A primer on
Numerical methods for elasticity

Douglas N. Arnold, University of Minnesota

Complex materials: Mathematical models and numerical methods

Oslo, June 10–12, 2015

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– D. N. Arnold, 2015 Complex Materials workshop, Oslo

Elasticity

Continuum mechanics:

- Material particle in body: $X = X_t \in \Omega_t \subset \mathbb{R}^3$
- Body force density: $f : \Omega_t \to \mathbb{R}^3$
- (Cauchy) stress tensor: $\sigma : \Omega_t \to \mathbb{M}^3$, $\int_{\partial D} \sigma n \, ds =$ surf. force on D
- Bal. of momentum: $\rho \ddot{X} = \operatorname{div} \sigma + f$
- Bal. of ang. momentum: $\operatorname{skw} \sigma = 0$

Elasticity: stress determined by deformation gradient

$$X_t = \phi_t(x), \quad \phi = \phi_t : \hat{\Omega} \xrightarrow{\cong} \Omega_t \quad \textit{deformation}$$

Material is characterized by its *constitutive equation*: $\sigma(X) = \hat{\sigma}(\nabla \phi(x))$

The constitutive function $\hat{\sigma} : \mathbb{M}^3 \to \mathbb{S}^3$ is constrained by frame-indifference, symmetries, growth conditions, ...

(IV)BVP for elasticity

Find ϕ, σ satisfying balance equations and constitutive equation:

$$\begin{gathered} \sigma(X) = \hat{\sigma}(\nabla\phi(x)) \\ \rho\,\ddot{X} - \operatorname{div}\sigma = f \\ \operatorname{skw}\sigma = 0 \end{gathered}$$

$+$ boundary & initial conditions

or

$$\begin{gathered} \sigma(X) = \hat{\sigma}(\nabla\phi(x)) \\ -\operatorname{div}\sigma = f \\ \operatorname{skw}\sigma = 0 \end{gathered}$$

$+$ boundary conditions

Linearization

Suppose

- $\hat{\sigma}$ is a smooth function of $\nabla\phi$
- $\hat{\sigma}(I) = 0$
- ∇u is small, where $u(x) := \phi(x) - x$ is the *displacement*

Then $\sigma \approx C\nabla u$ where $C = \dfrac{\partial\hat{\sigma}}{\partial\nabla\phi}$ is linear.

Since $\hat{\sigma}(F) = 0$ if $F \in \mathbb{O}(3)$, $C\,K = 0$ for K skew. Thus

$$C\nabla u = C\,\mathrm{sym}\,\nabla u := C\,\epsilon\,u$$

Assuming $\hat{\sigma}$ comes from an energy, $C : \mathbb{S}^3 \to \mathbb{S}^3$ is SPD

BVP for linear elasticity:

$$\sigma = C\,\epsilon\,u$$
$$\rho\ddot{u} - \mathrm{div}\,\sigma = f$$

$+$ boundary & initial conditions

Displacement formulation

$$\sigma = C\epsilon u, \quad -\operatorname{div}\sigma = f \quad \text{in } \Omega, \qquad u = 0 \ \text{ on } \partial\Omega$$

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Mutiplying by a test vector field and integrating over Ω by parts we get the weak form: $u \in \mathring{H}^1(\Omega;\mathbb{R}^3)$ satisfies

$$(C\epsilon u, \epsilon v) = (f, v) \quad \forall v \in \mathring{H}^1(\Omega;\mathbb{R}^3)$$

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These are the Euler–Lagrange equations of a minimization:

$$u = \operatorname*{arg\,min}_{u \in \mathring{H}^1(\Omega;\mathbb{R}^3)} [\frac{1}{2}(C\epsilon u, \epsilon u) - (f, u)]$$

the variational form.

