The Combinatorics of Finite Element Methods

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August 28, 2023

Outline

1. From finite elements to the Euler characteristic.
    - Finite element spaces let us numerically solve PDEs.
    - Using naïve finite element spaces can give us wrong answers.
    - Finite element spaces that do work well are related to the Euler characteristic $V - E + F$.
2. From the Euler characteristic to cohomology (1500s–1930s).
    - An introduction to Euler characteristic and cohomology.
    - Both numerical analysis and cohomology are ways of going between the continuous world and the discrete world.
        - Some finite element spaces developed by numerical analysts in the 1970s and 1980s were actually rediscoveries of spaces developed by geometers decades earlier.
3. From cohomology to finite elements (Arnold, Falk, Winther, 2006–2010).
    - Finite element spaces that respect cohomology work well.
    - Finite element spaces that do not respect cohomology might give wrong answers.

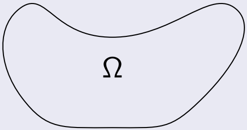
Numerically solving PDEs

Sample Problem

- Given $f\colon \Omega \to \mathbb{R}$, find $u\colon \Omega \to \mathbb{R}$ such that

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f$$

and u vanishes on the boundary.

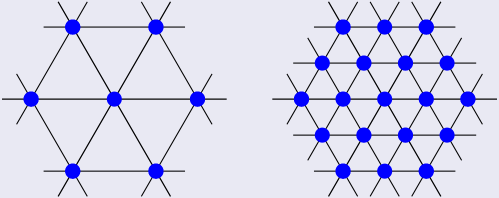


Discretization

- To solve numerically, we must discretize.
- We need a finite-dimensional space of functions that "approximates" the full infinite-dimensional space of possible u.

Finite-dimensional function spaces

Continuous piecewise linear functions to $\mathbb{R}$



Continuous piecewise polynomial functions to $\mathbb{R}$

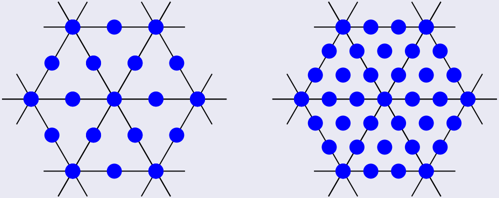
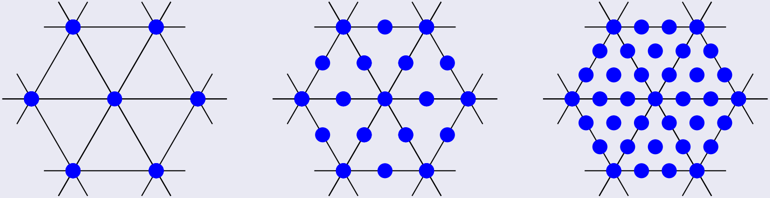


Figure: Piecewise quadratic (left) and piecewise cubic (right)

Degrees of freedom

Piecewise linear/quadratic/cubic continuous scalar-valued functions



Degrees of freedom (DOFs)

- One value per degree of freedom (blue dot)
  - yields a unique function on each triangle, and
  - enforces continuity between adjacent triangles.

Piecewise linear	$\mathbb{R}^{V}$
Piecewise quadratic	$\mathbb{R}^{V+E}$
Piecewise cubic	$\mathbb{R}^{V+2E+F}$

What about vector fields?

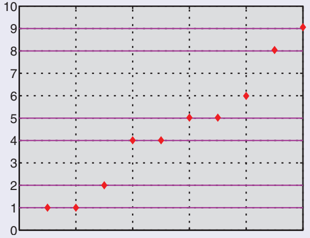
A naïve approach

Use continuous piecewise polynomial vector fields.

Eigenvalues of the curl curl operator

On a square domain, find a vector field u (with appropriate boundary conditions) such that $\operatorname{curl}\operatorname{curl} u = \lambda u$.

Bad things happen with the naïve approach (AFW, 2010)



- Using vector fields with full continuity yields false eigenvalue $\lambda = 6$.
- To get the right eigenvalues, we need better finite element spaces of vector fields.

