Modern Numerical Methods for Dynamical Cores

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Overview

- Why do we need modern numerical methods?
- An example: compatible finite elements
- Some finite element theory and practice
- Research directions

“Weather Forecasting Factory” by Stephen Conlin, 1986. Based on the description in Weather Prediction by Numerical Process, by L.F. Richardson `https://www.emetsoc.org/resources/rff/`

Evolution of the Met Office dynamical core

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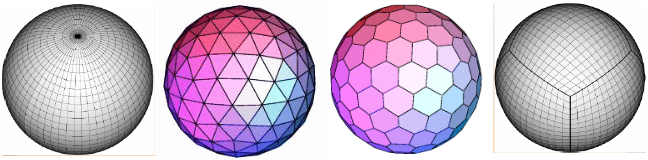


Gung Ho and LFRic

Motivation:

Can we have all the 'optimal properties' of ENDGame but on a grid that enables better scaling from parallel domain decomposition?

Optimal properties:

- Energy and mass conservation.
- No spurious modes (oscillations that are present in the discrete equations that are not there in the continuous equations) coming from certain terms.
- Geostrophic modes are exactly steady.

Gung Ho and LFRic

Motivation:

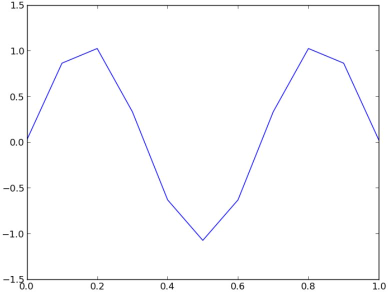
Can we have all the 'optimal properties' of ENDGame but on a grid that enables better scaling from parallel domain decomposition?

One solution: Compatible finite element methods

- The finite element method approximates the solution as piecewise polynomial.
- The dynamical core requires solving for multiple fields (wind velocity, pressure, density, ...).
- Different fields can be approximated by different degrees of polynomial; this is a *mixed* finite element method.
- *Compatible* finite element methods choose these polynomials in such a way that the discrete equations are *compatible* with the differential operators in the equations.

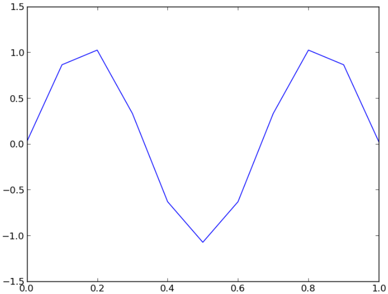
Piecewise polynomials: a 1D example

A piecewise linear approximation...

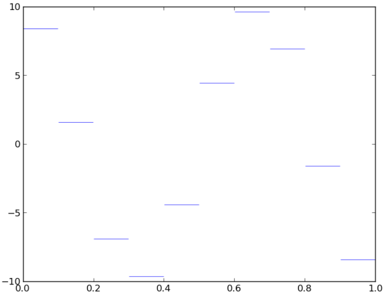


Piecewise polynomials: a 1D example

A piecewise linear approximation...



...and its derivative



- The piecewise linear function lies in the function space $P1$ of piecewise linear polynomials that are continuous between cells.
- The derivative lies in the function space $dP0$ of piecewise constant polynomials that are discontinuous between cells.
- The differential operator $\frac{d}{dx}$ takes a function $f(x) \in P1$ to a function $\frac{df}{dx} \in dP0$.

The Finite Element Method

"...an understanding of the FEM calls not just for a different frame of mind but also for the comprehension of several principles. Each principle is important but it is their combination that makes the FEM into such an effective computational tool."
A. Iserles, A first course in the numerical analysis of differential equations.

1. Approximate *the solution* in a finite dimensional space $\mathbb{H}_m$.
2. Choose the approximation so the *defect* is orthogonal to $\mathbb{H}_m$.
3. Integrate by parts to reduce differentiability requirements.
4. Choose each function in a basis of $\mathbb{H}_m$ such that it vanishes along much of the spatial domain, ensuring that the intersection between the supports of most of the basis functions is empty.

Approximate *the solution* in a finite dimensional space

An example problem:

$$-\frac{d^2u}{dx^2} + u = f, \quad 0 \le x \le 1$$

with periodic boundary conditions.