Galerkin's method

Let $V_h \subset \mathring{H}^1(\Omega;\mathbb{R}^3)$ be finite dimensional. The Galerkin solution is defined as $u_h \in V_h$ satisfying

$$(C\,\epsilon\, u_h, \epsilon\, v) = (f, v) \quad \forall v \in V_h.$$

Basis for V_h

Expand $u_h = \sum_{j=1}^{N} \alpha_j\, \phi_j$, so $\sum_j \underbrace{(C\,\epsilon\,\phi_j, \epsilon\,\phi_i)}\alpha_j = \underbrace{(f, \phi_i)}$

- compute the *stiffness matrix* A_{ij} and *load vector* b_i
- solve the matrix equation $A\alpha = b$ for $\alpha \in \mathbb{R}^N$
- sol'n is $u_h = \sum \alpha_j\, \phi_j, \quad \sigma = \sum \alpha_j\, C\,\epsilon\,\phi_j$

Convergence analysis

$(C\epsilon u, \epsilon v)$ (f, v)

V an H-space, $b : V \times V \to \mathbb{R}$ bdd bilinear form, $F \in V^*$

Problem: Find $u \in V$ s.t. $b(u, v) = F(v) \quad \forall v \in V$

Galerkin: Find $u_h \in V_h$ s.t. $b(u_h, v) = F(v) \quad \forall v \in V_h$

Stability: $$\gamma_h := \inf_{0 \neq w \in V_h} \sup_{0 \neq v \in V_h} \frac{b(w,v)}{\|w\| \|v\|} > 0$$

Basic error est:

$$\|u - u_h\| \leq \|b\| \gamma_h^{-1} \inf_{v \in V_h} \|u - v\|$$

Convergence analysis

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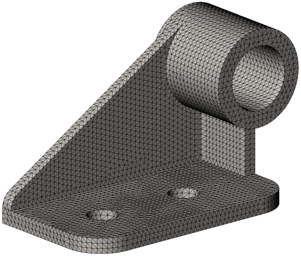
If b is *coercive*: $\quad b(w, w) \geq \gamma \|w\|^2, \quad$ then the Galerkin method is stable with $\gamma_h \geq \gamma$ for any subspace V_h.

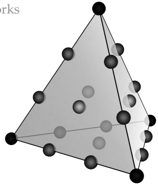
Lagrange finite element spaces

Like all finite element spaces, constructed from three ingredients:

- A triangulation $\mathcal{T}_h$ consisting of polyhedral elements T., e.g., tetrahedra.
- For each T, a space of shape functions $V(T)$, typically polynomial. E.g., $V(T) = \mathcal{P}_3(T; \mathbb{R}^3)$.
- For each T, a set of DOFs: *a basis for* $V(T)^*$, *with each element associated to a face of* T



Solidworks



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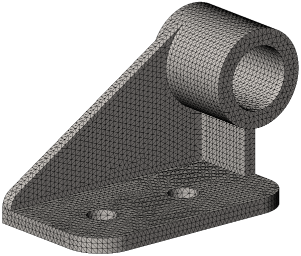

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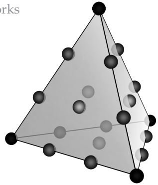


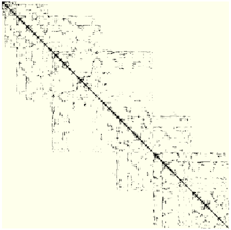
V_h is *defined* as functions piecewise in $V(T)$ with DOFs single-valued on faces. Interelement continuity is not specified *a priori*, but *inferred:* in this case V_h is the space of continuous piecewise cubics.

$$\inf_{v \in V_h} \|u - v\|_{H^1} \le ch^3 \|u\|_{H^4}$$

Implementation

This framework for finite elements ensures

- An easily computable basis with local supports.
- A sparse stiffness matrix.
- Efficient assembly
- Total number of operations $= O(N_{\text{elt}})$



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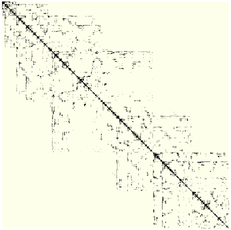
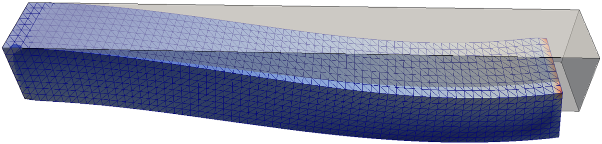