Gradients of piecewise smooth scalar fields

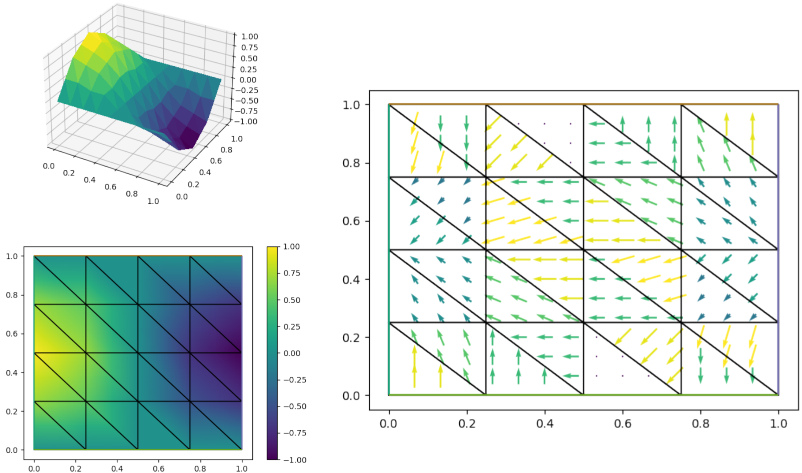


Figure: A piecewise linear function (left) and its gradient (right)

Finite-dimensional spaces of vector fields

Continuity conditions

- We want only tangential continuity, not full continuity.

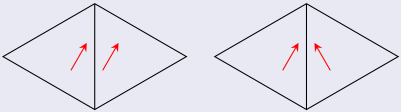


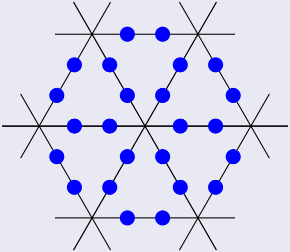
Figure: Full continuity (left) vs. tangential continuity (right)

- Why do these spaces work better?
  - Gradients of continuous piecewise smooth scalar fields only have tangential continuity.
    - Gradients of "valid objects" should be "valid objects".
  - Having well-defined line integrals requires only tangential continuity.

Degrees of freedom (DOFs)

DOFs of piecewise linear vector fields with tangential continuity?

- Values should
  - uniquely specify a linear vector field on each triangle, and
  - enforce tangential continuity between adjacent triangles.



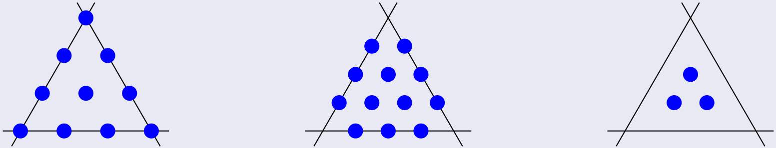
Higher degree?

Periodic Table of the Finite Elements

Complexes

A discrete complex

continuous piecewise cubic scalar fields $\xrightarrow{\text{grad}}$ tangentially continuous piecewise quadratic vector fields $\xrightarrow{\text{curl}}$ discontinuous piecewise linear scalar fields



$$\mathbb{R}^{V+2E+F} \longrightarrow \mathbb{R}^{3E+3F} \longrightarrow \mathbb{R}^{3F}$$

Euler characteristic

- This complex has the right Euler characteristic:

$$(V + 2E + F) - (3E + 3F) + 3F = V - E + F.$$

Euler characteristic

$V - E + F = 2$ (Maurolico, 1537)

Name	Image	Vertices V	Edges E	Faces F	Euler characteristic: $\chi = V - E + F$
Tetrahedron		4	6	4	**2**
Hexahedron or cube		8	12	6	**2**
Octahedron		6	12	8	**2**
Dodecahedron		20	30	12	**2**
Icosahedron		12	30	20	**2**

Figure: Wikipedia, "Euler characteristic"

Works for all convex polyhedra

Soccer ball:

$$V - E + F = 60 - 90 + 32 = 2.$$

Euler characteristic for other shapes

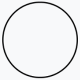
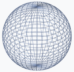
Name	Image	χ
Interval		**1**
Circle		**0**
Disk		**1**
Sphere		**2**
Torus *(Product of two circles)*		**0**
Double torus		**−2**
Triple torus		**−4**

