From Exact Sequences to Colliding Black Holes: Differential Complexes in Numerical Analysis

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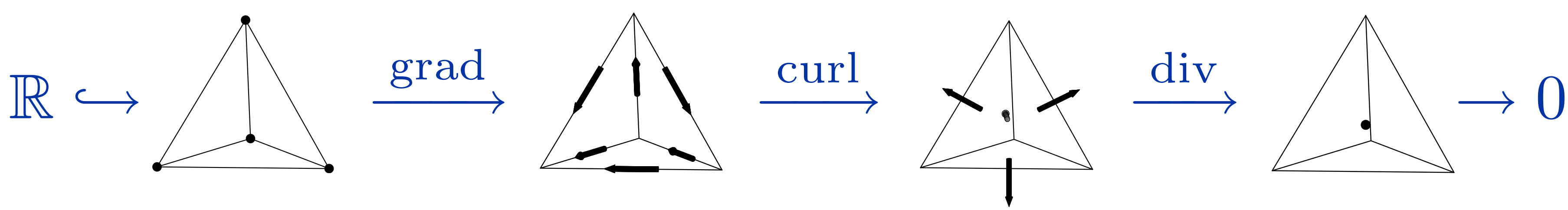

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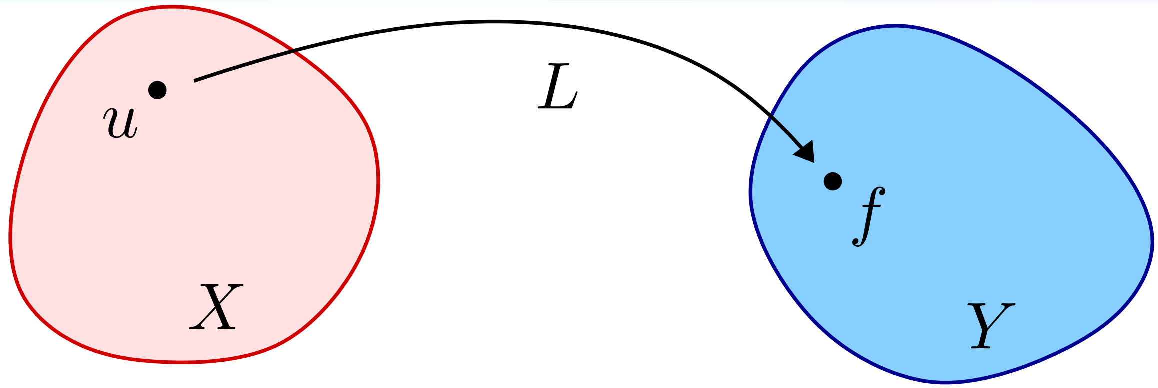
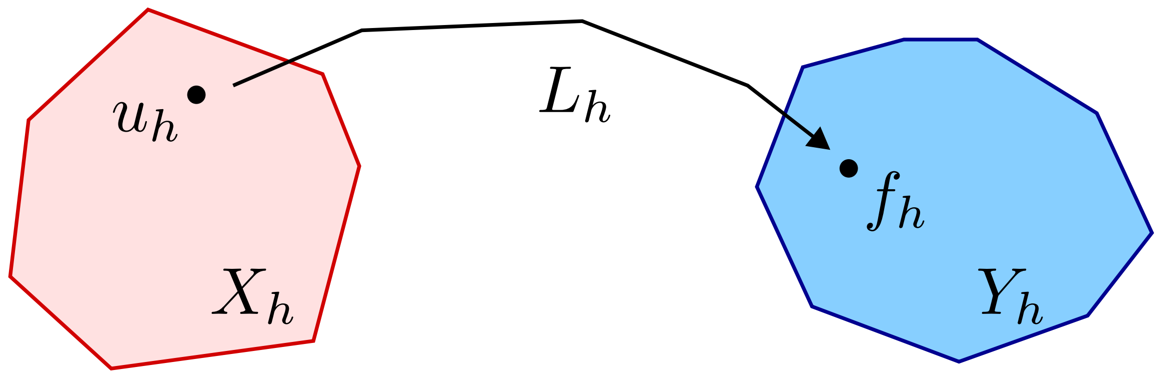
Fundamental metatheorem of numerical analysis



well-posed



consistency: (L_h, X_h, Y_h) close to (L, X, Y)
stability: continuity of L_h^{-1}

$\Longrightarrow$ *convergence*: u_h is close to u

A model boundary-value problem

Find $u : \Omega \to \mathbb{R}$ such that

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

strong

$$u = \operatorname*{argmin}_{v \in H_0^1(\Omega)} \left(\frac{1}{2} \int_\Omega C \operatorname{grad} v \cdot \operatorname{grad} v \, dx - \int_\Omega f v \, dx \right)$$

variational

Find $u \in H_0^1(\Omega)$ such that

$$\int_\Omega C \operatorname{grad} u \cdot \operatorname{grad} v \, dx = \int_\Omega f v \, dx$$

for all $v \in H_0^1(\Omega)$

weak

Ritz method:

$$u_h = \operatorname*{argmin}_{v \in W_h} \left(\frac{1}{2} B(v,v) - F(v) \right)$$

$W_h \subset W$ finite-diminsional

$\Longleftrightarrow$ *Galerkin method:*

Find $u_h \in W_h$ such that $\quad B\,(u_h, v) = F\,(v) \quad$ for all $v \in W_h$

Find $u_h \in W_h$ such that $\quad B_h(u_h, v) = F_h(v) \quad$ for all $v \in V_h$

discrete operator: $\quad L_h : W_h \to V_h^*, \qquad L_h u_h = F_h$

Approximability, consistency, stability, convergence

Given a norm on W the *error* $\|u - u_h\|$ depends on 3 factors:

Approximability: $\text{A.E.} = \inf_{\chi \in W_h} \|u - \chi\|$

Consistency: $\text{C.E.} = \sup_{v \in V_h} \frac{|B_h(u,v) - F_h(v)|}{\|v\|}$

$\|v\| := \sup_{\chi \in V_h} \frac{B_h(\chi, v)}{\|\chi\|}$

Stability: $\text{S.C.} = \|L_h^{-1}\|_{\mathcal{L}(V_h^*, W_h)}$

$$\|u - u_h\| \leq (1 + \text{S.C.})(\text{A.E.} + \text{C.E.})$$

Stability and quasioptimality

For the Ritz method for the model problem

$$u_h = \operatorname*{argmin}_{v \in W_h} \left(\frac{1}{2} B(v,v) - F(v) \right)$$

there is no consistency error. In the H^1 norm *stability is automatic*. Therefore we get *quasioptimality*:

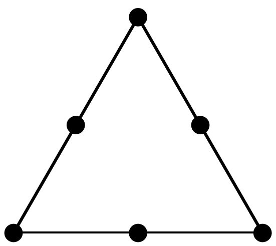
$$\|u - u_h\|_{H^1} \le c \inf_{v \in W_h} \|u - v\|_{H^1}$$

Estimates in other norms (L^2, L^∞, . . .) require additional work

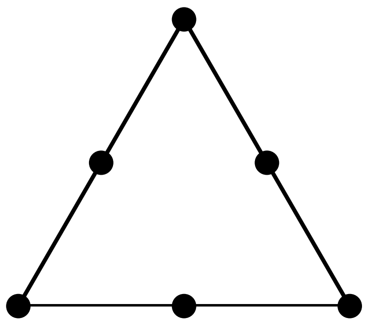
For a finite element method W_h is a piecewise polynomial space defined by the FE assembly procedure:

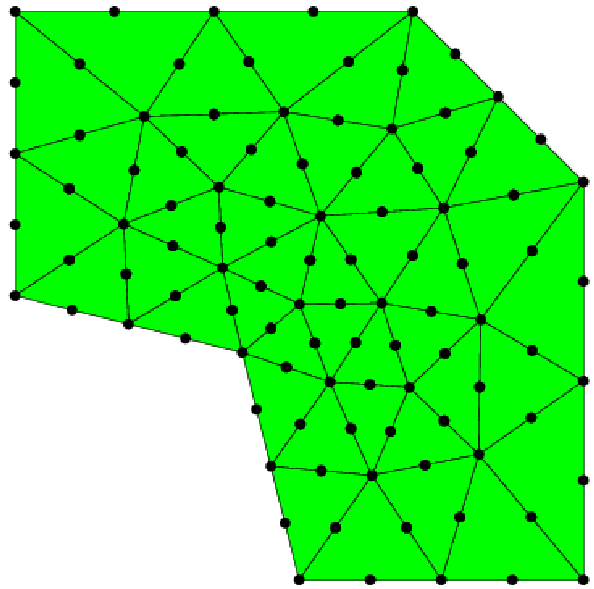
- the domain Ω is triangulated by simplices
- on each simplex T a f.d. space of *shape functions* W_T is given together with a set of *degrees of freedom*, each DOF associated to a subsimplex
- W_h consists of functions piecewise in W_T with equal DOFs on shared subsimplices

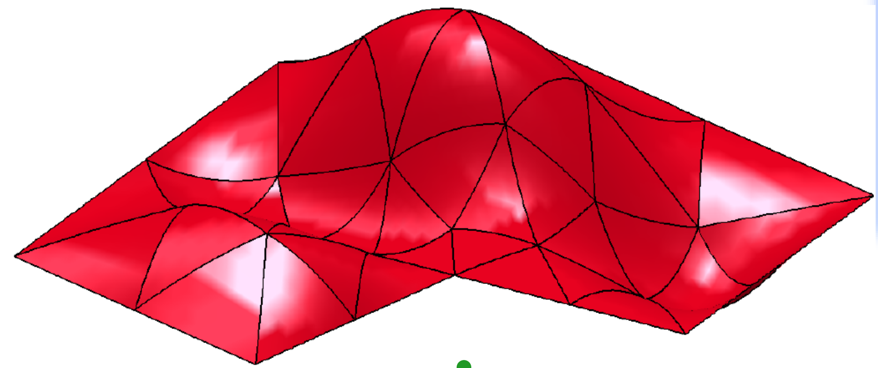
Ex: $W_T = \mathbb{P}_2(T)$, DOFs are vertex vals., edge avgs.



