TOWARDS FINITE ELEMENT TENSOR CALCULUS

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Main question: systematic and canonical discretization of tensor fields on triangulation?

de Rham complex: there have been comprehensive results for skew-symmetric tensor fields, i.e., differential forms, under the name of finite element differential forms or Finite Element Exterior Calculus (FEEC).

Canonical construction of finite elements, Ralf Hiptmair, Math. Comp. 1999.

This talk: focuses on a special kind of tensors $\Lambda^{k,\ell} := \text{Alt}^k \otimes \text{Alt}^\ell$, form-valued forms. Special cases include strain and stress fields in elasticity and metric and curvature tensors in geometry.

OUTLINE

1	Conti	inuous level: BGG construction (review)
2	Discr	rete level: finite elements
3	Exter	nsions and outlook
	3.1	Solving PDEs with distributional elements
	3.2	Twisted complexes: continuum microstructures, Riemann-Cartan geometry
	3.3	Young tableaux: an algebraic representation of tensor symmetries

CONTINUOUS LEVEL: BGG CONSTRUCTION (REVIEW)

1	Continuous level: BGG construction (re	review)	•	•		•		•	• •	•	•	•	•	-	• •	•	•	• •	-	-	• •		•	- 2	2
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2 Discrete level: finite elements	10
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3	Exten	sions and outlook
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DE RHAM COMPLEX (3D VERSION)

$$\begin{array}{cccc} 0 & \longrightarrow & \mathcal{C}^{\infty}(\Omega) \stackrel{\mathsf{grad}}{\longrightarrow} & \mathcal{C}^{\infty}(\Omega; \mathbb{R}^3) \stackrel{\mathsf{curl}}{\longrightarrow} & \mathcal{C}^{\infty}(\Omega; \mathbb{R}^3) \stackrel{\mathsf{div}}{\longrightarrow} & \mathcal{C}^{\infty}(\Omega) & \longrightarrow & 0.\\ \\ & \mathcal{d}^0 := \mathsf{grad}, \quad \mathcal{d}^1 := \mathsf{curl}, \quad \mathcal{d}^2 := \mathsf{div} \,. \end{array}$$

► complex property:
$$d^k \circ d^{k-1} = 0$$
, $\Rightarrow \mathcal{R}(d^{k-1}) \subset \mathcal{N}(d^k)$,
curl \circ grad $= 0 \Rightarrow \mathcal{R}($ grad $) \subset \mathcal{N}($ curl $)$, div \circ curl $= 0 \Rightarrow \mathcal{R}($ curl $) \subset \mathcal{N}($ div $)$

► cohomology:
$$\mathscr{H}^k := \mathcal{N}(d^k)/\mathcal{R}(d^{k-1})$$
,
 $\mathscr{H}^0 := \mathcal{N}(\text{grad}), \quad \mathscr{H}^1 := \mathcal{N}(\text{curl})/\mathcal{R}(\text{grad}), \quad \mathscr{H}^2 := \mathcal{N}(\text{div})/\mathcal{R}(\text{curl})$

• exactness (contractible domains): $\mathcal{N}(d^k) = \mathcal{R}(d^{k-1})$, i.e., $d^k u = 0 \Rightarrow u = d^{k-1}v$ curl $u = 0 \Rightarrow u = \text{grad } \phi$, div $v = 0 \Rightarrow v = \text{curl } \psi$.

In higher dimensions,

$$\cdots \longrightarrow \Lambda^{k-1} \xrightarrow{d^{k-1}} \Lambda^k \xrightarrow{d^k} \Lambda^{k+1} \longrightarrow \cdots$$

 Λ^k : differential *k*-forms, d^k : exterior derivatives

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DE RHAM COMPLEX AND TOPOLOGY

dimension of \mathscr{H}^{k} = number of "k-dimensional holes" (c.f. de Rham theorem)



Examples where dim $\mathscr{H}^1 = 1$ and dim $\mathscr{H}^2 = 1$, respectively. Left: curl-free field which is not grad, Right: div-free field with is not curl.