Figure: Wikipedia, "Euler characteristic"

Vector calculus in the plane (or on a surface)

$$\text{scalar fields} \xrightarrow{\text{grad}} \text{vector fields} \xrightarrow{\text{curl}} \text{scalar fields}$$

- If $E = \operatorname{grad} \phi$, then $\operatorname{curl} E = 0$. always true
- If $\operatorname{curl} E = 0$, then $E = \operatorname{grad} \phi$ for some ϕ. not always true

curl $E = 0$ but $E \neq \operatorname{grad} \phi$

The electric field around a solenoid

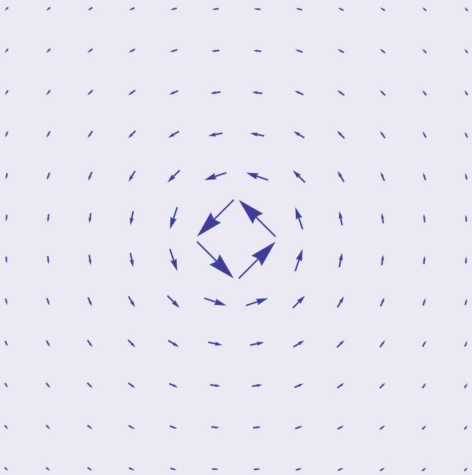


Figure: Wikipedia, "Irrotational vector field"

de Rham cohomology

The de Rham complex

$$\text{scalar fields} \xrightarrow{\text{grad}} \text{vector fields} \xrightarrow{\text{curl}} \text{scalar fields}$$

The first cohomology group H^1

- Informally, the first cohomology group of a domain Ω is the set of counterexamples:
  - Vector fields E on Ω
    - whose curls are zero, but
    - which aren't gradients of a scalar field.
- Caveat: If E is a counterexample, then so is $E' := E + \operatorname{grad}\psi$.
  - $\operatorname{curl} E' = \operatorname{curl} E + 0 = 0$.
  - If E is not a gradient then neither is E'.
- In the first cohomology group H^1, we view E and E' as "equivalent counterexamples".
- $\dim H^1$ counts the number of "holes" in the domain.

de Rham cohomology

The de Rham complex

$$\text{scalar fields} \xrightarrow{\text{grad}} \text{vector fields} \xrightarrow{\text{curl}} \text{scalar fields}$$

de Rham cohomology, informally

- H^0: scalar fields ϕ whose gradients are zero.
- H^1: vector fields E whose curls are zero but which aren't gradients.
- H^2: scalar fields ρ which aren't curls.

The zeroth cohomology group H^0

- If $\operatorname{grad} \phi = 0$ then ϕ is constant only for connected domains.
- So $\dim H^0 = 1$ for connected domains.
- $\dim H^0$ counts the number of connected components of the domain.

de Rham cohomology

The de Rham complex

$$\text{scalar fields} \xrightarrow{\text{grad}} \text{vector fields} \xrightarrow{\text{curl}} \text{scalar fields}$$

de Rham cohomology, informally

- H^0: scalar fields ϕ whose gradients are zero.
- H^1: vector fields E whose curls are zero but which aren't gradients.
- H^2: scalar fields ρ which aren't curls.

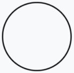
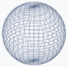
The second cohomology group H^2

- For planar domains $H^2 = 0$ (every scalar field is a curl).
- For a closed surface S (e.g. sphere), H^2 is the constants.
  - If B is tangent to S then $\int_S \operatorname{curl} B = 0$ by Stokes's theorem.
  - But $\int_S 1 \neq 0$, so 1 is not a curl.