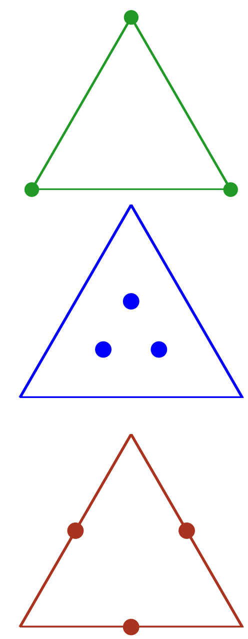
Lagrange finite elements

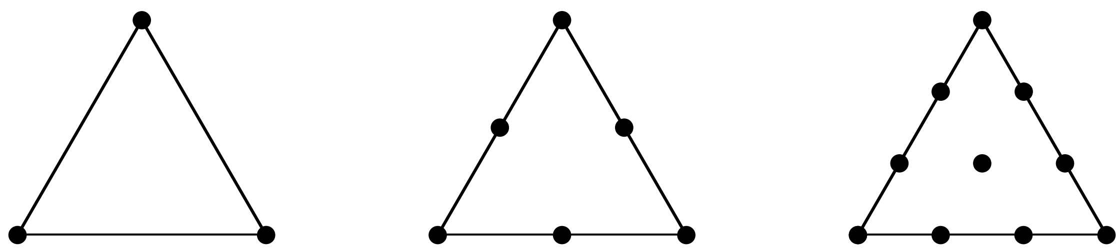




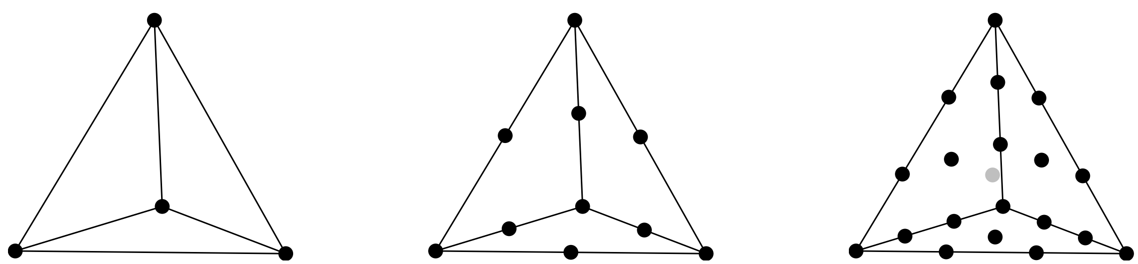


shape fns: $\mathbb{P}_2$
DOFs: vertex vals.
& edge averages





$\mathbb{P}_1$ $\mathbb{P}_2$ $\mathbb{P}_3$



A.E. in H^1 for $u \in H^k$

$\leq c p^{-k} h^{\min(p,k)}$

Computing the sound of a drum

Drum sound determined by standing wave solutions to wave equation with Dirichlet boundary conditions. These are expressed in terms of solutions of an eigenvalue problem:

Find nonzero $u : \Omega \to \mathbb{R}$, $\lambda \in \mathbb{R}$:

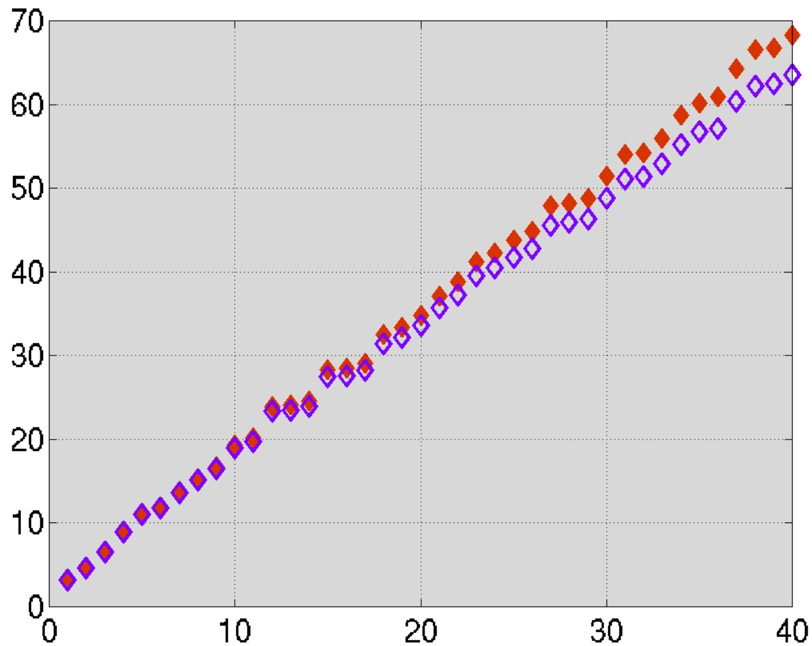
$$-\operatorname{div} C \operatorname{grad} u = \lambda u \text{ in } \Omega, \quad u = 0 \text{ on } \partial\Omega$$

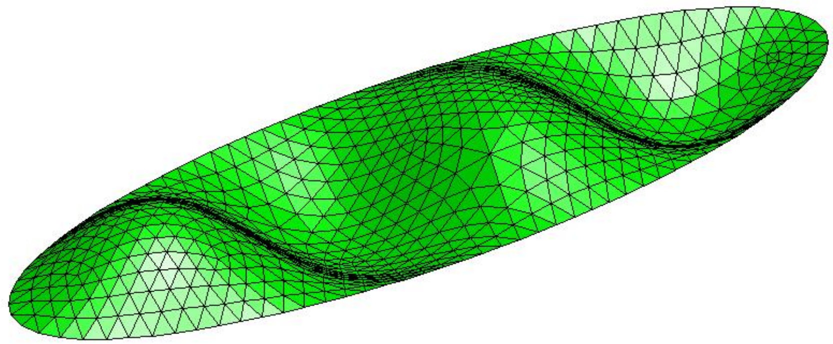
u, λ critical pts.,vals. of $\dfrac{\int_\Omega C \operatorname{grad} u \cdot \operatorname{grad} u \, dx}{\int_\Omega |u|^2 \, dx}$ on $H_0^1(\Omega) \setminus \{0\}$

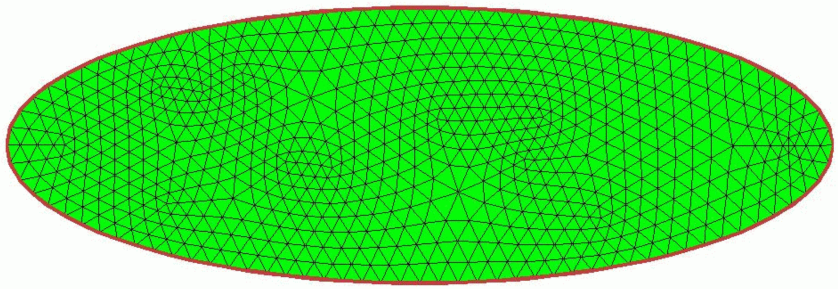
Eigenvalues form a sequence of positive numbers tending to infinity; give the fundamental frequencies; eigenfunctions give fundamental modes.

We can discretize by the Ritz method (find critical points over $W_h \subset H_0^1$), or equivalently the Galerkin method.

Discrete problem has finite sequence of eigenvalues for which the smaller ones will approximate well the true eigenvalues if approximability is good.







Similarly, to compute the resonant frequencies of an electromagnetic cavity, we need to find standing wave solutions of *Maxwell's equations*, which give rise to an eigenvalue problem on $\Omega \subset \mathbb{R}^3$:

Find nonzero $E : \Omega \to \mathbb{R}^3$, $\lambda \in \mathbb{R}$:

$$\operatorname{curl}\operatorname{curl} E = \lambda E, \quad \operatorname{div} E = 0, \quad E \times n = 0 \text{ on } \partial\Omega$$

The eigenvalues are all positive, finite multiplicity, and form a sequence tending to infinity.