(figure from Finite element exterior calculus, D.N.Arnold, SIAM 2008.)

(Linear) elasticity $-\operatorname{div}(A\operatorname{def} u) = f.$

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displacement (vector). $\boldsymbol{e} := \operatorname{def} \boldsymbol{u} := 1/2(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T)$ strain (linearized deformation), symmetric matrix, $\sigma := A \operatorname{def} u$ stress, symmetric matrix.

Metric: $g: T\mathcal{M} \times T\mathcal{M} \to \mathbb{R}$, symmetric. g(u, u): length of $u. g(\cdot)(\cdot)$: 1-form-valued 1-forms

Riemannian curvature: $R_i^{j}_{kl}$ transform(matrix)-valued 2-forms. Given two vectors u, v, Riem(u, v) is the transform measuring the change brought by parallel transport around the loop [u, v].

 $R_{ij,kl} := g_{js}R_{j}s_{kl}$ 2-form-valued 2-forms



Figure: J. M. Lee, Introduction to Riemannian Manifolds.

Ricci curvature: trace of $R_{ii,kl}$, $R_{ik} := g^{jl}R_{ii,kl}$. symmetric 2-tensor (matrix) Einstein tensor: Ricci with modified trace $G_{ik} := R_{ik} - \frac{1}{2}(g^{jl}R_{il})g_{ik}$. symmetric 2-tensor (matrix)

TENSORS FIT IN COMPLEXES

EXAMPLE: ELASTICITY (KRÖNER, CALABI) COMPLEX



 $\mathbb{V}:=\mathbb{R}^3$ vectors, $\quad \mathbb{S}:=\mathbb{R}^{3\times 3}_{sym}$ symmetric matrices

$$\begin{split} \det u &:= 1/2(\nabla u + \nabla u^T), \quad (\det u)_{ij} = 1/2(\partial_i u_j + \partial_j u_i).\\ & \text{inc} \ g := \nabla \times g \times \nabla, \quad (\text{inc} \ g)^{ij} = \epsilon^{ikl} \epsilon^{jst} \partial_k \partial_s g_{lt}.\\ & \text{div} \ v := \nabla \cdot v, \quad (\text{div} \ v)_i = \partial^j u_{ij}. \end{split}$$

 $g \text{ metric} \Rightarrow \text{inc } g \text{ linearized Einstein tensor} (\subseteq \text{Riem} \subseteq \text{Ric in 3D})$

inc \circ def = 0: Saint-Venant compatibility div \circ inc = 0: Bianchi identity

HOW TO DERIVE SUCH COMPLEXES: THE BGG MACHINERY

Bernstein-Gelfand-Gelfand (BGG) machinery: Derive complexes from de Rham complexes; carry over de Rham results. (B-G-G 1975, Čap,Slovák,Souček 2001, Eastwood 2000, Arnold,Falk,Winther 2006)

BGG in 1D

BGG diagram:



BGG complex:

$$0 \longrightarrow H^2 \xrightarrow{\partial_x^2} L^2 \longrightarrow 0.$$

- two de-Rham complexes with different continuity,
- cohomology: $\mathcal{N}(\partial_x^2) \cong \mathcal{N}(\partial_x) \oplus \mathcal{N}(\partial_x), \, \partial_x^2$ is onto.

ELASTICITY COMPLEX FROM BGG



Output : elasticity complex

Conclusion : elasticity cohomology = de Rham cohomology (Proof: homological algebra)

ND: FORM-VALUED FORMS

$$0 \longrightarrow H^{q} \otimes \operatorname{Alt}^{0,J-1} \xrightarrow{d} H^{q-1} \otimes \operatorname{Alt}^{1,J-1} \xrightarrow{d} \cdots \xrightarrow{d} H^{q-n} \otimes \operatorname{Alt}^{n,J-1} \longrightarrow 0$$

$$0 \longrightarrow H^{q-1} \otimes \operatorname{Alt}^{0,J} \xrightarrow{d} H^{q-2} \otimes \operatorname{Alt}^{1,J} \xrightarrow{d} \cdots \xrightarrow{d} H^{q-n-1} \otimes \operatorname{Alt}^{n,J} \longrightarrow 0$$
where $\operatorname{Alt}^{i,J} := \operatorname{Alt}^{i} \otimes \operatorname{Alt}^{J}$

