Towards a variational complex for the Finite Element Method

Can we use symbolic algebra to study numerical methods?

- Can you design a numerical method, automatically, to inherit a variational principle and selected conservation laws?
- Can one obtain symmetries and hence conservation laws, automatically, of variational numerical methods?

A variational complex is a tool which helps to formulate and answer questions such as;

- Is my scheme variational? What is the (discrete) Lagrangian?
- Do symmetries yield conservation laws? How can I derive them?

Compare the FEM differential complexes

D. Arnold, *Differential complexes and numerical stability*, Plenary address at ICM Beijing, 2002. See also Hiptmair, Raviart and Thomas, Chard and Shapiro, Matiussi, Schwalm, Bossavit . . .

$$\begin{tikzcd}
0 \arrow[r] & \mathbb{R} \arrow[r] & \Lambda^0 \arrow[r, "\overset{\text{grad}}{\mathrm{d}}"] \arrow[d, "\Pi"] & \Lambda^1 \arrow[r, "\overset{\text{curl}}{\mathrm{d}}"] \arrow[d, "\Pi"] & \Lambda^2 \arrow[r, "\overset{\text{div}}{\mathrm{d}}"] \arrow[d, "\Pi"] & \Lambda^3 \arrow[r] \arrow[d, "\Pi"] & 0 \\
0 \arrow[r] & \mathbb{R} \arrow[r] & W_h \arrow[r, "\mathrm{d}"] & Q_h \arrow[r, "\mathrm{d}"] & S_h \arrow[r, "\mathrm{d}"] & V_h \arrow[r] & 0
\end{tikzcd}$$

Π	projection operator, $\Pi \circ \mathrm{d} = \mathrm{d} \circ \Pi$
$W_h \ldots V_h$	finite dimensional function spaces wrt some triangulation

to the variational complex

$$0 \rightarrow \mathbb{R} \rightarrow \Lambda^0 \xrightarrow{\mathrm{D}} \Lambda^1 \xrightarrow{\mathrm{D}} \Lambda^2 \xrightarrow{\mathrm{D}} \Lambda^3 \xrightarrow{\mathrm{E}} \Lambda^1_* \xrightarrow{\mathcal{H}} \Lambda^2_* \cdots$$

where

D as above but now we have smooth functions of x, u, $u_x, \ldots$ with derivatives acting totally

E $\equiv$ Euler Lagrange operator

Theorem: Locally, the kernel of one map equals the image of the previous in all these sequences.

The preimages can be constructed.

Recall the smooth Euler Lagrange operator

- Step 1: $\frac{\mathrm{d}}{\mathrm{d}\epsilon}|_{\epsilon=0} L[u + \epsilon v]$
- Step 2: mod out by the boundary terms, that is, total derivatives.

The simplest FEM example using the mindset/technology/terminology of formal variational processes:

$$L[u] = u_x^2 + 2u, \qquad E(L) = -2(u_{xx} - 1)$$

The triangulation of $\mathbb{R}$ has vertices x_n and edges $e_n = (x_n, x_{n+1})$. The data is $u_n = u(x_n)$

The projection is

$$\Pi(u)|_{e_n} \quad = \quad x \mapsto \tfrac{u_{n+1}-u_n}{x_{n+1}-x_n} x + \tfrac{u_n x_{n+1} - u_{n+1} x_n}{x_{n+1}-x_n}$$

The discrete Lagrangian is $\Pi(u)_x^2 - 2\Pi(u)$ and hence

$$\begin{aligned}\mathcal{L}[u] &= \textstyle\int \Pi(u)_x^2 - 2\Pi(u)\,\mathrm{d}x = \sum_n \int_{e_n} \Pi(u)_x^2 - 2\Pi(u)\,\mathrm{d}x \\ &= \sum_n \frac{(u_{n+1}-u_n)^2}{x_{n+1}-x_n} + (u_n x_{n+1} - u_{n+1} x_n) \\ &\quad + (u_{n+1} x_{n+1} - u_n x_n)\end{aligned}$$

The blue term telescopes and hence is set to zero: this term is a boundary term.

Calculating $\frac{\mathrm{d}}{\mathrm{d}\epsilon}|_{\epsilon=0}\mathcal{L}[u+\epsilon\delta u]$ yields

$$\begin{aligned}\sum_n &\left(2\frac{u_{n+1}-u_n}{x_{n+1}-x_n} - x_n\right)\delta u_{n+1} \\ &+ \left(-2\tfrac{u_{n+1}-u_n}{x_{n+1}-x_n} + x_{n+1}\right)\delta u_n\end{aligned}$$

Using the identity

$$\sum a_n \delta u_{n+1} = \sum a_{n-1} \delta u_n + \text{boundary terms}$$

yields the variational derivative, modulo boundary terms, of $\mathcal{L}[u]$ to be

$$\sum_n \left(2\frac{u_n - u_{n-1}}{x_n - x_{n-1}} - x_{n-1} - 2\frac{u_{n+1} - u_n}{x_{n+1} - x_n} + x_{n+1} \right) \delta u_n$$

Since each δu_n is independent, the coefficient must be zero (at least in the function space ℓ_2), and this then is the discrete Euler Lagrange equation. Integrating twice gives

$$u_N = \tfrac{1}{2} x_N^2 + \kappa x_N + (u_0 - \tfrac{1}{2} x_0^2 - \kappa x_0)$$

which is the exact solution at each node.