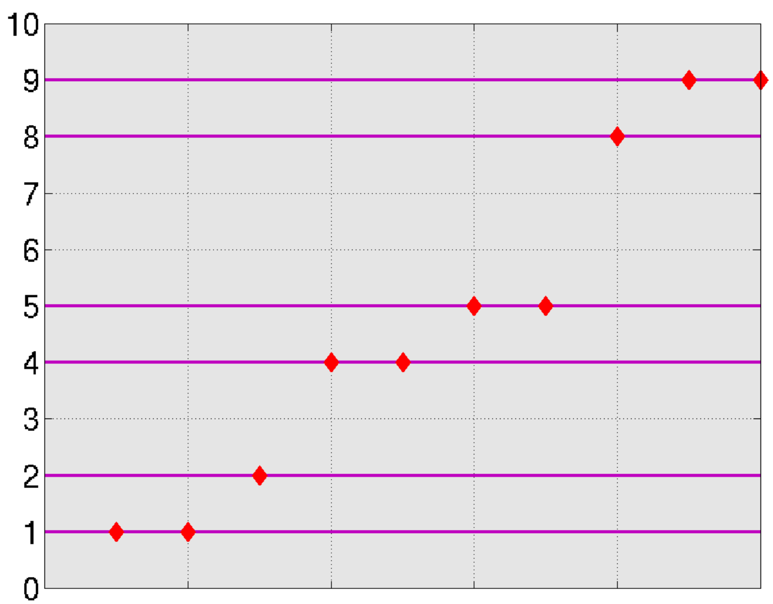
The divergence constraint is redundant except for when $\lambda = 0$. Dropping it adds an infinite dimensional space of (nonphysical) zero eigenfunctions.

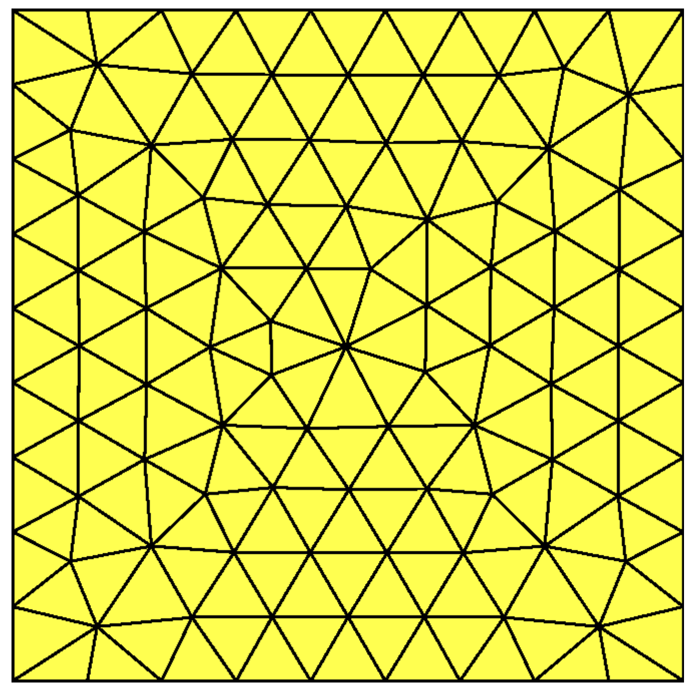
A numerical method is obtained by looking for the nonzero critical values of the Rayleigh quotient over nonzero $E \in Q_h \subset H(\mathrm{curl})$

$$\frac{\int |\operatorname{curl} E|^2}{\int |E|^2}$$

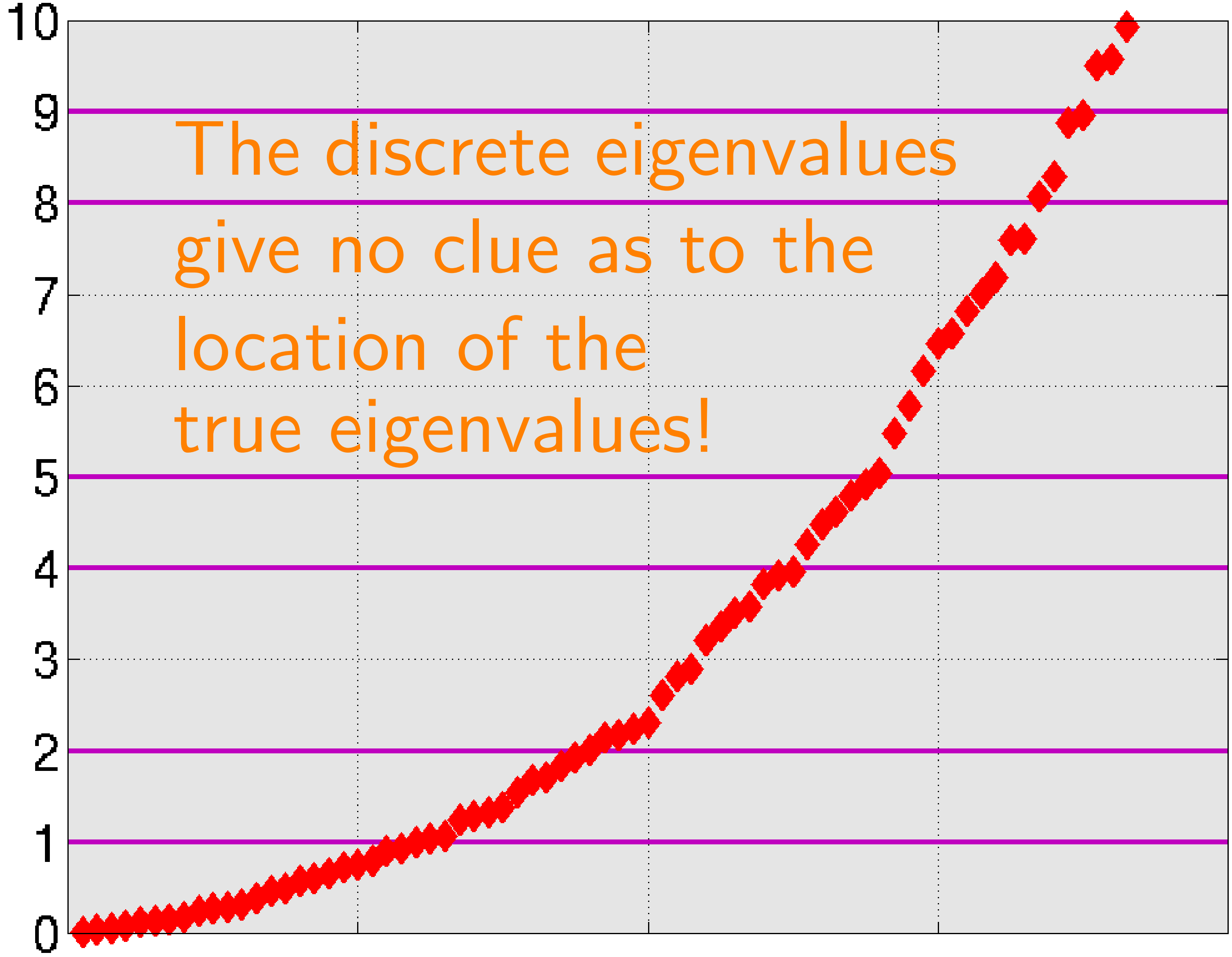
As a test case we choose Ω square, for which the positive eigenvalues are known:
$\lambda = m^2 + n^2, \quad 0 \le m, n \in \mathbb{Z}$.

We triangulate Ω and take Q_h to consist of continuous piecewise linear vectorfields.

