DISTRIBUTIONAL FINITE ELEMENTS AND COMPLEXES

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A BRIEF OVERVIEW

Finite element exterior calculus (FEEC) recognizes that understanding and preserving differential structures is important for numerical PDEs.

For scalar and vector problems (Poisson, Maxwell, Stokes...), de Rham complexes encode these structures. For tensor-valued problems (continuum mechanics, geometry, relativity...), we will see that the Bernstein-Gelfand (BGG) sequences play the corresponding role on the continuous level.

Classical de Rham finite elements (Whitney forms: Lagrange, Nédélec, Raviart-Thomas...) are canonical and have a topological meaning. Nevertheless, tensor-valued problems are much more difficult to discretize. We ask the question: Can we generalize the classics of finite elements? We also want to achieve discrete topological/geometric meanings, as they allow potential generalization to operators/PDEs on graphs/discrete structures.

We will argue that, to achieve this, we have to generalize the definition of finite elements.

DE RHAM COMPLEXES

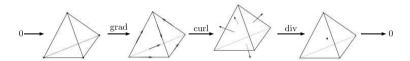
CONTINUOUS

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

- ▶ complex property: $d^k \circ d^{k-1} = 0$, $\Rightarrow \mathcal{R}(d^{k-1}) \subset \mathcal{N}(d^k)$, curl \circ grad $= 0 \Rightarrow \mathcal{R}(\mathsf{grad}) \subset \mathcal{N}(\mathsf{curl})$, div \circ curl $= 0 \Rightarrow \mathcal{R}(\mathsf{curl}) \subset \mathcal{N}(\mathsf{div})$
- ▶ cohomology: $\mathcal{H}^k := \mathcal{N}(d^k)/\mathcal{R}(d^{k-1})$, $\mathcal{H}^0 := \mathcal{N}(\mathsf{grad})$, $\mathcal{H}^1 := \mathcal{N}(\mathsf{curl})/\mathcal{R}(\mathsf{grad})$, $\mathcal{H}^2 := \mathcal{N}(\mathsf{div})/\mathcal{R}(\mathsf{curl})$
- 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 $u = 0 \Rightarrow u = \operatorname{grad} \phi$, div $v = 0 \Rightarrow v = \operatorname{curl} \psi$.

DE RHAM COMPLEXES

DISCRETE



$$0 \longrightarrow \mathcal{P}_1 \stackrel{\mathsf{grad}}{\longrightarrow} [\mathcal{P}_0]^3 + [\mathcal{P}_0]^3 \times x \stackrel{\mathsf{curl}}{\longrightarrow} [\mathcal{P}_0]^3 + \mathcal{P}_0 \otimes x \stackrel{\mathsf{div}}{\longrightarrow} \mathcal{P}_0 \longrightarrow 0.$$

Raviart-Thomas (1977), Nédélec (1980) in numerical analysis, Bossavit (1988), Hiptmair (1999) for differential forms, Whitney (1957) for studying topology.

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).

Question: how to discretize/define quantities (spaces, operators, PDEs etc.) on discrete structures (triangulation, graphs etc.) in a structured way?

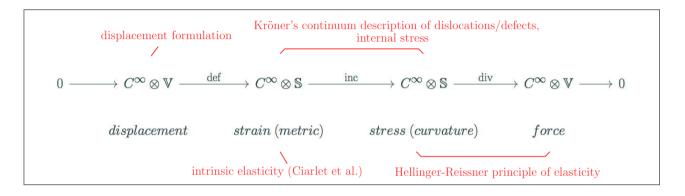
electromagnetism (electric/magnetic fields), fluid mechanics (velocity, vorticity), solid mechanics (strain, stress, defects, microstructures), plates and shells (bending moment, shear stress), geometry (metric, scalar/Ricci/Riemann curvature, Einstein/Weyl/Cotton tensors, torsion), gravitational waves (transverse-traceless tensors)...

Continuous level: Bernstein-Gelfand-Gelfand (BGG) construction (with surprising connections!)

Discrete level: What are the analogue of Whitney forms?