Not all choices of Finite Element are suited to variational methods

Using piecewise constant functions to approximate functions leads to poor results. Instead, use the zeroth moments for u on (x_n, x_{n+1}) and (x_{n+1}, x_{n+2}) to create a piecewise linear approximation for u on (x_n, x_{n+2}) with the same 2 moments:

$$\begin{aligned} \Pi(u)_n &= x \mapsto A_n x + B_n \\ A_n &= 2\left(\frac{\alpha_n - \alpha_{n+1}}{x_n - x_{n+2}}\right) \\ B_n &= \left(\frac{x_{n+1} + x_{n+2}}{x_{n+2} - x_n}\right)\alpha_n - \left(\frac{x_{n+1} + x_n}{x_{n+2} - x_n}\right)\alpha_{n+1} \end{aligned}$$

for an approximation on the partition

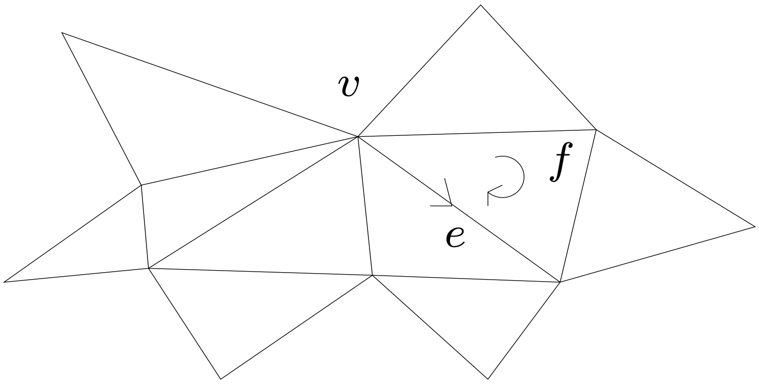
$$\cdots x_{n-4},\ x_{n-2},\ x_n,\ x_{n+2},\ x_{n+4},\cdots$$

This fixed projection fits into a coherent scheme.

In two dimensions, what is the equivalence class / cancelling sums / boundary terms needed to calculate the Euler Lagrange operator?

ANSWER: “coboundary of a 1-cochain”*

Take a triangulation: vertices v, oriented edges e and oriented faces f.



0 cochains are maps $< v_i > \longrightarrow \mathbb{R}$

1 cochains are maps $< e_i > \longrightarrow \mathbb{R}$

2 cochains are maps $< f_i > \longrightarrow \mathbb{R}$

All maps linear over $\mathbb{R}$ or some coefficient ring.

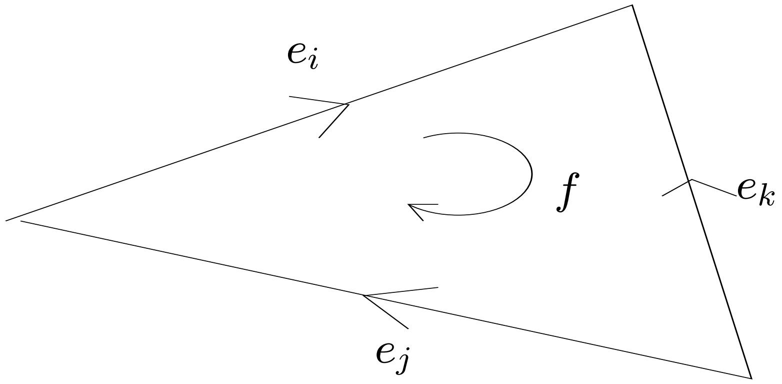
Change orientation $\equiv$ change sign.

*classical simplicial algebra

Given $F :< e_i > \longrightarrow \mathbb{R}$, define $\delta F :< f_i > \longrightarrow \mathbb{R}$ by (for f as in the diagram),

$$(\delta F)(f) = F(e_i) + F(e_j) - F(e_k)$$

and extended linearly. Note: the signs are according to whether the orientations match or not.



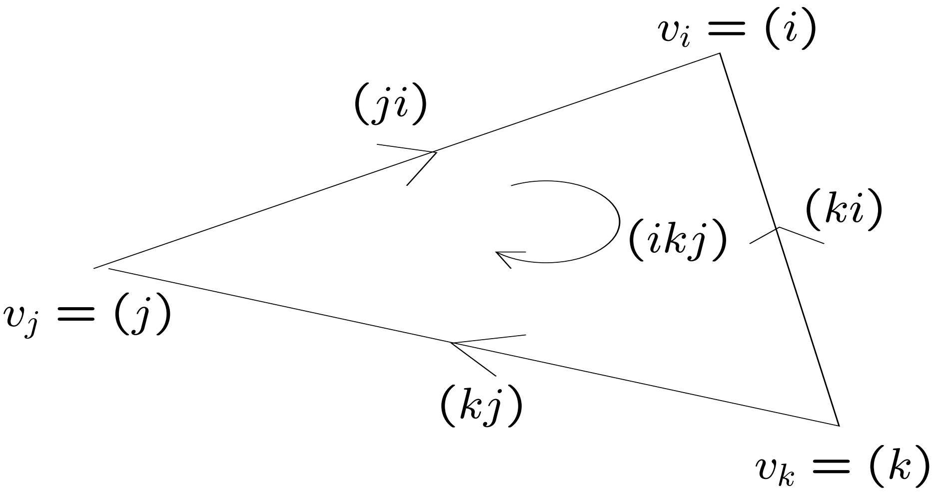
For the face in the diagram, the boundary is $\partial(f) = e_i + e_j - e_k$. In general, we write,