Cohomology tells you the Euler characteristic

The Euler characteristic is

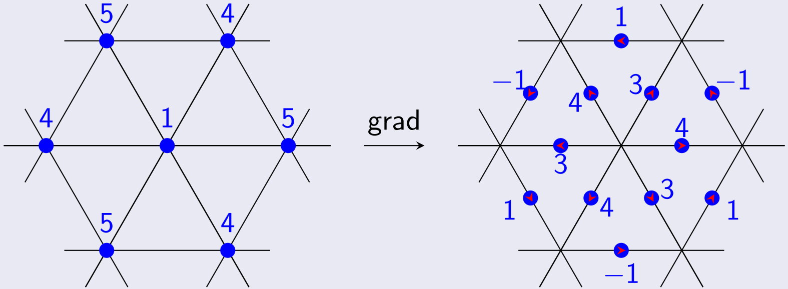
$$\begin{array}{ccccc} V & - & E & + & F, \\ \dim H^0 & - & \dim H^1 & + & \dim H^2. \end{array}$$

Name	Image	χ
Interval		1
Circle		0
Disk		1
Sphere		2
Torus *(Product of two circles)*		0
Double torus		−2
Triple torus		−4

From Euler characteristic to cohomology (1930s)

The discrete setting

Discrete gradient

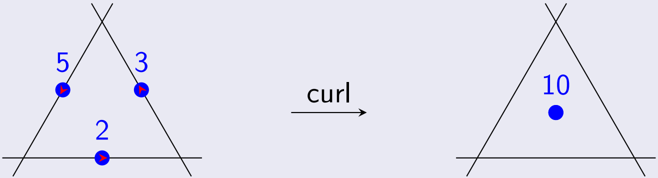


Fundamental theorem of line integrals

$$\int_C \operatorname{grad}\phi = \phi\Big|_{v_0}^{v_1}$$

for a curve C from point v_0 to point v_1.

Discrete curl



Green's/Stokes's Theorem

$$\int_S \operatorname{curl} E = \int_C E$$

where C is the boundary of the surface S.

From Euler characteristic to cohomology (1930s)

The continuous complex (de Rham complex)

$$\text{scalar fields} \xrightarrow{\text{grad}} \text{vector fields} \xrightarrow{\text{curl}} \text{scalar fields}$$

The discrete complex (simplicial cochain complex)

$$\begin{array}{ccccc} \text{discrete} & \xrightarrow{\text{grad}} & \text{discrete} & \xrightarrow{\text{curl}} & \text{discrete} \\ \text{scalar fields} & & \text{vector fields} & & \text{scalar fields} \\ \mathbb{R}^V & \longrightarrow & \mathbb{R}^E & \longrightarrow & \mathbb{R}^F \end{array}$$

Theorem (De Rham's Theorem, 1931)

de Rham cohomology equals simplicial cohomology

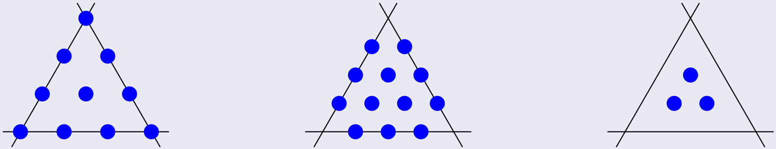
Corollary (Euler characteristic)

$$V - E + F = \dim H^0 - \dim H^1 + \dim H^2$$

Back to finite elements

We've already seen a different discrete complex

continuous piecewise cubic scalar fields $\xrightarrow{\text{grad}}$ tangentially continuous piecewise quadratic vector fields $\xrightarrow{\text{curl}}$ discontinuous piecewise linear scalar fields



$$\mathbb{R}^{V+2E+F} \longrightarrow \mathbb{R}^{3E+3F} \longrightarrow \mathbb{R}^{3F}$$

Euler characteristic and cohomology

- We saw this complex has the right Euler characteristic:

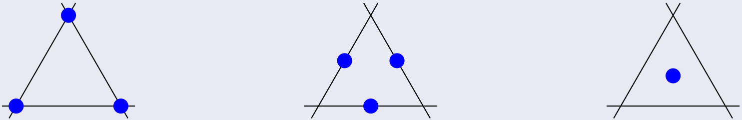
$$(V+2E+F)-(3E+3F)+3F = V-E+F.$$

- Moreover, the cohomology is right, too.
    - That's why the spaces work well (Arnold, Falk, Winther, 2006).