CONTINUOUS LEVEL: BGG CONSTRUCTION

EXAMPLE: ELASTICITY (KRÖNER, CALABI) COMPLEX



$$\mathbb{V} := \mathbb{R}^3 \text{ vectors}, \quad \mathbb{S} := \mathbb{R}^{3\times3}_{\text{sym}} \text{ symmetric matrices}$$

$$\text{def } u := 1/2(\nabla u + \nabla u^T), \quad (\text{def } u)_{ij} = 1/2(\partial_i u_j + \partial_j u_i).$$

$$\text{inc } g := \nabla \times g \times \nabla, \quad (\text{inc } g)^{ij} = \epsilon^{ikl} \epsilon^{jst} \partial_k \partial_s g_{lt}.$$

$$\text{div } v := \nabla \cdot v, \quad (\text{div } v)_i = \partial^j u_{ij}.$$

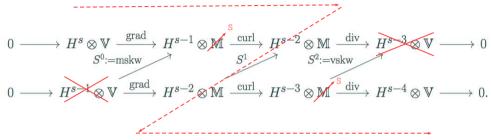
$$g \text{ metric } \Rightarrow \text{inc } g \text{ linearized Einstein tensor } (\backsimeq \text{Riem } \backsimeq \text{Ric in 3D})$$

$$\text{inc } \circ \text{def } = 0 \text{: Saint-Venant compatibility}$$

$$\text{div } \circ \text{inc } = 0 \text{: Bianchi identity}$$

DERIVATION: COMPLEXES FROM COMPLEXES

ARNOLD, KH 2021



$$S^1u:=u^T-\operatorname{tr}(u)I.$$

Output: elasticity complex

$$0 \longrightarrow H^s \otimes \mathbb{V} \xrightarrow{\text{def}} H^{s-1} \otimes \mathbb{S} \xrightarrow{\text{curl}} H^{s-3} \otimes \mathbb{S} \xrightarrow{\text{div}} H^{s-4} \otimes \mathbb{V} \longrightarrow 0.$$

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

From algebra to analysis: finite dimensional cohomology \Longrightarrow operators have closed range Hodge decomposition, Poincaré-Korn inequalities, existence of regular potentials, compactness, div-curl lemma, etc.

BGG: GENERAL RECIPE

- ▶ input: $(Z^{\bullet}, D^{\bullet})$, $(\tilde{Z}^{\bullet}, \tilde{D}^{\bullet})$, connecting maps $S^i : \tilde{Z}^i \to Z^{i+1}$, satisfying
 - (anti-)commutativity: $S^{i+1}\tilde{D}^i = -D^{i+1}S^i$,
 - injectivity/surjectivity condition: S^i injective for $i \leq J$, surjective for $i \geq J$.

$$0 \longrightarrow Z^{0} \xrightarrow{D^{0}} Z^{1} \xrightarrow{D^{1}} \cdots \xrightarrow{D^{n-1}} Z^{n} \longrightarrow 0$$

$$0 \longrightarrow \tilde{Z}^{0} \xrightarrow{\tilde{D}^{0}} \tilde{Z}^{1} \xrightarrow{\tilde{D}^{1}} \cdots \xrightarrow{\tilde{D}^{n-1}} \tilde{Z}^{n} \longrightarrow 0$$

output:

$$\cdots \longrightarrow \operatorname{coker}(S^{J-2}) \xrightarrow{D^{J-1}} \operatorname{coker}(S^{J-1}) \xrightarrow{D^J} \\ \stackrel{\tilde{D}^J}{\longrightarrow} \mathcal{N}(S^{J+1}) \xrightarrow{\tilde{D}^{J+1}} \mathcal{N}(S^{J+2}) \xrightarrow{\tilde{D}^{J+2}} \cdots$$

conclusion:

$$\dim \mathcal{H}^{i}\left(\Upsilon^{\bullet}, \mathcal{D}^{\bullet}\right) = \dim \mathcal{H}^{i}\left(Z^{\bullet}, D^{\bullet}\right) + \dim \mathcal{H}^{i}\left(\tilde{Z}^{\bullet}, \tilde{D}^{\bullet}\right), \quad \forall i = 0, 1, \cdots, n.$$

Inspired by Bernstein-Gelfand (BGG) resolution (Eastwood 2000, Čap,Slovák,Souček 2001, Arnold,Falk,Winther 2006)