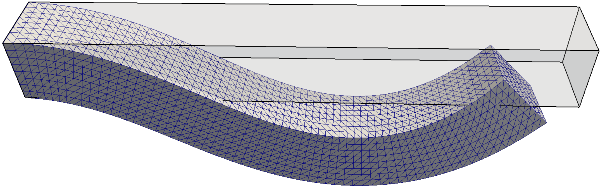


$\mathcal{P}_2$ Lagrange, 24,576 tets, dim $V_h = 111,843$, NNZ = 8,934,921, sparsity $= 99.93\%$

FEniCS project

Nonlinear problems

For larger deformation we need a nonlinear model. Just use Newton's method to solve the nonlinear equations.



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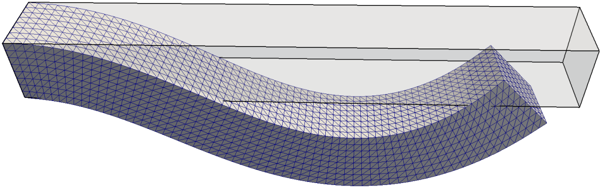
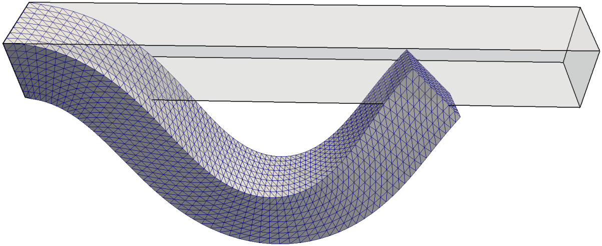
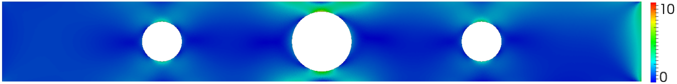
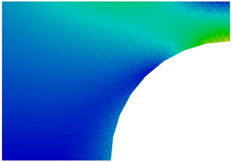


For even larger deformation, Newton's method may not converge. Just use continuation to get the initial iterate.



Poisson locking





$\mathcal{P}_1$ Lagrange, 88,374 triangles, $\dim V_h = 89,972$, $E = 10$, $\nu = 0.2$

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The method does *not* lose H^1 stability as $\nu \uparrow 0.5$.
The problem is that $\|b\| \to \infty$.

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Other issues with the displacement approach: thin domains, rough coefficients, loss of accuracy for σ, inapplicability to some materials, ...

Dual variational principles

Finite elements based on dual variational principles were advocated from the start (Fraeijs de Veubeke '65).

Primal variational form

$$u = \operatorname*{arg\,min}_{u \in \mathring{H}^1(\Omega;\mathbb{R}^3)} [\frac{1}{2}(C\epsilon\, u, \epsilon\, u) - (f, u)]$$

Dual variational form

$$\sigma = \operatorname*{arg\,min}_{\substack{\sigma \in H(\operatorname{div};\mathbb{S}^3) \\ -\operatorname{div}\sigma = f}} \frac{1}{2}(A\sigma, \sigma)$$

$A := C^{-1}$

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Dual variational form

$$\sigma = \operatorname*{arg\,min}_{\substack{\sigma \in H(\operatorname{div};\mathbb{S}^3)\\ -\operatorname{div}\sigma = f}} \frac{1}{2}(A\sigma, \sigma)$$

$A := C^{-1}$

It is not practical to find finite element subspaces that satisfy the constraint $-\operatorname{div}\sigma = f$, so we use a Lagrange multiplier:

$$(\sigma, u) = \operatorname*{arg\,crit}_{\substack{\sigma \in H(\operatorname{div};\mathbb{S}^3)\\ u \in L^2(\Omega;\mathbb{R}^3)}} \left[\frac{1}{2}(A\sigma, \sigma) + (u, \operatorname{div}\sigma + f)\right]$$

Hellinger–Reissner

The saddle-point problem

$$(\sigma, u) = \operatorname*{arg\,crit}_{\substack{\sigma \in H(\operatorname{div};\mathbb{S}^3) \\ u \in L^2(\Omega;\mathbb{R}^3)}} \underbrace{[\frac{1}{2}(A\sigma,\sigma) + (u, \operatorname{div}\sigma + f)]}_{L(\sigma,u)}$$