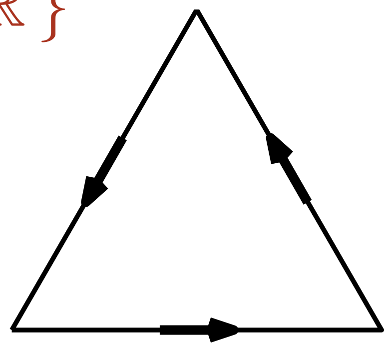




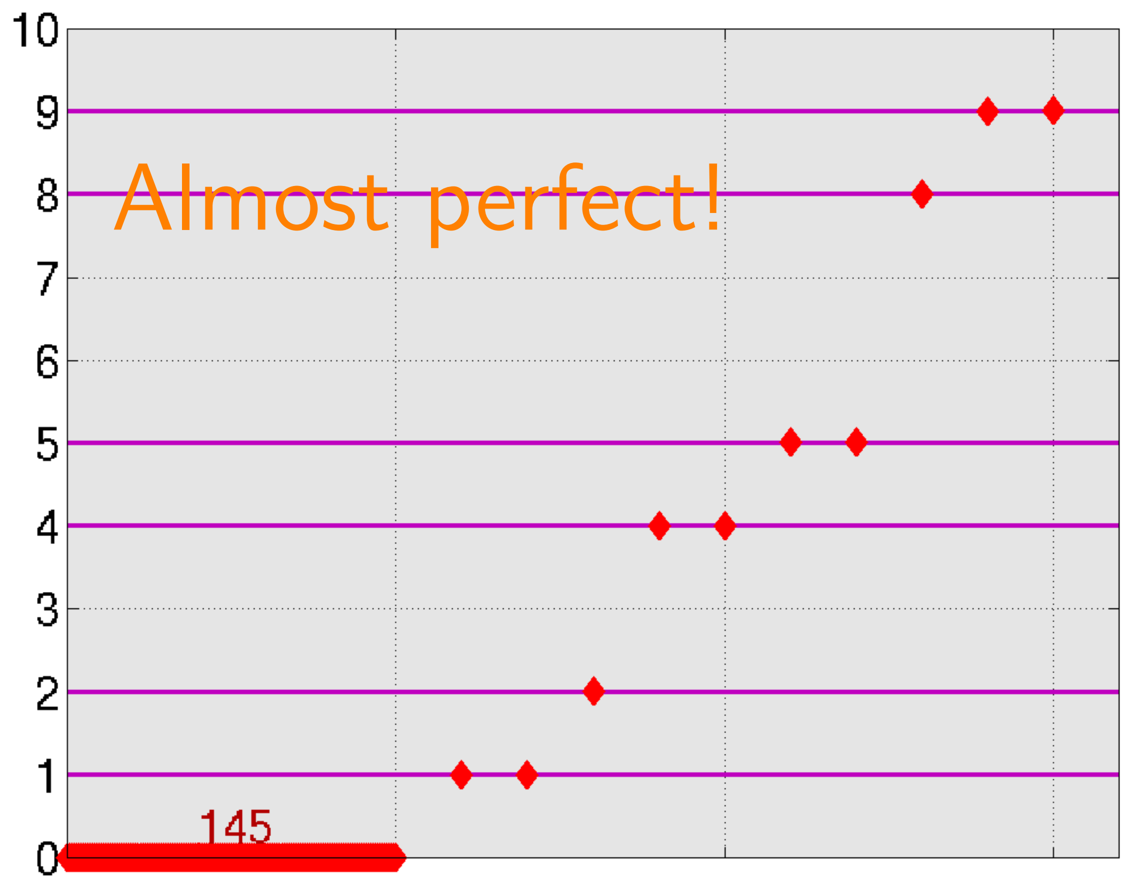
Eigenvalues computed with piecewise linear finite elements

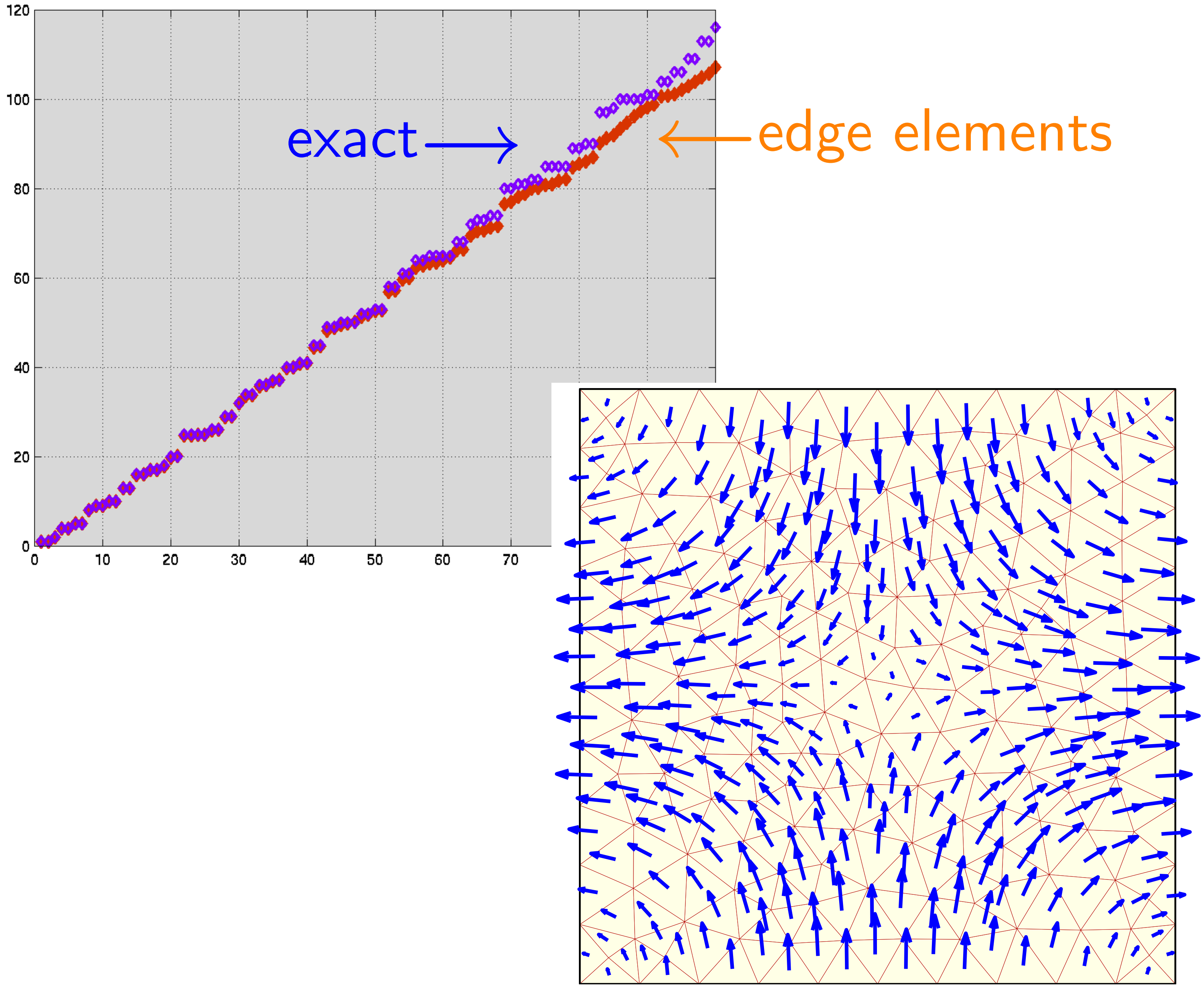


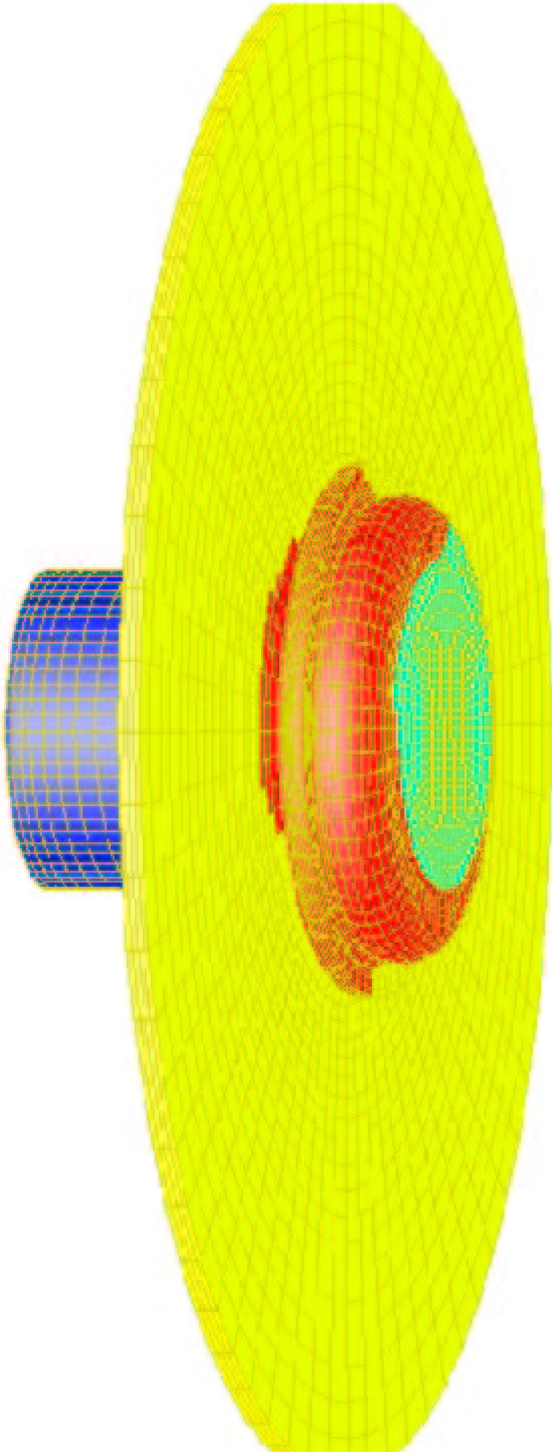
Shape fns: $\mathbb{T} := \{\, (a - bx_2, c + bx_1) \,|\, a, b, c \in \mathbb{R} \,\}$