BGG IN 1D

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

$$0 \longrightarrow H^2 \xrightarrow{\partial_x} H^1 \longrightarrow 0$$

$$0 \longrightarrow H^1 \xrightarrow{\partial_x} L^2 \longrightarrow 0.$$

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

ND: FORMS WITH DOUBLE INDICES

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

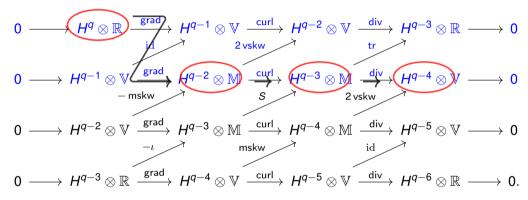
$$0 \longrightarrow H^{q-1} \otimes \operatorname{Alt}^{0,J} \xrightarrow{d} H^{q-2} \otimes \operatorname{Alt}^{1,J} \xrightarrow{d} \cdots \xrightarrow{d} H^{q-n-1} \otimes \operatorname{Alt}^{n,J} \longrightarrow 0$$
where $\operatorname{Alt}^{i,J} := \operatorname{Alt}^{i} \otimes \operatorname{Alt}^{J}$

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

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

3D VECTOR/MATRIX PROXIES

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



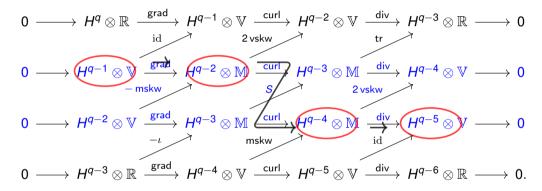
Hessian complex:

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

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

3D VECTOR/MATRIX PROXIES

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



elasticity complex:

$$0 \longrightarrow H^{q-1} \otimes \mathbb{V} \stackrel{\mathsf{def}}{\longrightarrow} H^{q-2} \otimes \mathbb{S} \stackrel{\mathsf{inc}}{\longrightarrow} H^{q-4} \otimes \mathbb{S} \stackrel{\mathsf{div}}{\longrightarrow} H^{q-5} \otimes \mathbb{V} \longrightarrow 0.$$
 elasticity, defects, metric, curvature

3D VECTOR/MATRIX PROXIES

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

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

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

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

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

divdiv complex:

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

DISCRETE LEVEL

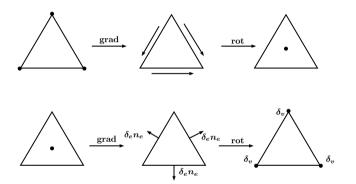
Goal: discrete spaces fitting in complexes.

- ▶ 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
- ▶ nD: Chen-Huang 2021 (last two spaces), 2D arbitrary regularity: Chen-Huang 2022, Bonizzoni-KH-Kanschat-Sap 2023
- conformal complexes: open.

What is the analogue of Whitney forms (lowest order Lagrange, Nédélec, RT...)?

encode topological/geometric information
 canonical dofs (allowing generalizations)

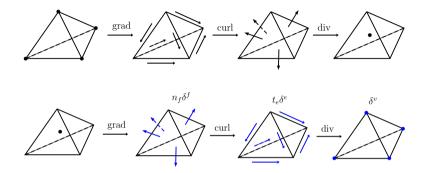
DISTRIBUTIONAL COMPLEXES: 2D DE RHAM (BRAESS, SCHÖBERL 2008)



$$\begin{array}{ll} \textit{grad of p.w. constants:} & \text{for } \phi \in \textit{\textbf{C}}_0^\infty \colon \\ \langle \operatorname{grad} u, \phi \rangle := -(u, \operatorname{div} \phi) = -\sum_T \int_T u \operatorname{div} \phi = \sum_{\partial T} \int_{\partial T} u(\textbf{\textit{n}} \cdot \phi) = \sum_e \langle [u]_e \textbf{\textit{n}} \delta_e, \phi \rangle \\ & \Longrightarrow \operatorname{grad} u = [u]_e \textbf{\textit{n}} \delta_e. \\ \\ \textit{rot of normal deltas } \textbf{\textit{v}} = \sum_e c_e \textbf{\textit{n}} \delta_e \colon & \text{for } \psi \in \textit{\textbf{C}}_0^\infty \colon \\ \langle \operatorname{rot} \textbf{\textit{v}}, \psi \rangle := -\langle \textbf{\textit{v}}, \operatorname{curl} \psi \rangle = -\sum_e \int_e c_e \textbf{\textit{n}} \cdot \operatorname{curl} \psi = -\sum_e \int_e c_e \partial_\tau \psi = \sum_{} \operatorname{vertex terms} \\ & \Longrightarrow \operatorname{rot} \textbf{\textit{v}} = [\textbf{\textit{v}} \cdot \boldsymbol{\tau}]_v \delta_v. \end{array}$$

(... and some traces of DG emerge here.)