$$s^{i,J}\mu(v_0,\cdots,v_i)(w_1,\cdots,w_{J-1}) := \sum_{l=0}^{i} (-1)^l \mu(v_0,\cdots,\widehat{v_l},\cdots,v_l)(v^l,w_1,\cdots,w_{J-1}),$$

$$\forall v_0,\cdots,v_i,w_1,\cdots,w_{J-1} \in \mathbb{R}^n.$$

All the cases in 3D:

 $\Lambda^{i,j}$: Alt^{*i*} \otimes Alt^{*j*} with Sobolev or smooth coefficients

3D EXAMPLES

 \mathbb{R} : scalar \mathbb{V} : vector \mathbb{M} : matrix \mathbb{S} : symmetric matrix \mathbb{T} : trace-free matrix



Hessian complex:

$$0 \longrightarrow H^{q} \otimes \mathbb{R} \xrightarrow{hess} H^{q-2} \otimes \mathbb{S} \xrightarrow{curl} H^{q-3} \otimes \mathbb{T} \xrightarrow{div} H^{q-4} \otimes \mathbb{V} \longrightarrow 0.$$

biharmonic equations, plate theory, Einstein-Bianchi system of general relativity

3D EXAMPLES

 \mathbb{R} : scalar \mathbb{V} : vector \mathbb{M} : matrix \mathbb{S} : symmetric matrix \mathbb{T} : trace-free matrix



elasticity complex:

$$0 \longrightarrow H^{q-1} \otimes \mathbb{V} \xrightarrow{\text{def}} H^{q-2} \otimes \mathbb{S} \xrightarrow{\text{inc}} H^{q-4} \otimes \mathbb{S} \xrightarrow{\text{div}} H^{q-5} \otimes \mathbb{V} \longrightarrow 0$$

elasticity, defects, metric, curvature

3D EXAMPLES

 \mathbb{R} : scalar \mathbb{V} : vector \mathbb{M} : matrix \mathbb{S} : symmetric matrix \mathbb{T} : trace-free matrix

$$0 \longrightarrow H^{q} \otimes \mathbb{R} \xrightarrow{\text{grad}} H^{q-1} \otimes \mathbb{V} \xrightarrow{\text{curl}} H^{q-2} \otimes \mathbb{V} \xrightarrow{\text{div}} H^{q-3} \otimes \mathbb{R} \longrightarrow 0$$

$$0 \longrightarrow H^{q-1} \otimes \mathbb{V} \xrightarrow{\text{grad}} H^{q-2} \otimes \mathbb{M} \xrightarrow{\text{curl}} H^{q-3} \otimes \mathbb{M} \xrightarrow{\text{div}} H^{q-4} \otimes \mathbb{V} \longrightarrow 0$$

$$- \operatorname{mskw} \xrightarrow{\uparrow} S \xrightarrow{\uparrow} 2 \operatorname{vskw} \xrightarrow{\uparrow} 0$$

$$0 \longrightarrow H^{q-2} \otimes \mathbb{V} \xrightarrow{\text{grad}} H^{q-3} \otimes \mathbb{M} \xrightarrow{\text{curl}} H^{q-4} \otimes \mathbb{V} \xrightarrow{\text{div}} H^{q-5} \otimes \mathbb{V} \longrightarrow 0$$

$$0 \longrightarrow H^{q-3} \otimes \mathbb{R} \xrightarrow{\text{grad}} H^{q-4} \otimes \mathbb{V} \xrightarrow{\text{curl}} H^{q-5} \otimes \mathbb{V} \xrightarrow{\text{div}} H^{q-6} \otimes \mathbb{R} \longrightarrow 0.$$

divdiv complex:

$$0 \longrightarrow H^{q-2} \otimes \mathbb{V} \xrightarrow{\text{dev grad}} H^{q-3} \otimes \mathbb{T} \xrightarrow{\text{sym curl}} H^{q-4} \otimes \mathbb{S} \xrightarrow{\text{div div}} H^{q-6} \otimes \mathbb{R} \longrightarrow 0.$$

plate theory, elasticity

DISCRETE LEVEL: FINITE ELEMENTS

2 Discrete level: finite elements	10
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CANONICAL FINITE ELEMENTS FOR THE DE RHAM COMPLEX

$$0 \longrightarrow \underbrace{\operatorname{grad}}_{\operatorname{curl}} \underbrace{\operatorname{curl}}_{\operatorname{div}} \underbrace{\operatorname{div}}_{\operatorname{div}} \longrightarrow 0$$

Raviart-Thomas (1977), Nédélec (1980) in numerical analysis

"The main advantage of these finite elements is the possibility of approximating Maxwell's equations while exactly verifying one of the physical law." – J.C. Nédélec, Mixed Finite Elements in \mathbb{R}^3 (1980)

Bossavit (1988): differential forms and complex

"A rationale for the use of Lhese special 'mixed' clements can be obtained if one expresses basic equations in terms of differential forms, instead of vector fields. ... Whitney forms were described in 1957, long before the use of finite elements." – A. Bossavit, Whitney forms: a class of finite elements for three-dimensional computations in electromagnetism (1988)

Hiptmair (1999), Arnold, Falk, Winther (2006): systematic study, "Finite Element Exterior Calculus"

Finite element exterior calculus (FEEC): structure-preserving FEM Discrete exterior calculus (DEC): defining spaces and operators on primal and dual meshes Topological data analysis (TDA): cohomology and Hodge-Laplacian on graphs

Lim, Lek-Heng. "Hodge Laplacians on graphs." SIAM Review 62.3 (2020).

DISCRETE LEVEL: FINITE ELEMENTS

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Periodic Table of the Finite Elements

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1_

Arnold, Logg 2014, SIAM news

DISCRETIZATION OF COMPLEXES: FINITE ELEMENTS AND SPLINES

- > 2D stress: Arnold-Winther 2002, J.Hu-S.Zhang 2014, Christiansen-KH 2018,
- 2D strain: Chen-J.Hu-Huang 2014 (Regge/HHJ), Christiansen-KH 2018 (conforming), Chen-Huang 2020, DiPietro-Droniou 2021 (polygonal meshes), KH 2023
- 3D elasticity: various results on last part of complex, Hauret-Kuhl-Ortiz 2007 (discrete geometry/mechanics), Arnold-Awanou-Winther 2008, Christiansen 2011 (Regge), Christiansen-Gopalakrishnan-Guzmán-KH 2020, Chen-Huang 2021, J.Hu-Liang-Lin 2023, Gong-Gopalakrishnan-Guzmán-Neilan 2023
- ▶ 3D Hessian: Chen-Huang 2020, J.Hu-Liang 2021, Arf-Simeon 2021 (splines)
- 3D divdiv: Chen-Huang 2021, J.Hu-Liang-Ma 2021, Sander 2021 (H(sym curl), H(dev sym curl)), J.Hu-Liang-Ma-Zhang 2022, J.Hu-Liang-Lin 2023, DiPietro-Hanot 2023
- nD: Chen-Huang 2021 (last two spaces), 2D arbitrary regularity: Chen-Huang 2022, Bonizzoni-KH-Kanschat-Sap 2023
- conformal complexes: KH-Lin-Shi 2023.

Most on conforming finite elements, high order polynomials and super(redundant)-smoothness

Goal: A canonical construction, generalizing Whitney forms.

GENERALIZING FINITE ELEMENTS: BACK TO DE RHAM'S CURRENTS

Use currents (measures, Dirac delta), rather than functions.

Geometric Measure Theory, graphics

(Codimensional geometry: A point cloud represents a probability measure; curve cloud, surface cloud...)



Figure 2.4 Differential k-forms can be represented by clouds of codimension-k geometries.

Figure: *Exterior Calculus in Graphics*, Stephanie Wang, Mohammad Sina Nabizadeh and Albert Chern; ACM SIGGRAPH 2023 courses.