- *Weak formulation:* Find $(\sigma, u) \in H(\operatorname{div}, \mathbb{S}^3) \times L^2(\Omega; \mathbb{R}^3)$ s.t.

$$(A\sigma, \tau) + (u, \operatorname{div}\tau) = 0 \quad \forall \tau \in H(\operatorname{div}, \mathbb{S}^3),$$
$$(\operatorname{div}\sigma, v) = -(f, v) \quad \forall v \in L^2(\Omega; \mathbb{R}^3)$$

- *Euler–Lagrange equations:* $A\sigma - \epsilon\, u = 0, \quad -\operatorname{div}\sigma = f.$
- Lagrange multiplier is the displacement.
- Critical point is a *saddle point*:

$$L(\sigma, v) \le L(\sigma, u) \le L(\tau, v) \quad \forall \sigma \in H(\operatorname{div}, \mathbb{S}^3),\ v \in L^2(\Omega; \mathbb{R}^3)$$

- Displacement boundary conditions are *natural*, not essential.
- The bilinear form $b(\sigma, u; \tau, v) = (A\sigma, \tau) + (u, \operatorname{div}\tau) + (\operatorname{div}\sigma, v)$ is symmetric, but *not coercive.* $\begin{pmatrix} \mathcal{A} & \mathcal{B}^T \\ \mathcal{B} & 0 \end{pmatrix}$
- Finding stable finite elements is a major challenge.

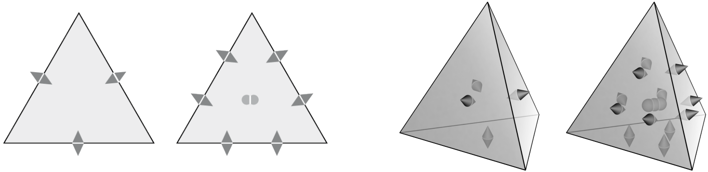
Stable mixed finite elements for the Laplacian

The same bilinear form

$$b(\sigma, u; \tau, v) = (A\sigma, \tau) + (u, \operatorname{div} \tau) + (\operatorname{div} \sigma, v)$$

arises for the mixed Laplacian, except that then u is scalar-valued and σ is vector-valued (rather than u vector-valued and σ $\mathbb{S}^3$-valued).

Finite elements for this case were found by Raviart–Thomas in ’77 in 2D, and extended to $3D$ by Nédélec in ’80. These are the analogues of Lagrange elements for $H(\text{div})$ (i.e., differential $(n-1)$-forms).

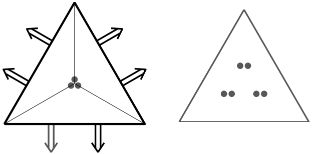


A second major family was discovered by Brezzi–Douglas–Marini in ’85, exended by Nédélec to 3D in ’86.

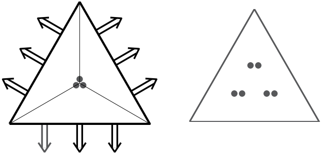
Stable mixed finite elements for elasticity

It proved to be very difficult to carry over such element to $H(\mathrm{div}, \mathbb{S}^3)$.
Composite elements:

Watwood–Hartz '68
Johnson–Mercier '78

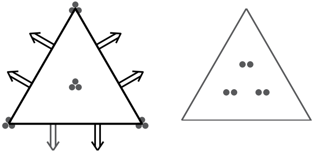


Arnold–Douglas–Gupta '84



First stable elements with polynomial trial functions:

Arnold–Winther '02



Nothing practical has been found for 3D.