DISTRIBUTIONAL COMPLEXES: 3D DE RHAM



Perspectives:

- Finite element perspective: dual, complex of degrees of freedom
- ► DEC perspective: complex on dual meshes
- ► Fluid perspective: point vortex, vortex lines... (delta on codim 2) (V.I.Arnold,B.Khesin, Topological methods in hydrodynamics)





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

SOLVING PDES USING DISTRIBUTIONAL ELEMENTS

General principle: evaluating Dirac delta only on continuous functions.

Poisson (trivial example): $(\nabla u, \nabla v) = (f, v)$, $\forall v \in \text{Lagrange}$. Equivalently, $\langle -\Delta u, v \rangle = (f, v)$. u in Lagrange, ∇u in Nédélec, div $\nabla u \in \delta_F$. Evaluating δ_F on v (legal since u single-valued!)

Linear elasticity: (div σ , \boldsymbol{u}). σ : symmetric matrix, \boldsymbol{u} : vector

Displacement formulation: $\mathbf{u} \in C^0$, $\sigma \in DG$, locking

Hellinger-Reissner: $\boldsymbol{u} \in DG, \boldsymbol{n} \cdot \sigma \in C^0$ hard to discretize

Tangential-Displacement-Normal-Normal-Stress (TDNNS, Pechstein, Schöberl 2011):

 $\mathbf{n} \cdot \sigma \cdot \mathbf{n} \in C^0$ (weaker than H(div)). $\text{div } \sigma \in \tau \delta_F$. $(\text{div } \sigma, v)$ is legal if v in Nédélec!

Biharmonic: $\sigma = \text{hess } u$, div div $\sigma = f$.

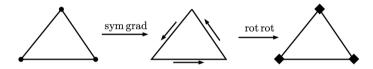
Hellen-Herrmann-Johnson (HHJ): $\mathbf{n} \cdot \sigma \cdot \mathbf{n} \in C^0$, div div $\sigma \in \delta_V$. Pair (div div σ, v) is legal if v is in Lagrange.

. . .

DISTRIBUTIONAL COMPLEXES?

2D rot rot COMPLEX





Rotation of HHJ (div \sim rot, $\boldsymbol{n} \sim \boldsymbol{\tau}$), rot rot: linearized Gauss curvature.

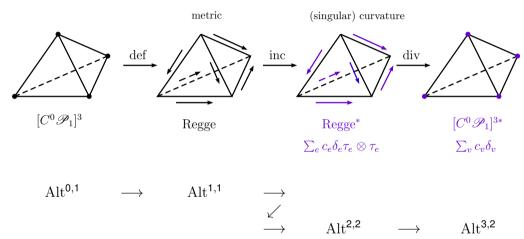
Discrete curvature: angle deficit at vertices (discrete geometric approach), δ_V (finite element approach).



Cohomology can be reduced to de Rham with BGG diagrams.

3D ELASTICITY COMPLEX: ANALOGUE OF WHITNEY FORMS?

Christiansen 2011: Regge calculus = finite elements

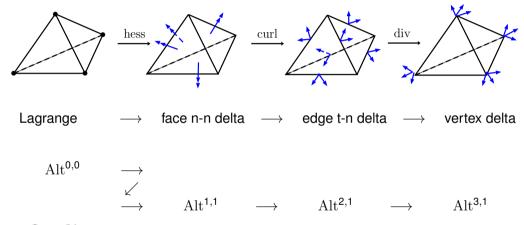


Regge calculus: quantum and numerical relativity, discrete geometry. Metric given by edge lengths; curvature as angle deficit.

