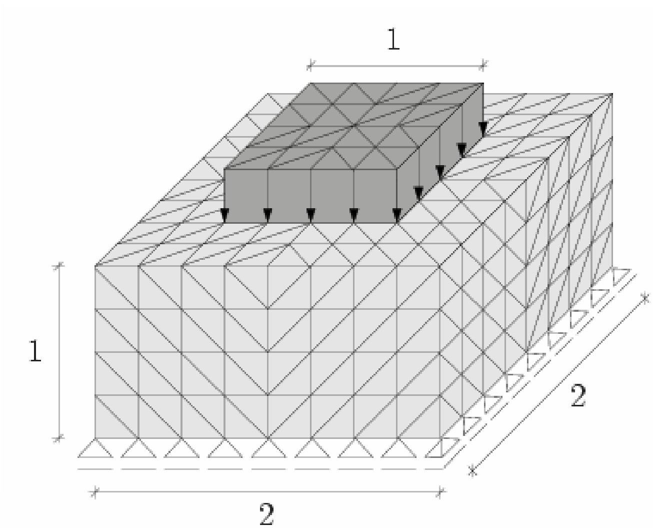
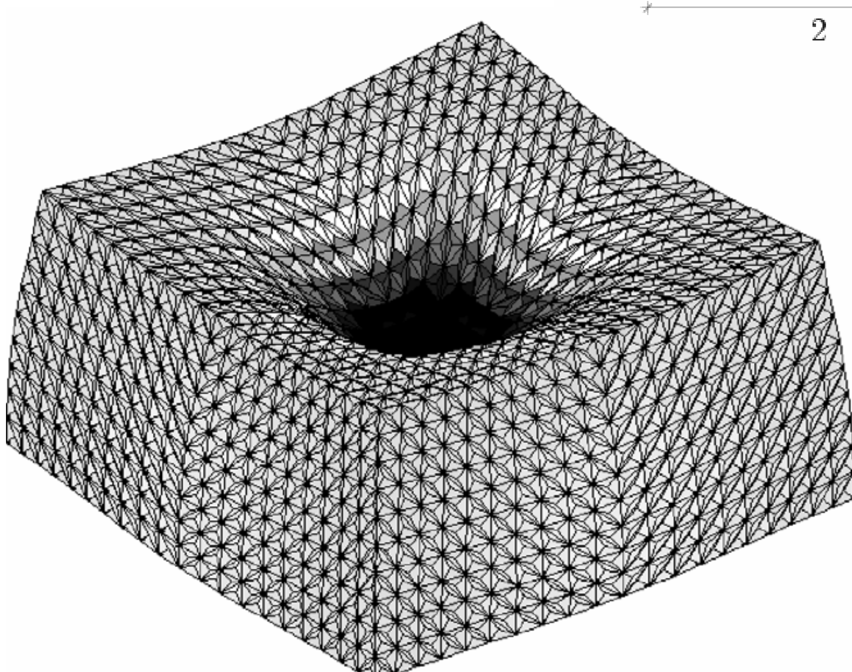
Diamonds – Numerical tests

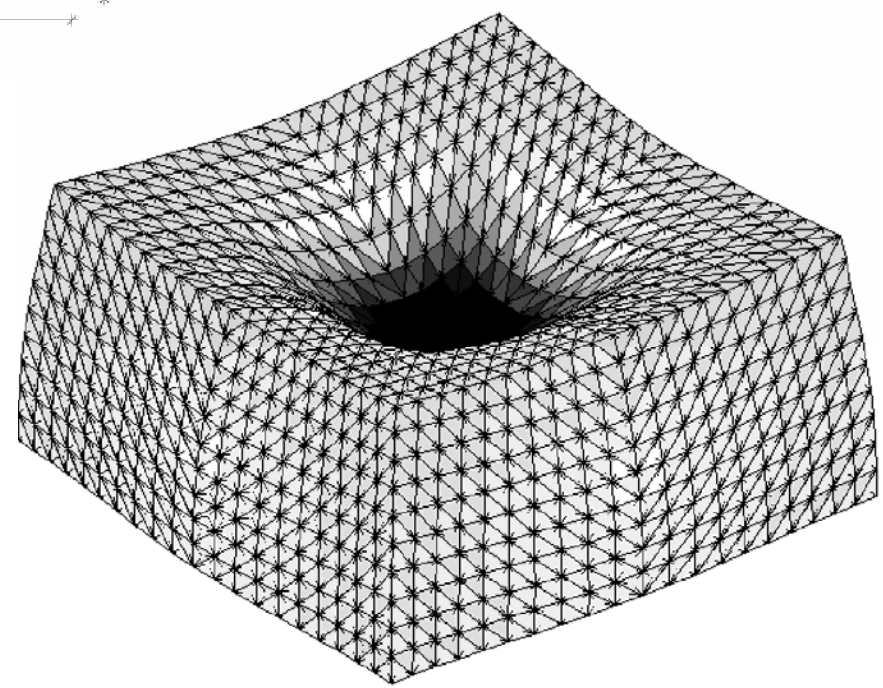


Two-dimensional flat punch test

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:

$$\Omega^0_*(\mathbb{R}^3) \xrightarrow{\text{div}} \Omega^3_*(\mathbb{R}) \xrightarrow{0} \Omega^3_*(\mathbb{R}) \xrightarrow{\text{grad}} \Omega^0_*(\mathbb{R}^3),$$

- Isotropic complex cohomology:

$$\left.\begin{aligned} H^2 &= \Omega^3_*(\mathbb{R})/\text{im}(\text{div}) \\ H^3 &= \ker(\text{grad}) \end{aligned}\right\}$$

Proposition. *The following statements are equivalent:*

i) $H^2 = \{0\}$, *ii)* $H^3 = \{0\}$,

iii) the inf-sup *condition is satisfied.*

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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 conservations 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?...