Can we interpret simplicial cochains as finite elements?

Yes (Whitney, 1957)

$$\mathbb{R}^V \longrightarrow \mathbb{R}^E \longrightarrow \mathbb{R}^F$$



continuous piecewise linear scalar fields $\xrightarrow{\text{grad}}$ span of Whitney forms $\xrightarrow{\text{curl}}$ discontinuous piecewise constant scalar fields

Barycentric coordinates (the standard simplex)

$$\{(\lambda_1, \lambda_2, \lambda_3) \in \mathbb{R}^3_{\geq 0} \mid \lambda_1 + \lambda_2 + \lambda_3 = 1\}$$

Whitney one-forms:

$$\lambda_1\, d\lambda_2 - \lambda_2\, d\lambda_1,$$
$$\lambda_2\, d\lambda_3 - \lambda_3\, d\lambda_2,$$
$$\lambda_3\, d\lambda_1 - \lambda_1\, d\lambda_3.$$

A modern language for vector calculus

The complex

- Vector calculus:

$$\text{scalar fields} \xrightarrow{\text{grad}} \text{vector fields} \xrightarrow{\text{curl}} \text{vector fields} \xrightarrow{\text{div}} \text{scalar fields}$$

- Cartan, 1899:

$$\text{0-forms} \xrightarrow{d} \text{1-forms} \xrightarrow{d} \text{2-forms} \xrightarrow{d} \text{3-forms}$$

Fundamental theorem

- Vector calculus:
  - fundamental theorem of calculus/line integrals,
  - Green's/Stokes's theorem,
  - the divergence theorem.
- Cartan, 1945:

$$\int_{\Omega} d\omega = \int_{\partial\Omega} \omega.$$

Definition (the $\mathcal{P}_r\Lambda^k$ spaces)

- Let $\mathcal{T}$ be a triangulation of a manifold of dimension n.
- Let $\mathcal{P}_r\Lambda^k(\mathcal{T})$ be the space of k-forms that
  - are piecewise polynomial of degree at most r, and
  - are tangentially continuous.

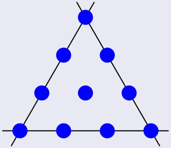
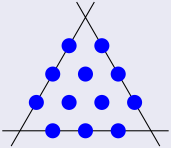
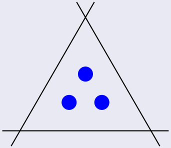
Example

$\mathcal{P}_r\Lambda^0(\mathcal{T})$	continuous piecewise polynomial scalar fields
$\mathcal{P}_r\Lambda^1(\mathcal{T})$	tangentially continuous piecewise polynomial vector fields
$\mathcal{P}_r\Lambda^{n-1}(\mathcal{T})$	normally continuous piecewise polynomial vector fields
$\mathcal{P}_r\Lambda^n(\mathcal{T})$	discontinuous piecewise polynomial scalar fields

Complexes revisited

We've seen

continuous piecewise cubic scalar fields $\xrightarrow{\text{grad}}$ tangentially continuous piecewise quadratic vector fields $\xrightarrow{\text{curl}}$ discontinuous piecewise linear scalar fields

$$\mathcal{P}_3\Lambda^0(\mathcal{T}) \xrightarrow{\quad d \quad} \mathcal{P}_2\Lambda^1(\mathcal{T}) \xrightarrow{\quad d \quad} \mathcal{P}_1\Lambda^2(\mathcal{T})$$

On a single simplex T

- The Whitney k-forms have one DOF per k-dimensional face.
- Call their span $\mathcal{P}_1^-\Lambda^k(T)$.
  - Note: $\mathcal{P}_0\Lambda^k(T) \subseteq \mathcal{P}_1^-\Lambda^k(T) \subseteq \mathcal{P}_1\Lambda^k(T)$.
- Multiply Whitney forms by arbitrary scalar-valued polynomials of degree at most $r-1$. Call the span of these $\mathcal{P}_r^-\Lambda^k(T)$.
  - So, $\mathcal{P}_{r-1}\Lambda^k(T) \subseteq \mathcal{P}_r^-\Lambda^k(T) \subseteq \mathcal{P}_r\Lambda^k(T)$.