Regge finite element: Metric: p.w. constant sym matrices, $\int_e t_e \cdot g \cdot t_e$ as dofs. Curvature: distributional (delta on codim 2).

nD: Lizao Li (2018 UMN thesis), nonlinear curvature with Regge elements (Berchenko-Kogan, Gawlik 2022, Gopalakrishnan, Neunteufel, Schöberl, Wardetzky 2022, Gawlik, Neunteufel 2023)

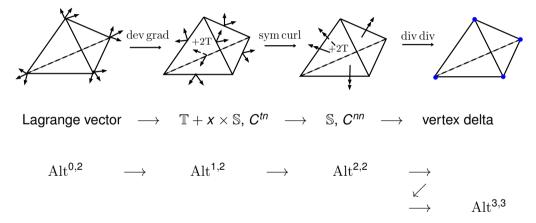
3D HESSIAN



Cohomology: $\mathcal{P}_1 \otimes \mathcal{H}_{deRham}$

- ▶ Step 1: define an auxiliary sequence, cohomology = homology with \mathcal{P}_1 coefficients (resolution of \mathcal{P}_1)
- ► Step 2: cohomology of original complex = cohomology of auxiliary sequence (diagram chase, snake lemme)

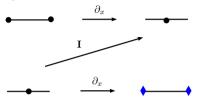
3D DIVDIV



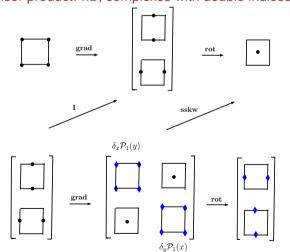
Almost dual of Hessian complex , except for two interior dofs for unisolvency. $\mathbb{T} + x \times \mathbb{S}$: analogy of Koszul (automatically trace-free, symbol version of curl $\mathbb{S} \subset \mathbb{T}$).

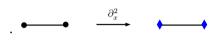
CUBES: TENSOR PRODUCT STRUCTURES

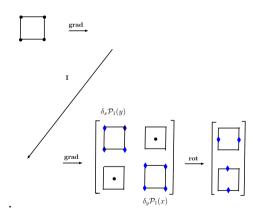
1D diagram



Tensor product: nD, complexes with double indices



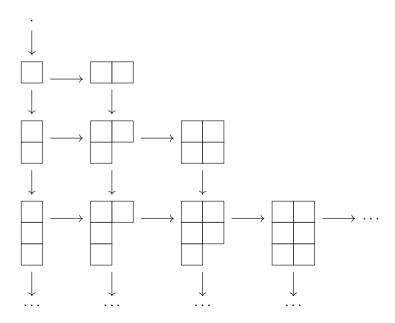


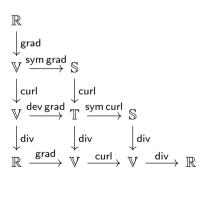


A DIFFERENT PICTURE: HOW TO CHARACTERIZE HIGH-ORDER TENSORS?

Young tableaux (representation theory)

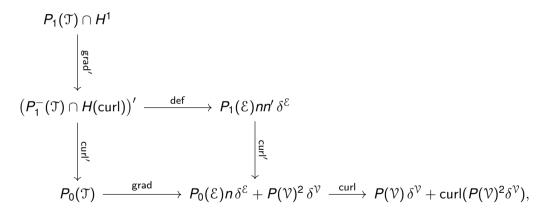
- number of boxes: order of tensors,
- ► shape: symmetry of tensors.





20/22

Distributional elements in 2D, 3D (Gopalakrishnan,KH,Schöberl).



SUMMARY

- What is the generalization of Whitney forms? Distributional elements seem to be flexible to allow a topological/geometric interpretation, and yet promising for analysis and computation.
- ▶ nD in progress.
- Further directions: solving PDEs, comparing to discrete curvature on graphs, discrete Riemann-Cartan geometry (torsion, defects of materials)...

References:

- Complexes from complexes, Douglas Arnold, KH; Foundations of Computational Mathematics (2021).framework, analytic results from homological algebraic structures
- BGG sequences with weak regularity and applications, Andreas Čap, KH; Foundations of Computational Mathematics (2023) more general framework, conformal complexes, applications
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- works with Ting Lin, Qian Zhang; Jay Gopalakrishnan, Joachim Schöberl. In preparation.