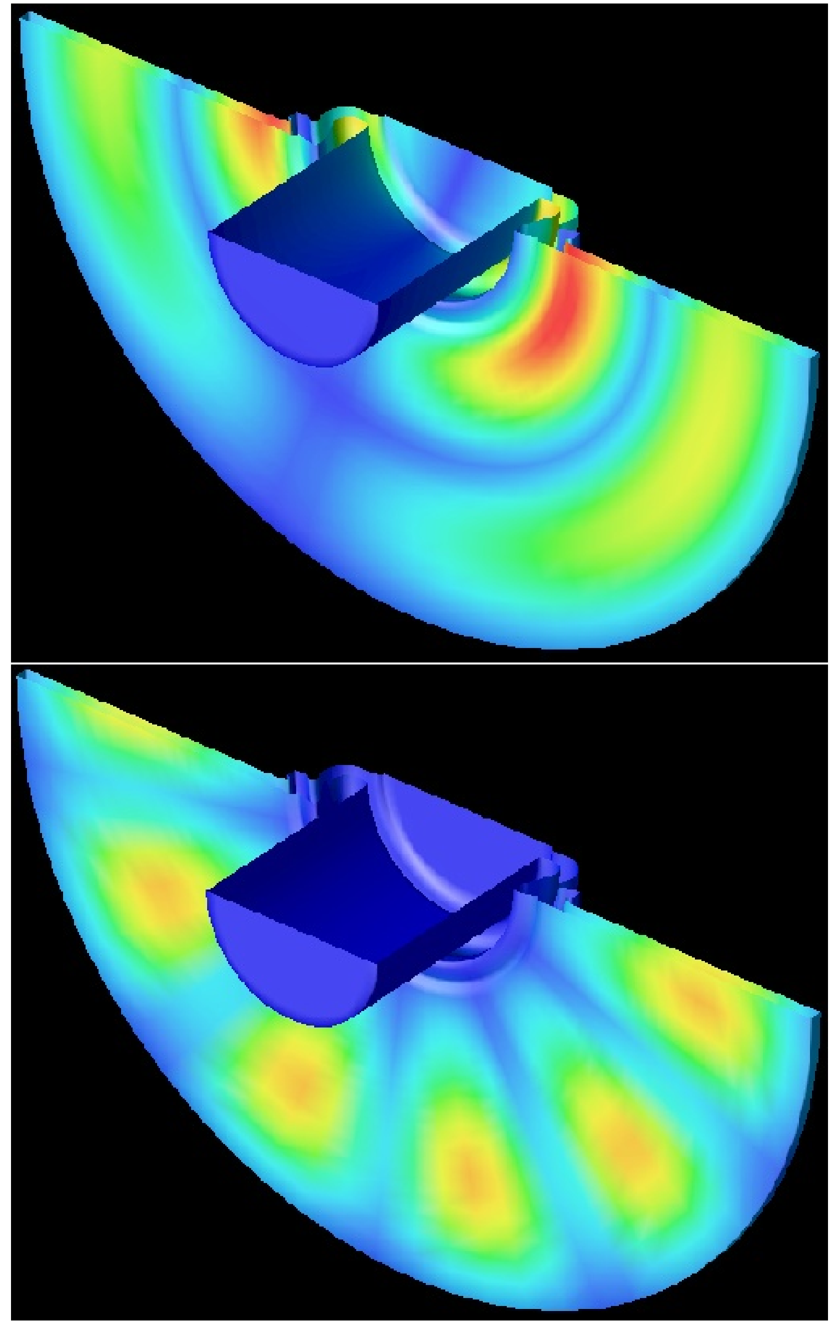


DOFs: values of the (constant) tangential component on each edge




exact
edge elements
120
100
80
60
40
20
0
0
10
20
30
40
50
60
70





D. White, EMSolve, LLNL

Mixed methods for the model problem

$$-\operatorname{div} C \operatorname{grad} u = f$$

Sometimes it is better to work with a first-order system:

$$\sigma = C \operatorname{grad} u, \qquad -\operatorname{div} \sigma = f$$

$$(\sigma, u) = \operatorname*{argcrit}_{H(\operatorname{div}) \times L^2} \left[\int (\frac{1}{2} C^{-1} \tau \cdot \tau + v \operatorname{div} \tau) \, dx + \int f v \, dx \right]$$

It's not an extremum, but a *saddle-point.*

Discretization leads to a *mixed method*.

$$(\sigma_h, u_h) = \underset{S_h \times V_h}{\text{argcrit}} \left[\int (\frac{1}{2} C^{-1}\tau \cdot \tau + v \operatorname{div} \tau)\, dx + \int f v\, dx \right]$$

Stability is not automatic. Discrete system could be singular, or inverse could blow up as mesh is refined.

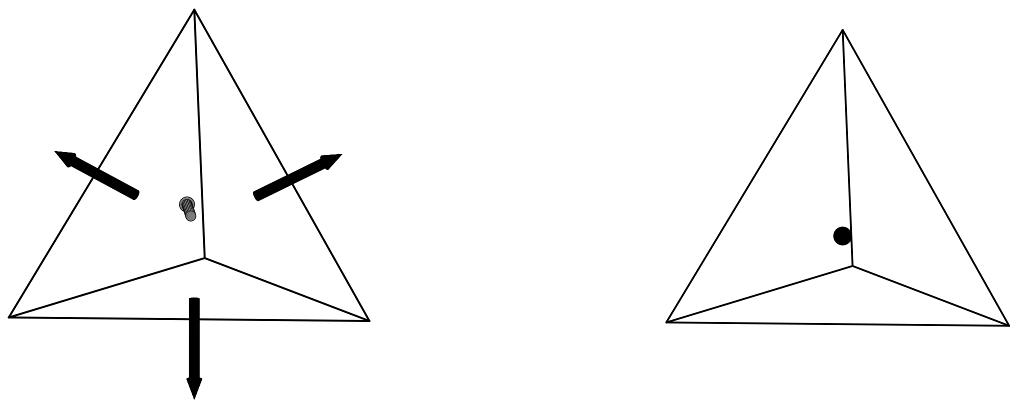
Stability conditions (Brezzi '74):

- For all $\tau \in S_h$ satisfying $\operatorname{div} \tau \perp V_h$, $\int C^{-1}\tau \cdot \tau \geq \gamma \|\tau\|^2_{H(\operatorname{div})}$
  (E.g., $\operatorname{div} S_h \subset V_h$.)
- For all $v \in V_h$, $\exists\, 0 \neq \tau \in S_h$ s.t. $\int v \operatorname{div} \tau \geq \gamma \|v\|_{L^2} \|\tau\|_{H(\operatorname{div})}$
  (E.g., $\operatorname{div} S_h \supset V_h$ and $\operatorname{div}|_{S_h}$ admits a bounded 1-sided inverse.)

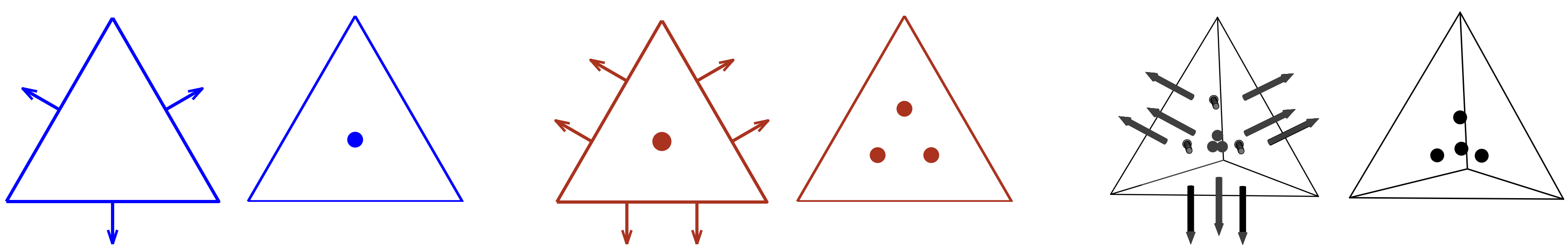
Brezzi's conditions $\implies$ stability $\implies$ quasioptimality.