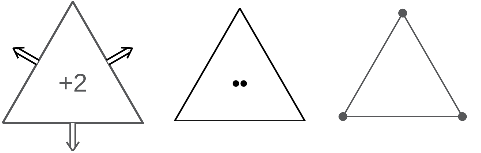
Weak symmetry

Since the symmetry constraint is the rub, a natural idea is to enforce it via another Lagrange multiplier:

$$(\sigma, u, p) = \underset{\substack{\sigma \in H(\mathrm{div};\mathbb{M}^3) \\ u \in L^2(\Omega;\mathbb{R}^3) \\ p \in L^2(\Omega;\mathbb{K}^3)}}{\arg\operatorname{crit}} \left[\frac{1}{2}(A\sigma, \sigma) + (u, \operatorname{div}\sigma + f) + (p, \sigma)\right]$$

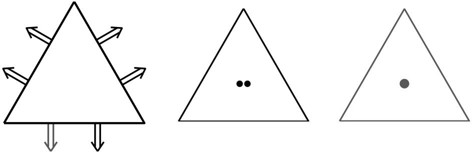
- A is extended so $A : \mathbb{S}^3 \to \mathbb{S}^3$ and $A : \mathbb{K}^3 \to \mathbb{K}^3$ are SPD
- *EL eqs:* $A\sigma - \operatorname{grad} u + p = 0, \quad -\operatorname{div}\sigma = f, \quad \operatorname{skw}\sigma = 0$
- Lagrange multiplier $p = \operatorname{skw}\operatorname{grad} u$, the *rotation*.
- Finding stable finite elements is still a challenge, but much less so.

Arnold–Brezzi–Douglas ’84
(PEERS)



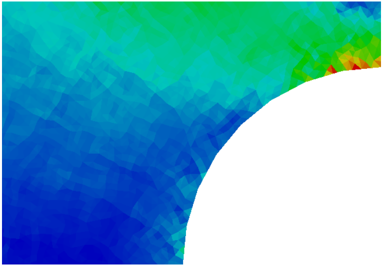
Stenberg derived several higher order methods in ’86, 88.
Since the advent of Finite Element Exterior Calculus, there have been lots of methods, in both 2D and 3D

Arnold–Falk–Winther ’07

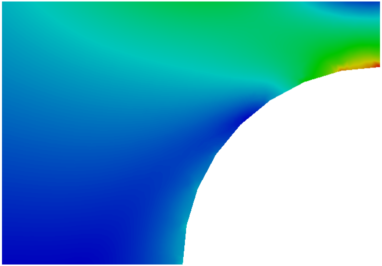


The analogous element works for all polynomial degrees, in n-D.
Variations have also been developed by Boffi-Brezzi-Fortin, Cockburn-Gopalakrishnan-Guzman, Gopalakrishnan-Guzman, Awanou, Hu, …

Mixed methods are robust wrt incompressibility



Displacement method, Lagrange $\mathcal{P}_1$



Mixed method, lowest order AFW

Detail of stress computed for $\nu = 0.4999$

Elastodynamics

For dynamic problem, we seek $\sigma, p = \operatorname{skw}\operatorname{grad} u, v = \dot{u}$

Static

$$A\sigma - \operatorname{grad} u + p = 0$$
$$-\operatorname{div}\sigma = f$$
$$\operatorname{skw}\sigma = 0$$

Dynamic

$$A\dot{\sigma} - \operatorname{grad} v + \dot{p} = 0$$
$$\rho\dot{v} - \operatorname{div}\sigma = f$$
$$\operatorname{skw}\dot{\sigma} = 0$$

$$(A\sigma, \tau) + (u, \operatorname{div}\tau) + (p, \tau) = 0 \quad \forall\tau$$
$$-(\operatorname{div}\sigma, w) = (f, w) \quad \forall w$$
$$(\sigma, q) = 0 \quad \forall q$$