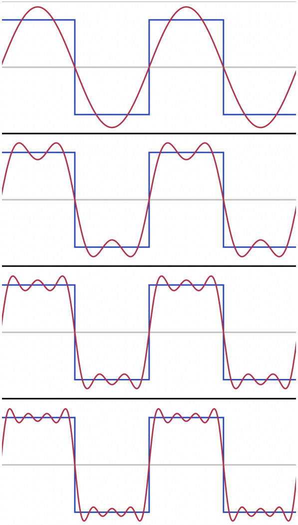
Goal:

Write the solution u as a linear combination of *basis functions* ϕ_i, $i = 1, ..., m$:

$$u_m(x) = \sum_{i=1}^{m} \gamma_i \phi_i(x), \quad 0 \le x \le 1$$

where the $\{\gamma_i\}$ are the *coefficients* that we need to calculate to specify the solution.

Aside: you may have seen this idea in another context:



Fourier Series

Approximate $g(x)$, a square wave (the blue line), as the sum of sine functions:

$$g(x) \approx \sum_{k=1}^{\infty} a_k sin(kx),$$

where the $\{\sin(kx)\}$ are the *basis functions* and the $\{a_k\}$ are the *coefficients*.

Using sine and cosine basis functions leads to a spectral or pseudospectral method; we will use different basis functions for the finite element method.

The Finite Element Method

✓ Approximate *the solution* in a finite dimensional space $\mathbb{H}_m$.
  - Note, we have not yet specified our basis functions $\{\phi_i\}$; this comes in step 4.
  - All we need to do to find the solution is compute the coefficients $\{\gamma_i\}$.

2. Choose the approximation so the *defect* is orthogonal to $\mathbb{H}_m$.
3. Integrate by parts to reduce differentiability requirements.
4. Choose each function in a basis of $\mathbb{H}_m$ such that it vanishes along much of the spatial domain, ensuring that the intersection between the supports of most of the basis functions is empty.

Choose the approximation so the *defect* is orthogonal to $\mathbb{H}_m$

Recall our example problem:

$$-\frac{d^2u}{dx^2} + u = f, \quad 0 \leq x \leq 1 \tag{1}$$

The *defect* d_m is defined by:

$$d_m(x) := -\frac{d^2u_m(x)}{dx^2} + u_m(x) - f(x), \quad 0 \leq x \leq 1.$$

If u_m is the solution of equation 1, then $d_m \equiv 0$.

If $d_m \in \mathbb{H}_m$ then we can identify it by equipping $\mathbb{H}_m$ with an inner product $\langle ., . \rangle$ and seek $\gamma_0, ..., \gamma_m$ such that

$$\langle d_m, \phi_k \rangle = 0, \quad k = 1, ..., m$$

i.e. we require d_m to be orthogonal to $\mathbb{H}_m$.

In general $d_m \notin \mathbb{H}_m$ but the principle holds *if $\mathbb{H}_m$ is a good approximation of the infinite dimensional linear space of solutions*.

Recall we have a finite dimensional approximation for u

$$u_m(x) = \sum_{i=1}^{m} \gamma_i \phi_i(x)$$

Substituting in to the equation for the defect gives

$$\begin{aligned} d_m(x) &:= -\frac{d^2 u_m(x)}{dx^2} + u_m(x) - f(x) \\ &= -\sum_{i=1}^{m} \gamma_i \frac{d^2 \phi_i(x)}{dx^2} + \sum_{i=1}^{m} \gamma_i \phi_i(x) - f(x) \end{aligned}$$

The orthogonality conditions are

$$\langle d_m, \phi_k \rangle = 0, \quad k = 1, ..., m$$

so we have

$$\sum_{i=1}^{m} \gamma_i \big(\langle -\phi_i'', \phi_k \rangle + \langle \phi_i, \phi_k \rangle \big) = \langle f, \phi_k \rangle, \quad k = 1, ..., m$$

The Finite Element Method

- ✓ Approximate *the solution* in a finite dimensional space $\mathbb{H}_m$.
  - Note, we have not yet specified our basis functions $\{\phi_i\}$; this comes in step 4.
  - All we need to do to find the solution is compute the coefficients $\{\gamma_i\}$.
- ✓ Choose the approximation so the *defect* is orthogonal to $\mathbb{H}_m$.
  - This has given us m equations, which is exactly how many we need to find the m unknown coefficients!

3. Integrate by parts to reduce differentiability requirements.
4. Choose each function in a basis of $\mathbb{H}_m$ such that it vanishes along much of the spatial domain, ensuring that the intersection between the supports of most of the basis functions is empty.

Integrate by parts to reduce differentiability requirements

This is key to the computational efficiency of the finite element method as it allows us to choose basis functions that are only *piecewise* differentiable.