$$(\delta F)(f) = F(\partial f)$$

The map δ is called the coboundary operator.

If you are using an interpolation scheme, all the data lie on the vertices. The set of faces is then a set $\mathcal{F}$ of ordered triples of indices and the set of edges $\mathcal{E}$ is a set of ordered pairs of indices.

The ordering gives the orientation.



A telescoping/coboundary sum looks like

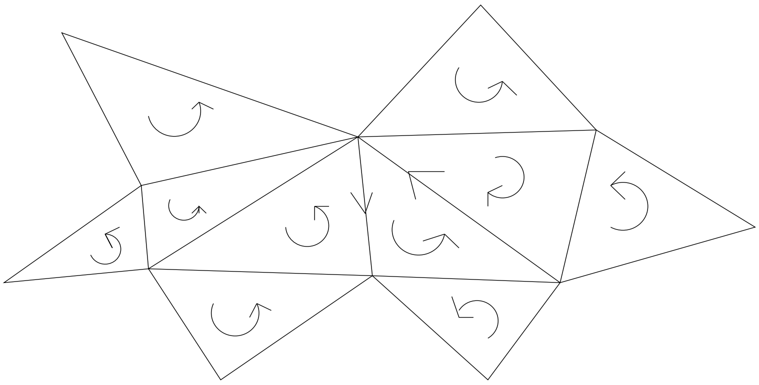
$$(\delta F)(ikj) = F(kj) + F(ji) + F(ik)$$

that is, cyclic sums on edges.

The projection of $\int_X L[u]\,\mathrm{d}x$ is

$$\sum_{f_i} (-1)^{|f_i|} \int_{f_i} \Pi(L[u])\,\mathrm{d}x \tag{1}$$

where $|f_i| = 1$ if f_i has the anti-clockwise orientation, and $|f_i| = -1$ for the reverse orientation.



If $\Pi(L)$ is a coboundary, the sums over the internal edges will cancel: (1) will depend only on the boundary data. In fact we have a discrete Stokes' theorem,

$$\int_X \delta F = \int_{\partial X} F.$$

The simplicial theory is attractive. It allows us to use results and intuition from classical work on triangulations. It generalizes to n dimensions.

From FE forms to simplicial cochains

Let the top, i.e. n dimensional simplices be denoted by τ. Given a piecewise defined n-form on the τ, a simplicial n-cochain is achieved by integrating the form on the τ. This map is the de Rham map. We will denote it by $\int$:

$$\omega \in \mathcal{F}^n, \quad (\int \omega)(\tau) = \int_\tau \omega.$$

Theorem

The FE variational complex, shown here for a three dimensional base space,

$$0 \longrightarrow \mathbb{R} \longrightarrow \widetilde{\mathcal{F}}_0 \xrightarrow{\mathrm{d}} \widetilde{\mathcal{F}}_1 \xrightarrow{\mathrm{d}} \widetilde{\mathcal{F}}_2 \xrightarrow{\mathrm{d}} \widetilde{\mathcal{F}}_3 \xrightarrow{\mathcal{EL}} \mathcal{F}^1_* \xrightarrow{\mathrm{d}^*} \mathcal{F}^2_* \xrightarrow{\mathrm{d}^*} \cdots$$

is locally exact: the kernel of one map equals the preimage of the previous. The preimage can be constructed.

$\widetilde{\mathcal{F}}_*$ is the algebra generated by the W_h, $Q_h \ldots$ with unevaluated degrees of freedom

$\mathcal{EL} = \pi \circ \widehat{\mathrm{d}} \circ \int$

$\mathrm{d}^* = \pi \circ \widehat{\mathrm{d}}$ is the analogue of the vertical exterior derivative, modulo boundary terms

$\mathcal{F}^*_*$ is the algebra of vertical forms tensored with the space of n-dimensional simplicial co-chains

Proofs and details appear in the preprint "Towards a variational complex for the Finite Element Method", to appear in a Centre de Recherches Mathematiques Proceedings volume for the workshop "Group Theory and Numerical Analysis", May 2003. Available from the URL `http://www.kent.ac.uk/ims/personal/elm2`

Ongoing work

To do:

1. Incorporate the Poincaré dual mesh model of the Hodge star operator.
2. Develop a computationally useful notion of the EL equations in terms of the incidence matrix of the mesh.
3. Derive formulae for discrete Noether's theorem relative to a given mesh.

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