Definition (the $\mathcal{P}_r^-\Lambda^k$ spaces on a triangulation)

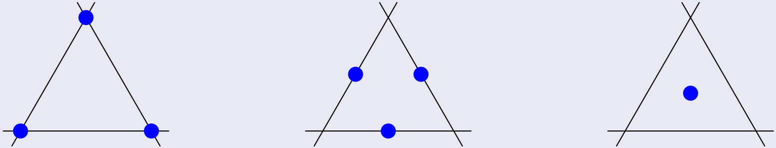
- Let $\mathcal{T}$ be a triangulation of a manifold of dimension n.
- Let $\mathcal{P}_r^-\Lambda^k(\mathcal{T})$ be the space of k-forms that
  - are in $\mathcal{P}_r^-\Lambda^k(T)$ for each element T of the triangulation, and
  - are tangentially continuous.

Duality between $\mathcal{P}$ and $\mathcal{P}^-$

Complexes revisited

We've also seen

continuous piecewise linear scalar fields $\xrightarrow{\text{grad}}$ Whitney forms $\xrightarrow{\text{curl}}$ discontinuous piecewise constant scalar fields



$$\mathcal{P}_1^-\Lambda^0(\mathcal{T}) \xrightarrow{\quad d \quad} \mathcal{P}_1^-\Lambda^1(\mathcal{T}) \xrightarrow{\quad d \quad} \mathcal{P}_1^-\Lambda^2(\mathcal{T})$$

More complexes

Theorem (Arnold, Falk, Winther, 2006)

For a triangulation $\mathcal{T}$, the cohomology of the complexes

$$\mathcal{P}_r\Lambda^0(\mathcal{T}) \xrightarrow{d} \mathcal{P}_{r-1}\Lambda^1(\mathcal{T}) \xrightarrow{d} \cdots \xrightarrow{d} \mathcal{P}_{r-n}\Lambda^n(\mathcal{T})$$

$$\mathcal{P}_r^-\Lambda^0(\mathcal{T}) \xrightarrow{d} \mathcal{P}_r^-\Lambda^1(\mathcal{T}) \xrightarrow{d} \cdots \xrightarrow{d} \mathcal{P}_r^-\Lambda^n(\mathcal{T})$$

agrees with de Rham cohomology (provided $r \geq n$ in the first line).

Remark

The second line with $r = 1$ is isomorphic to simplicial cochains.

Theorem (Arnold, Falk, Winther, 2006)

We can "mix and match" using any of the maps

$$\mathcal{P}_r\Lambda^k(\mathcal{T}) \xrightarrow{d} \mathcal{P}_{r-1}\Lambda^{k+1}(\mathcal{T}), \qquad \mathcal{P}_r\Lambda^k(\mathcal{T}) \xrightarrow{d} \mathcal{P}_r^-\Lambda^{k+1}(\mathcal{T})$$

$$\mathcal{P}_r^-\Lambda^k(\mathcal{T}) \xrightarrow{d} \mathcal{P}_r^-\Lambda^{k+1}(\mathcal{T}), \qquad \mathcal{P}_r^-\Lambda^k(\mathcal{T}) \xrightarrow{d} \mathcal{P}_{r-1}\Lambda^{k+1}(\mathcal{T})$$

References

Douglas N. Arnold, Richard S. Falk, and Ragnar Winther.
Finite element exterior calculus, homological techniques, and applications.
Acta Numer., 15:1–155, 2006.

Douglas N. Arnold, Richard S. Falk, and Ragnar Winther.
Finite element exterior calculus: from Hodge theory to numerical stability.
Bull. Amer. Math. Soc. (N.S.), 47(2):281–354, 2010.

How do finite element spaces yield numerical methods?