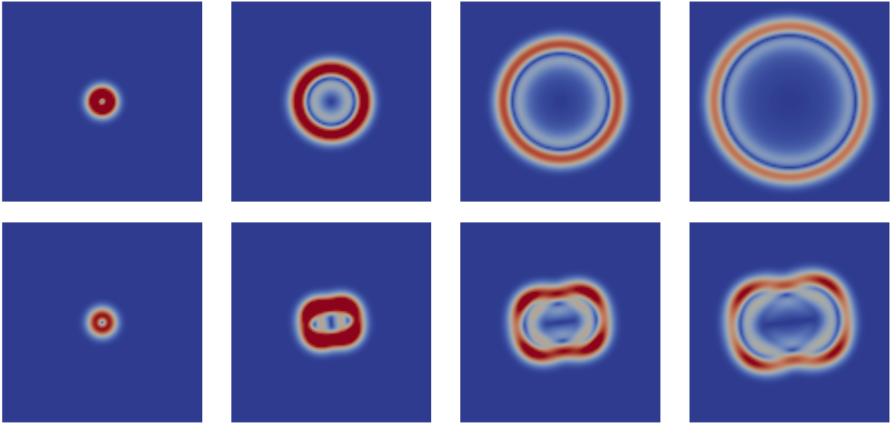
$$(A\dot{\sigma}, \tau) + (v, \operatorname{div}\tau) + (\dot{p}, \tau) = 0 \quad \forall\tau$$
$$(\rho\dot{v}, w) - (\operatorname{div}\sigma, v) = (f, v) \quad \forall v$$
$$(\dot{\sigma}, q) = 0 \quad \forall q$$

$$\begin{pmatrix} \mathcal{A} & \mathcal{B}^T & \mathcal{C}^T \\ -\mathcal{B} & 0 & 0 \\ \mathcal{C} & 0 & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = \cdots \qquad \begin{pmatrix} \mathcal{A} & 0 & \mathcal{C}^T \\ 0 & \mathcal{M} & 0 \\ \mathcal{C} & 0 & 0 \end{pmatrix} \begin{pmatrix} \dot{\alpha} \\ \dot{\beta} \\ \dot{\gamma} \end{pmatrix} + \begin{pmatrix} 0 & \mathcal{B}^T & 0 \\ -\mathcal{B} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = \cdots$$

To solve the ODEs we use a time-stepping scheme like Crank–Nicolson. At each time step the system is similar to the the static one.

Arnold–Lee '14

Computation of elastic waves



Jeonghun Lee ’12

Viscoelasticity

One of the simplest models of a viscoelastic solid is the Maxwell model:

$$u = u_e + u_v, \quad A_e \sigma = \epsilon\, u_e, \quad A_v \sigma = \epsilon\, \dot{u}_v.$$

Therefore we get the constitutive law

$$A_e \dot{\sigma} + A_v \sigma = \epsilon\, \dot{u}$$

which is supplemented by the equilibrium equation $-\operatorname{div}\sigma = f$ in the quasi-static case or the evolution equation $\rho\ddot{u} - \operatorname{div}\sigma = f$.

Such methods are amenable to the mixed methods discussed here, but σ cannot be easily eliminated to get a displacement method.

quasistatic: Rognes–Winther '10; dynamic: Lee

Complexes

$$0 \to H^1 \xrightarrow{\text{grad}} H(\text{curl}) \xrightarrow{\text{curl}} H(\text{div}) \xrightarrow{\text{div}} L^2 \to 0$$

de Rham complex

$$\begin{array}{ccccccc} 0 \to H^1(\mathbb{R}^3) & \xrightarrow{\epsilon} & H(\text{curl}\,T\,\text{curl}, \mathbb{S}^3) & \xrightarrow{\text{curl}\,T\,\text{curl}} & H(\text{div}, \mathbb{S}^3) & \xrightarrow{\text{div}} & L^2(\mathbb{R}^3) \to 0 \\ \uparrow & & \uparrow & & \uparrow & & \uparrow \\ \text{displacement} & & \text{strain} & & \text{stress} & & \text{load} \end{array}$$

elasticity complex

$$\begin{array}{ccccc} \text{displacement} & \text{rotation} & & \text{strain} & \\ \downarrow & \downarrow & & \downarrow & \\ 0 \to H^1(\mathbb{R}^3) & \times L^2(\mathbb{K}) & \xrightarrow{(\text{grad}, -I)} & H(\text{curl}\,\tilde{T}\,\text{curl}, \mathbb{M}) & \longrightarrow \end{array}$$