Mixed finite elements

It is not easy to satisfy both stability conditions!
Simplest stable elements are due to Raviart, Thomas and Nedelec. Face elements for σ_h, piecewise constants for u_h.



shape fns: $\boldsymbol{a} + b\boldsymbol{x}$, $\boldsymbol{a} \in \mathbb{R}^3$, $b \in \mathbb{R}$
DOFs: $\sigma_h \cdot n$ on each face



What does this have to do with differential complexes?

$$\mathbb{R} \hookrightarrow \bigwedge^0(\Omega) \xrightarrow{d} \bigwedge^1(\Omega) \xrightarrow{d} \cdots \xrightarrow{d} \bigwedge^n(\Omega) \to 0$$

$\omega \in \bigwedge^k(\Omega)$ means $\omega(x) : T_x\Omega \times \cdots \times T_x\Omega \to \mathbb{R}$ alternating k-linear

0-forms are smooth maps $\Omega \to \mathbb{R}$

1-forms are co-tangent vector fields

For Ω a domain in $\mathbb{R}^3$ the de Rham complex becomes

$$\mathbb{R} \hookrightarrow C^\infty(\Omega, \mathbb{R}) \xrightarrow{\text{grad}} C^\infty(\Omega, \mathbb{R}^3) \xrightarrow{\text{curl}} C^\infty(\Omega, \mathbb{R}^3) \xrightarrow{\text{div}} C^\infty(\Omega, \mathbb{R}) \to 0$$

Mixed formulation revisited

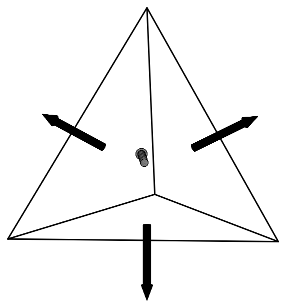
Separating the algebraic and differential operations we have

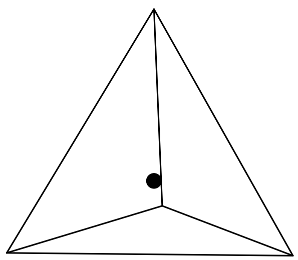
$$\operatorname{grad} \underset{\substack{\uparrow\\0}}{u} = \underset{\substack{\uparrow\\1}}{\gamma}, \qquad -\operatorname{div} \underset{\substack{\uparrow\\2}}{\sigma} = \underset{\substack{\uparrow\\3}}{f}, \qquad \sigma = C\gamma$$

First two equations are just exterior differentiation.
Last is a linear algebraic map from 1-forms to 2-forms:
Hodge star operator

The coefficient matrix C furnishes the inner product determining the Hodge operator.

$$
\begin{tikzcd}
\mathbb{R} \arrow[r, hook] & C^\infty(\Omega,\mathbb{R}) \arrow[r, "\mathrm{grad}"] & C^\infty(\Omega,\mathbb{R}^3) \arrow[r, "\mathrm{curl}"] & C^\infty(\Omega,\mathbb{R}^3) \arrow[r, "\mathrm{div}"] \arrow[d, "\Pi_h^S"'] & C^\infty(\Omega,\mathbb{R}) \arrow[r] \arrow[d, "\Pi_h^V"] & 0 \\
 & & & S_h \arrow[r, "\mathrm{div}"] & V_h \arrow[r] & 0
\end{tikzcd}
$$



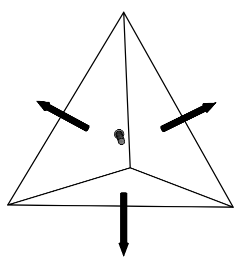


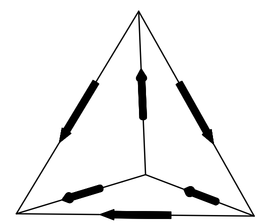
The electromagnetic resonator revisited

$$\mathrm{curl}\,\underbrace{\mu^{-1}\,\overbrace{\mathrm{curl}\,E}^{B}}_{H} = \lambda\,\overbrace{\epsilon\,E}^{D}$$

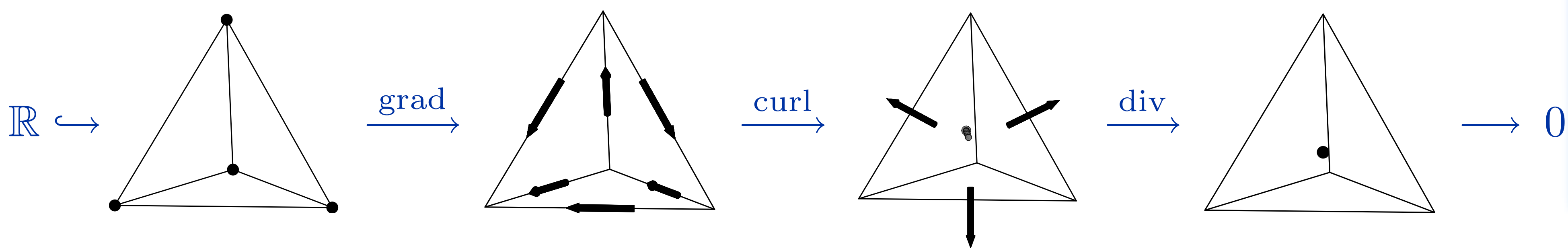
$$\mathrm{curl}\underset{\substack{\uparrow\\ 1}}{E} = \underset{\substack{\uparrow\\ 2}}{B}, \quad \mathrm{curl}\underset{\substack{\uparrow\\ 1}}{H} = \lambda \underset{\substack{\uparrow\\ 2}}{D}, \quad B = \mu H, \quad D = \epsilon E.$$

Two exterior differentiations, two Hodge star operations.

2-forms: face elts 

1-forms: edge elts 

$$\begin{array}{ccccccccccc}
\mathbb{R} \hookrightarrow & C^\infty(\Omega,\mathbb{R}) & \xrightarrow{\text{grad}} & C^\infty(\Omega,\mathbb{R}^3) & \xrightarrow{\text{curl}} & C^\infty(\Omega,\mathbb{R}^3) & \xrightarrow{\text{div}} & C^\infty(\Omega,\mathbb{R}) & \longrightarrow 0 \\
& \downarrow & & \downarrow & & \downarrow & & \downarrow & \\
\mathbb{R} \hookrightarrow & W_h & \xrightarrow{\text{grad}} & Q_h & \xrightarrow{\text{curl}} & S_h & \xrightarrow{\text{div}} & V_h & \longrightarrow 0
\end{array}$$

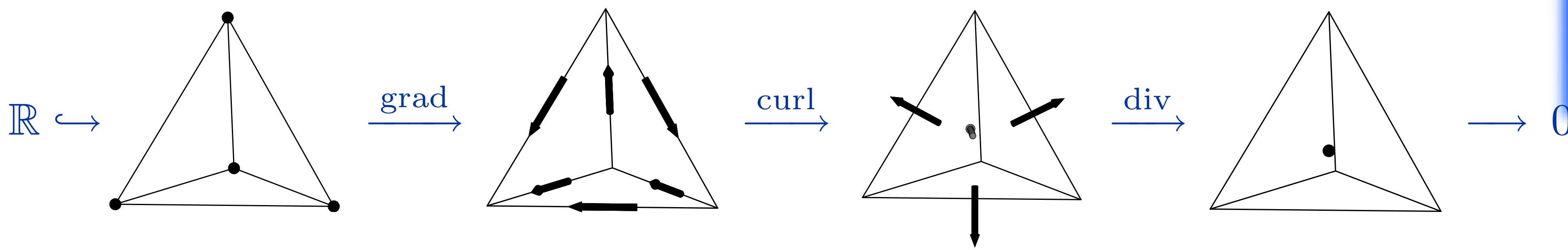


The exactness and commutativity of the diagram are exactly what is needed to analyze eigenvalue discretization based on edge elements using mixed method stability theory. Boffi–Fernandes–Gastaldi–Perugia '99.

The completion of the diagram is the statement that the curl-free edge elements are precisely the gradients of standard piecewise linear elements.

This explains completely the zero eigenspace for the discrete problem.

The complex of discrete differential forms

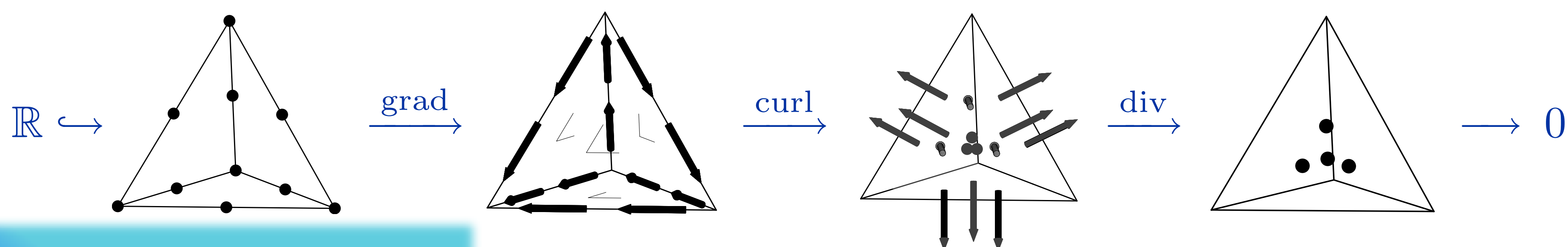


was constructed already by Whitney '57. Connection to mixed FEM first realized by Bossavit '88.

Hiptmair, Demkowicz, Monk, Winther,. . .

Yee scheme; Mimetic finite differences. Hyman, Shashkov,. . .