Take $\langle \cdot, \cdot \rangle$ to be the usual Euclidian inner product:

$$\langle v, w \rangle = \int_0^1 v(x)w(x)dx$$

$$\sum_{i=1}^{m} \gamma_i \left(\int_0^1 (-\phi_i'' \phi_k) dx + \int_0^1 \phi_i \phi_k dx \right) = \int_0^1 f \phi_k dx$$

Integrating by parts:

$$\sum_{i=1}^{m} \gamma_i \left(\int_0^1 (\phi_i' \phi_k') dx + \int_0^1 \phi_i \phi_k dx \right) = \int_0^1 f \phi_k dx$$

The Finite Element Method

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✓ Integrate by parts to reduce differentiability requirements.
  - These are the equations that we will solve.

4. Choose each function in a basis of $\mathbb{H}_m$ such that it vanishes along much of the spatial domain, ensuring that the intersection between the supports of most of the basis functions is empty.

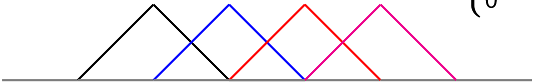
Choose the basis of $\mathbb{H}_m$

Aim:

Choose each ϕ_i such that it vanishes along much of the spatial domain, ensuring that the intersection between the supports of most of the basis functions is empty.

Hat functions

$$\phi_i(x) = \begin{cases} 1 - i + \frac{x}{\Delta x} & (i-1)\Delta x \leq x \leq i\Delta x, \\ 1 + i - \frac{x}{\Delta x} & i\Delta x \leq x \leq (i+1)\Delta x, \\ 0 & \text{otherwise.} \end{cases}$$



Advantages:

- reduce number of integrals that we compute
- sparse matrices
- computational efficiency

The Finite Element Method

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  - This has given us m equations, which is exactly how many we need to find the m unknown coefficients!
- ✓ Integrate by parts to reduce differentiability requirements.
  - These are the equations that we will solve.
- ✓ Choose each function in a basis of $\mathbb{H}_m$ such that it vanishes along much of the spatial domain.
  - We have reduced the problem to solving a matrix-vector equation $A\boldsymbol{\gamma} = \boldsymbol{f}$ where the elements of A are integrals of products of basis functions and their derivatives.
  - Due to the choice of basis functions, most of these products are zero, resulting in a sparse matrix.

Compatible finite element methods

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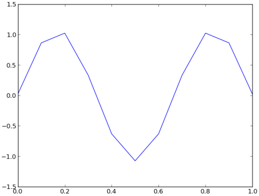
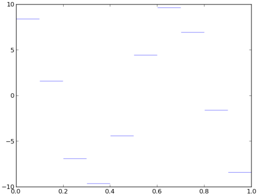




Example: 1D wave equation

- We have seen an example of compatible finite element function spaces.
- These spaces are appropriate for discretising the 1D wave equation:

$$\begin{aligned} u_t + h_x &= 0, \\ h_t + u_x &= 0. \end{aligned}$$

- We chose finite element spaces $\mathbb{V}_0$, $\mathbb{V}_1$ such that
    1. if $u \in \mathbb{V}_1$ then $u_x \in \mathbb{V}_0$,
    2. if $h \in \mathbb{V}_0$ then $\exists u \in \mathbb{V}_1$ with $u_x = h$.

$$\underbrace{\mathbb{V}_1}_{\text{Continuous}} \xrightarrow{\frac{d}{dx}} \underbrace{\mathbb{V}_0}_{\text{Discontinuous}}$$

$$\begin{aligned} \int_0^L w u_t - w_x h \, \mathrm{d}x &= 0, & \forall w \in \mathbb{V}_1, \\ \int_0^L \phi(h_t + u_x) \, \mathrm{d}x &= 0, & \forall \phi \in \mathbb{V}_0, \end{aligned}$$

Example: linear shallow water equations

$$\boldsymbol{u}_t + f\boldsymbol{u}^{\perp} + c^2\nabla\eta = 0, \quad \eta_t + \nabla\cdot\boldsymbol{u} = 0$$