DISCRETE LEVEL: FINITE ELEMENTS



Braess, Schöberl 2008

Perspectives:

- ▶ Topological perspective: *k*-th space \cong (*n* − *k*)-chains, distributional *d^k* \cong ∂_{n-k}
- ► Finite Element perspective: dual, complex of degrees of freedom
- Discrete Exterior Calculus perspective: cochain complex on dual meshes



Fluid perspective: point vortex, vortex lines... (vorticity 2-form: delta on codim 2)



- Numerical applications: equilibrated residual error estimators (Braess, Schöberl 2008)
- Cohomologies, analysis: Licht 2017 (double complex)

1D FINITE ELEMENTS BGG



3D ELASTICITY COMPLEX: REGGE CALCULUS

Christiansen 2011: Regge calculus = finite elements



Regge calculus: Metric given by edge lengths; curvature as angle deficit (quantum relativity, discrete geometry).

T. Regge (1961). *General relativity without coordinates*. Il Nuovo Cimento (1955-1965), 19, 558-571.



Regge finite element: Metric: p.w. constant sym matrices, $\int_{e} t_e \cdot g \cdot t_e$ as dofs. Curvature: distributional.

nD: Lizao Li (2018 Minnesota thesis), nonlinear curvature with Regge elements (Berchenko-Kogan, Gawlik

Theorem (Christiansen, KH, Lin 2023). The cohomology of the Regge complex is isomorphic to $\mathcal{H}^{\bullet}_{dR}(\Omega) \otimes \mathcal{RM}$, the infinitesimal-rigid-body-motion-valued de Rham cohomology.

Proof.

Step 1: cohomology of an auxiliary sequence is isomorphic to the simplicial homology Construct an auxiliary sequence starting with discontinuous piecewise polynomials (rigid body motions, $\mathcal{N}(def)$), sequence isomorphic to the chain complex ($D^{\bullet} \cong \partial_{\bullet}$).

Step 2: cohomology of the auxiliary sequence is isomorphic to the Regge sequence Increase the regularity using several auxiliary sequences. Use *diagram chase* (snake lemma) to derive the cohomology.

3D HESSIAN [KH, LIN, ZHANG 2023]



Theorem. The cohomology is isomorphic to $\mathfrak{P}_1\otimes \mathfrak{H}_{\mathrm deRham}.$

3D DIVDIV [KH, LIN, ZHANG 2023]



Dual of Hessian complex .

 $\mathbb{T} + x \times \mathbb{S}$: analogy of Koszul operator (automatically trace-free).

Theorem. The cohomology is isomorphic to $\mathcal{P}_1\otimes \mathcal{H}_{\mathrm deRham}.$

Hellan-Herrmann-Johnson (HHJ) element for biharmonic equation. Implemented in NGSolve (J.Schöberl). Applications in numerical relativity (in progress).

WHY DO WE BELIEVE THIS IS THE CANONICAL DISCRETIZATION?



Patterns for discretization for $Alt^i \otimes Alt^j$ (*j*-form-valued *i*-forms):

- cohomology is correct, isomorphic to continuous version
- ▶ $i \leq j$: functions, i > j: Dirac deltas, transition happens at BGG zig-zag
- (*i*, *j*) dual to (j, i); (i, j) dual to (n i, n j), Hessian complex dual to divdiv, elasticity 'self-adjoint'
- Function part ($i \le j$): *j*-form-valued *i*-forms discretized on *i*-cells attaching a *j*-form to an *i*-cochain
- delta part (i > j): j-form-valued i-forms means attaching j-forms to dual i-cells

EXTENSIONS AND OUTLOOK

1 Continuous level: BGG construction (review)

2 Discrete level: finite elements	0
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3	Exter	nsions and outlook
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General principle: choosing spaces such that Dirac delta is evaluated only on continuous functions.

Poisson (reinterpretation): seek $u \in C^0 \mathcal{P}_1(\mathcal{T}_h)$, such that

. . .