Mixed FEM provides higher order versions as well:



Given the load $f : \Omega \to \mathbb{R}^3$, linearized elasticity finds

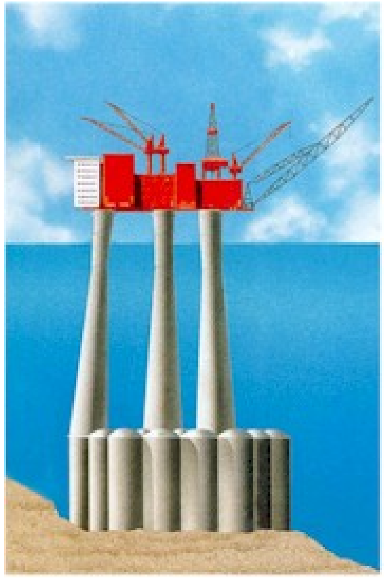
displacement field $u : \Omega \to \mathbb{R}^3$

strain field $\kappa : \Omega \to \mathbb{S} := \mathbb{R}^{3\times 3}_{\text{sym}}$

stress field $\sigma : \Omega \to \mathbb{S}$

$$\epsilon\, u = \kappa, \quad \operatorname{div} \sigma = f, \quad \sigma = C\kappa$$

$\epsilon\, u := [\nabla u + (\nabla u)^T]/2$


Mixed finite elements for elasticity

$$(\sigma, u) = \operatorname*{argcrit}_{\substack{H(\mathrm{div},\Omega,\mathbb{S}) \\ \times L^2(\Omega,\mathbb{R}^3)}} \left[\int \left(\frac{1}{2} C^{-1}\tau : \tau + v \cdot \operatorname{div}\tau\right) dx - \int f \cdot v \, dx \right]$$

A question which attracted a lot of attention over four decades:
How to construct stable mixed finite elements for elasticity

$$\Sigma_h \subset H(\mathrm{div}, \Omega, \mathbb{S}), \qquad V_h \subset L^2(\Omega, \mathbb{R}^3)$$

2D: first stable elements with polynomial shape fns:
Arnold–Winther, Numer. Math. 2001

3D case remains open

$$\epsilon\, u = \kappa, \quad \operatorname{div} \sigma = f, \quad \sigma = C\kappa$$

These are *not* differential forms. However, there is a relevant differential complex:

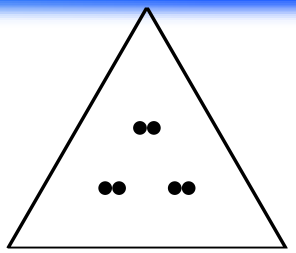
$$\mathbb{T} \hookrightarrow \underset{\substack{\uparrow \\ \text{displacement}}}{C^\infty(\Omega, \mathbb{R}^3)} \xrightarrow{\epsilon} \underset{\substack{\uparrow \\ \text{strain}}}{C^\infty(\Omega, \mathbb{S})} \xrightarrow{J} \underset{\substack{\uparrow \\ \text{stress}}}{C^\infty(\Omega, \mathbb{S})} \xrightarrow{\operatorname{div}} \underset{\substack{\uparrow \\ \text{load}}}{C^\infty(\Omega, \mathbb{R}^3)} \longrightarrow 0$$

$J = \operatorname{curl}_{\mathsf{c}} \operatorname{curl}_{\mathsf{r}}$ is a second order differential operator.

This complex can be derived from the de Rham complex by the Bernstein–Gelfand–Gelfand resolution (Eastwood '99).

New mixed elements for plane elasticity

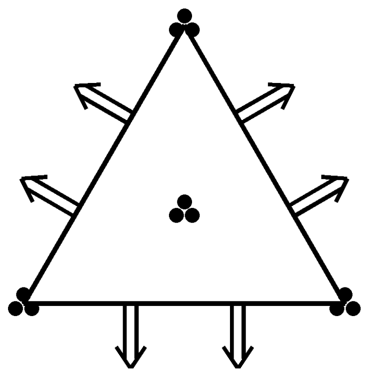
Pick any polynomial degree $p \geq 1$. For the *displacement* in $L^2(\Omega, \mathbb{R}^2)$ we simply use discontinuous p.w. polynomials of degree $\leq p$.



$p = 1$

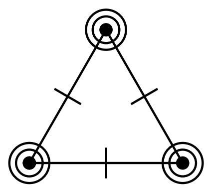
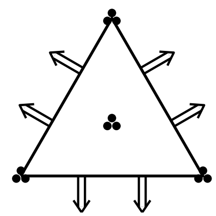
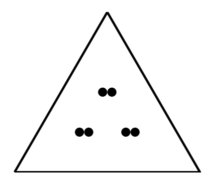
On each triangle the polynomial space for the *stress* is
$\Sigma_T = \{\, \tau \in \mathbb{P}_{p+2}(T, \mathbb{S}) \mid \operatorname{div} \tau \in \mathbb{P}_p(T, \mathbb{R}^2) \}$.
For $p = 1$, the 24 unisolvent degrees of freedom are:

- the values of three components at each vertex (9)
- the values of the moments of degree 0 and 1 of the normal components on each edge (12)
- the value of the moment of degree 0 on the triangle (3)



The discrete plane elasticity complex

$$\begin{tikzcd}
\mathbb{P}_1(\Omega) \arrow[r, hook] & C^\infty(\Omega) \arrow[r, "J"] \arrow[d] & C^\infty(\Omega, \mathbb{S}) \arrow[r, "\operatorname{div}"] \arrow[d] & C^\infty(\Omega, \mathbb{R}^2) \arrow[r] \arrow[d] & 0 \\
\mathbb{P}_1(\Omega) \arrow[r, hook] & Q_h \arrow[r, "J"] & \Sigma_h \arrow[r, "\operatorname{div}"] & V_h \arrow[r] & 0
\end{tikzcd}$$

$\mathbb{P}_1(\Omega) \hookrightarrow$  $\xrightarrow{J}$  $\xrightarrow{\operatorname{div}}$  $\longrightarrow 0$

$\uparrow$

Hermite quintic

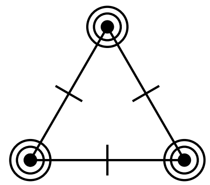
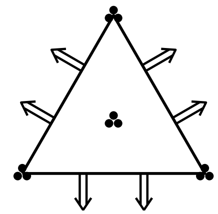
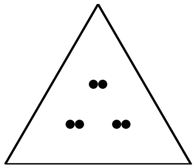
$$J\phi = \begin{pmatrix} \dfrac{\partial^2 \phi}{\partial y^2} & -\dfrac{\partial^2 \phi}{\partial x \partial y} \\ -\dfrac{\partial^2 \phi}{\partial x \partial y} & \dfrac{\partial^2 \phi}{\partial x^2} \end{pmatrix}$$

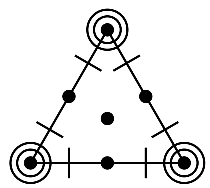
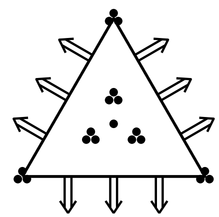
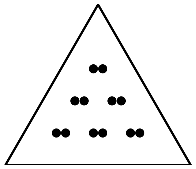
$$\|\sigma - \sigma_h\|_{L^2} \le Ch^3 \|\sigma\|_{H^3}$$

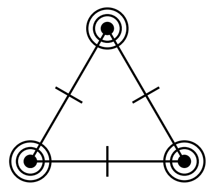
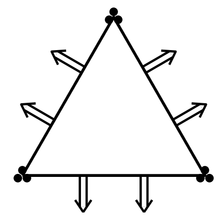
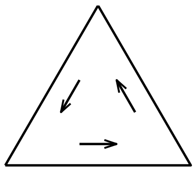
$$\|\operatorname{div} \sigma - \operatorname{div} \sigma_h\|_{L^2} \le Ch^2 \|\operatorname{div} \sigma\|_{H^3}$$

$$\|u - u_h\|_{L^2} \le Ch^2 \|u\|_{H^3}$$

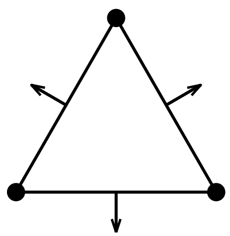
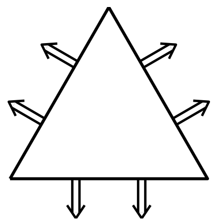
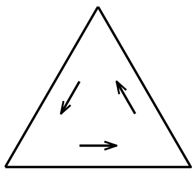
Discretizations of the plane elasticity complex

$\mathbb{P}_1(\Omega) \hookrightarrow$  $\xrightarrow{J}$  $\xrightarrow{\mathrm{div}}$  $\longrightarrow 0$

$\mathbb{P}_1(\Omega) \hookrightarrow$  $\xrightarrow{J}$  $\xrightarrow{\mathrm{div}}$  $\longrightarrow 0$

$\mathbb{P}_1(\Omega) \hookrightarrow$  $\xrightarrow{J}$  $\xrightarrow{\mathrm{div}}$  $\longrightarrow 0$

non-conforming:

$\mathbb{P}_1(\Omega) \hookrightarrow$  $\xrightarrow{J}$  $\xrightarrow{\mathrm{div}}$  $\longrightarrow 0$

A grand challenge: gravitational wave simulation

A subtle but ineluctable consequence of Einstein's theory of general relativity is that relatively accelerating masses emit gravitational waves. These waves are slight perturbations in the metric of spacetime which propagate at the speed of light: *ripples in the rigid fabric of spacetime.*

One of the largest scientific endeavors of our time is the construction of a network of massive interferometers to measure the tiny dynamic changes in distances caused by a passing gravity wave. The Laser Interferometer Gravitational-wave Observatory (LIGO) is designed to pick up changes in distance of a hundred millionth of a hydrogen atom diameter across its four kilometer length.