$$\begin{array}{ccccccc} \xrightarrow{\text{curl}\,\tilde{T}\,\text{curl}} & H(\text{div}, \mathbb{M}) & \xrightarrow{\begin{pmatrix}\text{div}\\ \text{skw}\end{pmatrix}} & L^2(\mathbb{R}^3) & \times L^2(\mathbb{K}) \to 0 \\ & \uparrow & & \uparrow & \uparrow \\ & \text{stress} & & \text{load} & \text{couple} \end{array}$$

elas complex w/ weak symm

Complexes

$$0 \to H^1 \xrightarrow{\text{grad}} H(\text{curl}) \xrightarrow{\text{curl}} H(\text{div}) \xrightarrow{\text{div}} L^2 \to 0$$

de Rham complex

$$\begin{array}{ccccccc} 0 \to H^1(\mathbb{R}^3) & \xrightarrow{\epsilon} & H(\text{curl}\,T\,\text{curl}, \mathbb{S}^3) & \xrightarrow{\text{curl}\,T\,\text{curl}} & H(\text{div}, \mathbb{S}^3) & \xrightarrow{\text{div}} & L^2(\mathbb{R}^3) \to 0 \\ \uparrow & & \uparrow & & \uparrow & & \uparrow \\ \text{displacement} & & \text{strain} & & \text{stress} & & \text{load} \end{array}$$

elasticity complex

$$\begin{array}{ccc} \text{displacement} \quad \text{rotation} & & \text{strain} \\ \downarrow \qquad\quad \downarrow & & \downarrow \\ 0 \to H^1(\mathbb{R}^3) \times L^2(\mathbb{K}) & \xrightarrow{(\text{grad}, -I)} & H(\text{curl}\,\tilde{T}\,\text{curl}, \mathbb{M}) \longrightarrow \end{array}$$

$$\begin{array}{ccccc} \xrightarrow{\text{curl}\,\tilde{T}\,\text{curl}} & H(\text{div}, \mathbb{M}) & \xrightarrow{\begin{pmatrix}\text{div}\\ \text{skw}\end{pmatrix}} & L^2(\mathbb{R}^3) \times L^2(\mathbb{K}) \to 0 \\ & \uparrow & & \uparrow \qquad\quad \uparrow \\ & \text{stress} & & \text{load} \qquad \text{couple} \end{array}$$

elas complex w/ weak symm

Complexes

$$0 \to H^1 \xrightarrow{\text{grad}} H(\text{curl}) \xrightarrow{\text{curl}} H(\text{div}) \xrightarrow{\text{div}} L^2 \to 0$$

de Rham complex

$$\begin{array}{ccccccccc} 0 \to H^1(\mathbb{R}^3) & \xrightarrow{\epsilon} & H(\text{curl}\, T\, \text{curl}, \mathbb{S}^3) & \xrightarrow{\text{curl}\, T\, \text{curl}} & H(\text{div}, \mathbb{S}^3) & \xrightarrow{\text{div}} & L^2(\mathbb{R}^3) \to 0 \\ \uparrow & & \uparrow & & \uparrow & & \uparrow \\ \text{displacement} & & \text{strain} & & \text{stress} & & \text{load} \end{array}$$

elasticity complex

$$\begin{array}{ccccc} \text{displacement} \quad \text{rotation} & & \text{strain} & & \\ \downarrow \qquad\quad \downarrow & & \downarrow & & \\ 0 \to H^1(\mathbb{R}^3) \times L^2(\mathbb{K}) & \xrightarrow{(\text{grad}, -I)} & H(\text{curl}\, \tilde{T}\, \text{curl}, \mathbb{M}) & \longrightarrow & \end{array}$$

$$\begin{array}{ccccc} \xrightarrow{\text{curl}\, \tilde{T}\, \text{curl}} & H(\text{div}, \mathbb{M}) & \xrightarrow{\begin{pmatrix} \text{div} \\ \text{skw} \end{pmatrix}} & L^2(\mathbb{R}^3) \times L^2(\mathbb{K}) \to 0 \\ & \uparrow & & \uparrow \qquad\quad \uparrow \\ & \text{stress} & & \text{load} \qquad \text{couple} \end{array}$$

elas complex w/ weak symm