 $(\nabla u, \nabla v) = (f, v), \forall v \in C^0 \mathcal{P}_1(\mathcal{T}_h) \subset H^1.$

 $\langle -\Delta u, v \rangle = (f, v), \Delta u = \text{div grad } u$: edge (tangential) measure, can be paired with $v \in C^0$ \checkmark

Linear elasticity: $(\operatorname{div} \sigma, \boldsymbol{u}) = -(\sigma, \operatorname{def} \boldsymbol{u})$. σ : symmetric matrix, \boldsymbol{u} : vector

regular *u* (displacement formulation): *u* ∈ C⁰, σ discontinuous locking: deterioate with parameters
 regular σ (Hellinger-Reissner): σ ⋅ *n* continuous difficult to construct
 in between (distributional): *n* ⋅ σ ⋅ *n* continuous robust

div σ : tangential delta, **u** has continuous tangential \checkmark (TDNNS, Pechstein, Schöberl 2011)

Benefit of distributional-FE-based methods:

- canonical degrees of freedom,
- intrinsic (coordinate-independent, e.g., Regge elements using edge lengths as DoFs) and discrete geometric interpretations,

Intrinsic Finite Elements, potential generalizations to other contexts

invariance under pullbacks useful for assembling FE matrices and mapping to curved manifolds such as shells.

Consequences of the canonical algebraic/geometric structures.



In 1D, 2D, 3D:

- twisted complexes: Timoshenko beam, Reissner-Mindlin plate, Cosserat elasticity
- BGG complexes: Euler-Bernoulli beam, Kirchhoff-Love plate, standard elasticity.

Mechanics interpretation of BGG construction: eliminating microstructure variables (e.g., pointwise rotation) or torsion from twisted complexes via cohomology-preserving projections.

EXTENDED REGGE COMPLEX: A DISCRETE RIEMANN-CARTAN GEOMETRY

Extending Regge complex to the entire diagram - extending discrete curvature to discrete Riemann-Cartan geometry (curvature+torsion).



A DIFFERENT PICTURE: HOW TO CHARACTERIZE HIGH-ORDER TENSORS?

Young tableau



Peter Olver, 'Differential hyperforms' 1982.

Discretization: ongoing work with Jay Gopalakrishnan (Portland), Joachim Schöberl (Vienna).

SUMMARY

- Take-home message : using currents as distributional finite elements to obtain canonical discretization of tensor fields and intrinsic finite elements.
- Further directions
 - higher dimension, general form degree and tensor type (e.g., Riemannian tensor), towards a Finite Element Tensor Calculus;
 - two traditions: lattice methods (e.g., Discrete Exterior Calculus (DEC), discrete physics; intuitive but not much convergence theory) and finite element type methods (systematic and rigorous, but less flexible) getting closer with distributional elements.

DEC: *defining* operators, heuristic and not unique. Distributional FEs: rigorous calculation in the sense of distributions, unique.

- distributions bring in subtle analytic issues (esp. nonlinear problems) → measure-valued solutions of PDEs.
- An Erlangen program for mechanics?

[sequences \Leftrightarrow geometry/algebra \Leftrightarrow mechanics models] \longleftarrow finite element exterior calculus

Einstein equations.

- Complexes from complexes, D.N. Arnold, KH; Foundations of Computational Mathematics (2021). framework, analytic results from homological algebraic structures
- BGG sequences with weak regularity and applications, A. Čap, KH; Foundations of Computational Mathematics (2023) more general framework, conformal complexes
- Nonlinear elasticity complex and a finite element diagram chase, KH; Springer INdAM Series "Approximation Theory and Numerical Analysis Meet Algebra, Geometry, Topology" (2023). nonlinear complex, diagram chase
- Extended Regge complex for linearized Riemann-Cartan geometry and cohomology, S.H. Christiansen, KH, T. Lin, arXiv (2023) cohomology of Regge sequence, extensions to torsion
- Distributional Hessian and divdiv complexes on triangulation and cohomology, KH, T. Lin, Q. Zhang arXiv (2023) distributional Hessian and divdiv complexes