If gravitational wave observatories are to succeed numerical computation must be used to infer from detected waveforms the massive cosmological events that gave birth to them (e.g., black hole or neutron star collisions).

The first step is numerical solution of Einstein's equations, but it is currently beyond our abilities: good algorithms not available, not just because the problem is huge and complicated, but also because the basic structure of the equations and the consequences for discretization are not sufficiently understood.

Despite tremendous efforts, no one has succeeded in developing a stable numerical scheme for simulating black hole collisions. *Simulating blackhole collisions may be harder than detecting them!*

In the 3+1 formulation, the Einstein equations determine a time-dependent spatial metric (3×3 positive definite matrix) on a 3-dimensional domain according to an evolution equation

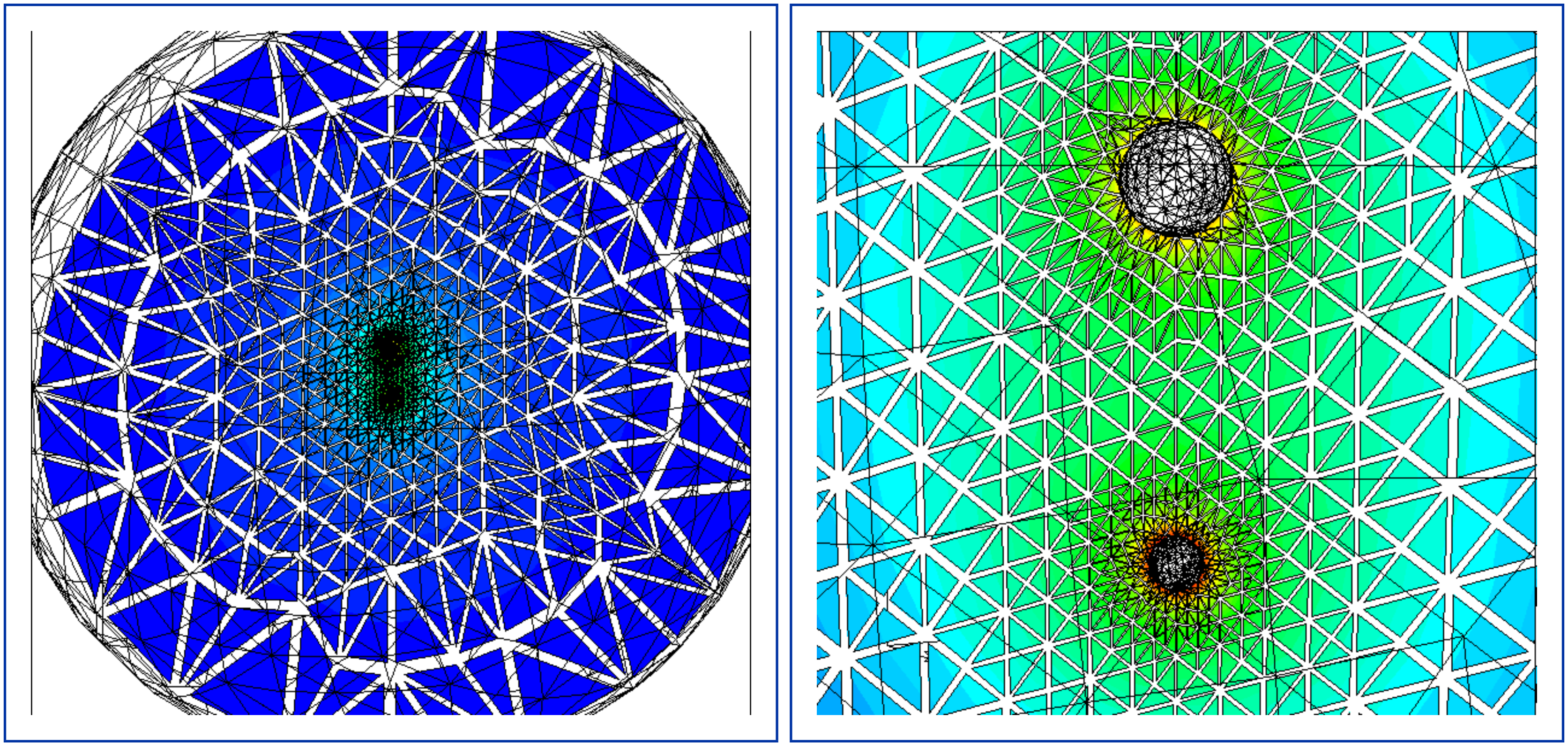
$$\ddot{\gamma} = F(\gamma)$$

subject to constraints

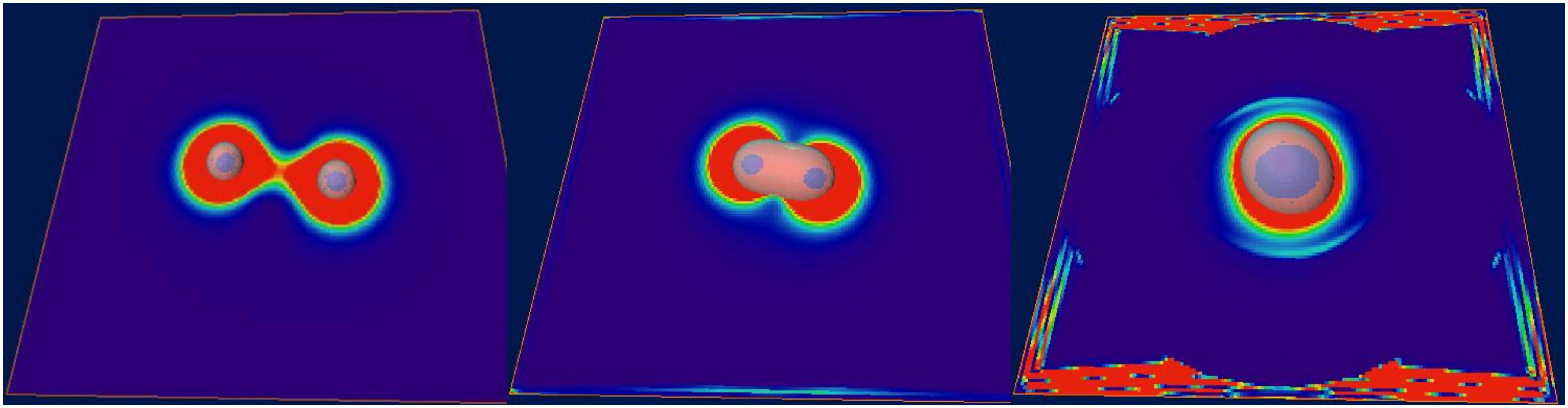
$$H(\gamma) = 0, M(\gamma, \dot{\gamma}) = 0.$$

F, H, and M are nonlinear partial differential operators in the 3 space variables. The leading term of $F(\gamma)$ is the Ricci curvature of the metric γ.

The computation proceeds by finding Cauchy data satisfying the constraints and then evolving it.



Arnold–Mukherjee ’96



Brandt, Correll, Gomez, Huq, Laguna, Lehner, Marronetti, Matzner, Neilsen, Pullin, Schnetter, Shoemaker, Winicour ’2000

Linearizing Einstein's equations about flat space and making a simple coordinate choice we get

$$\ddot{\gamma} = \Delta\gamma + \nabla\nabla \operatorname{tr}\gamma - 2\epsilon \operatorname{div}\gamma,$$

$$\operatorname{div}\operatorname{div}\gamma - \Delta \operatorname{tr}\gamma = 0, \quad \operatorname{div}\dot{\gamma} - \operatorname{grad}\operatorname{tr}\dot{\gamma} = 0.$$

Introducing the extrinsic curvature $\kappa = \dot{\gamma}$, and combining the constraints with evolution equation it turns out that

$$\boxed{\ddot{\kappa} = -J\kappa}$$

$$\mathbb{T} \hookrightarrow C^\infty(\Omega, \mathbb{R}^3) \xrightarrow{\epsilon} C^\infty(\Omega, \mathbb{S}) \xrightarrow{J} C^\infty(\Omega, \mathbb{S}) \xrightarrow{\operatorname{div}} C^\infty(\Omega, \mathbb{R}^3) \longrightarrow 0$$

This suggests that appropriate discretizations for the extrinsic curvature must be related to the (as yet unknown) stable mixed elasticity elements in 3D.

Conclusions

Stability of numerical methods for PDE is a subtle matter.

Often depends on geometric/homological props. of discretization reflecting similar props. at PDE level.

Discrete complexes commutatively related to differential complexes are a succint and useful tool.

This viewpoint has succeeded in unifying, clarifying, and advancing many techniques developed over the preceding few decades, e.g. in electromagnetism.

Recently lead to first stable mixed finite elements for elasticity in 2D; seems poised to do so in 3D.

Hopefully will be an important weapon in the of attack on the massive challenge presented by numerical relativity.