Recall our sample problem

- Given $f : \Omega \to \mathbb{R}$, find $u : \Omega \to \mathbb{R}$ vanishing on $\partial\Omega$ such that

$$\Delta u = f.$$

- Equivalently,

$$\int_\Omega (\Delta u) v = \int_\Omega f v \qquad \forall\, v \text{ vanishing on } \partial\Omega.$$

- Intergating by parts,

$$-\int_\Omega \operatorname{grad} u \cdot \operatorname{grad} v = \int_\Omega f v \quad \forall\, v \text{ vanishing on } \partial\Omega. \tag{1}$$

Galerkin method

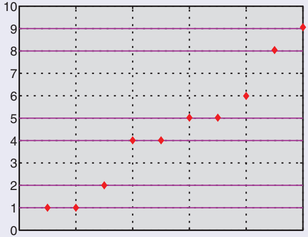
- Given f, solve (1) for u, where u and v are restricted to be in the finite element space.
- Get a finite-dimensional linear system of equations.

Bad things happen if we don't respect cohomology

Eigenvalues of the curl curl operator

On a square domain, find a vector field u (with appropriate boundary conditions) such that $\operatorname{curl}\operatorname{curl} u = \lambda u$.

Bad things happen if we do not respect cohomology (AFW, 2010)



- Using vector fields with full continuity yields false eigenvalue $\lambda = 6$.
- In contrast, using the spaces we've discussed yields the correct spectrum.

How does cohomology play a role?

- $\dim(\ker \operatorname{curl}) = \infty$, so zero eigenspace hard to control.
- Can control if $\ker \operatorname{curl} = \operatorname{im} \operatorname{grad}$ holds on the discrete level.

Good things happen if we do respect cohomology

Noether's Theorem, conservation laws, and discretization

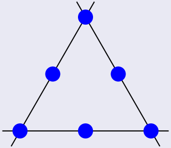
- Noether's theorem: a system that is invariant under a transformation has a corresponding conservation law:
  - translation invariance $\Rightarrow$ conservation of momentum
  - rotation invariance $\Rightarrow$ conservation of angular momentum
  - time-translation invariance $\Rightarrow$ conservation of energy
- Discretizations that respect Noether's theorem will conserve these quantities exactly.
  - Otherwise, the quantities will be conserved only approximately and may drift over time.

Charge conservation in electromagnetism / Yang-Mills

- $\operatorname{curl} u$ invariant under $u \mapsto u + \operatorname{grad} f$
- $\Rightarrow$ weighted average $\int \rho f$ conserved (ρ is charge).
  - continuous setting: all f allowed $\Rightarrow \rho$ conserved.
  - discrete setting: only f in finite element space (Nédélec, 1980).
- can conserve ρ even in discrete setting (—, Stern, 2021).

Bases for scalar fields

- Recall barycentric coordinates:
  $$\left\{(\lambda_1, \lambda_2, \lambda_3) \in \mathbb{R}^3_{\geq 0} \mid \lambda_1 + \lambda_2 + \lambda_3 = 1\right\}.$$
- Quadratic scalar fields have *monomial basis*
  $$\lambda_1^2, \quad \lambda_2^2, \quad \lambda_3^2, \quad \lambda_1\lambda_2, \quad \lambda_2\lambda_3, \quad \lambda_3\lambda_1.$$



Symmetry

- For scalar fields, the monomial basis is invariant under permuting $\lambda_1, \lambda_2, \lambda_3$.
- For vector fields, such an invariant basis may or may not exist, even up to sign.
  - In 2D and 3D, depends on the type of finite element space (e.g. $\mathcal{P}\Lambda^1$, $\mathcal{P}^-\Lambda^2$), and the polynomial degree modulo 3 (Licht, 2019; —, 2023).

Further directions

Riemannian geometry

So far we've discussed

- discretizing differential forms:
  - differential topology / smooth manifolds.

Riemannian geometry / Riemannian manifolds

- Must discretize the Riemannian metric:
  - Lowest order is just specifying the length of every edge of the triangulation (Regge, 1961).
  - Higher polynomial degree (Li, 2018).
- Must understand curvature:
  - Lowest order scalar curvature is just angle defect.
    - 2D: Gauss–Bonnett. General dimension: Regge, 1961.
  - Several papers towards full Riemann curvature tensor in general piecewise polynomial/smooth setting:
    - various combinations of —, Gawlik, Neunteufel, and others; 2019–2023 and in preparation.

Thank you