The finite element approximation is:

$$\begin{aligned} \frac{d}{dt}\int_\Omega \boldsymbol{w}\cdot\boldsymbol{u}\,\mathrm{d}V + \int_\Omega f\boldsymbol{w}\cdot\boldsymbol{u}^{\perp}\,\mathrm{d}V - c^2\int_\Omega \nabla\cdot\boldsymbol{w}\eta\,\mathrm{d}V &= 0, \forall \boldsymbol{w}\in\mathbb{V}_1 \\ \frac{d}{dt}\int_\Omega \phi\eta\,\mathrm{d}V + \int_\Omega \phi\nabla\cdot\boldsymbol{u}\,\mathrm{d}V &= 0, \forall\phi\in\mathbb{V}_2. \end{aligned}$$

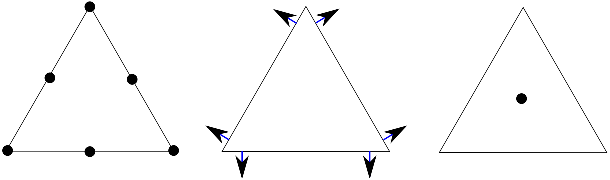
$$\underbrace{\mathbb{V}_0}_{\text{Continuous}} \xrightarrow{\nabla^{\perp}} \underbrace{\mathbb{V}_1}_{\text{Continuous normals}} \xrightarrow{\nabla\cdot} \underbrace{\mathbb{V}_2}_{\text{Discontinuous}}$$

Mimetic property: $\nabla\cdot\nabla^{\perp}\boldsymbol{u} = 0$

1. $\nabla\cdot$ maps from $\mathbb{V}_1$ onto $\mathbb{V}_2$.
2. $\nabla^{\perp}$ maps from $\mathbb{V}_0$ onto the kernal of $\nabla\cdot$ in $\mathbb{V}_1$.

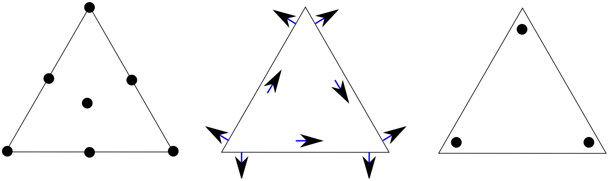
Example finite element spaces

$$\underbrace{\mathbb{V}_0 = P2}_{\text{Quadratic, Continuous}} \xrightarrow{\nabla^\perp} \underbrace{\mathbb{V}_1 = BDM1}_{\text{Linear, Continuous normals}} \xrightarrow{\nabla\cdot} \underbrace{\mathbb{V}_2 = P0}_{\text{Constant, Discontinuous}}$$



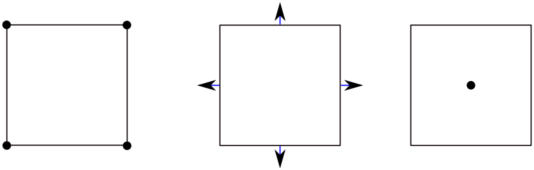
Example finite element spaces

$$\underbrace{\mathbb{V}_0 = P2+}_{\text{Quadratic (+1 Cubic) Continuous}} \xrightarrow{\nabla^\perp} \underbrace{\mathbb{V}_1 = BDFM1}_{\text{Linear (+2 Quadratic) Cont. normals}} \xrightarrow{\nabla\cdot} \underbrace{\mathbb{V}_2 = P1_{DG}}_{\text{Linear Discontinuous}}$$



Example finite element spaces

$$\underbrace{\mathbb{V}_0 = Q1}_{\text{Bilinear Continuous}} \xrightarrow{\nabla^{\perp}} \underbrace{\mathbb{V}_1 = RT0}_{\text{Constant/Linear, Cont. normals}} \xrightarrow{\nabla\cdot} \underbrace{\mathbb{V}_2 = Q0_{DG}}_{\text{Constant, Discontinuous}}$$



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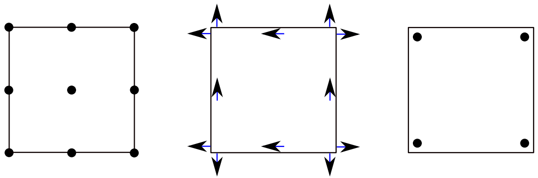
$$\underbrace{\mathbb{V}_0 = Q2}_{\text{Biquadratic Continuous}} \xrightarrow{\nabla^\perp} \underbrace{\mathbb{V}_1 = RT1}_{\text{Bilinear/Biquadratic, Cont. normals}} \xrightarrow{\nabla\cdot} \underbrace{\mathbb{V}_2 = Q1_{DG}}_{\text{Bilinear, Discontinuous}}$$



Properties

Compatible FEM applied to linear shallow water equations shares the properties of the C-grid staggered finite difference method.

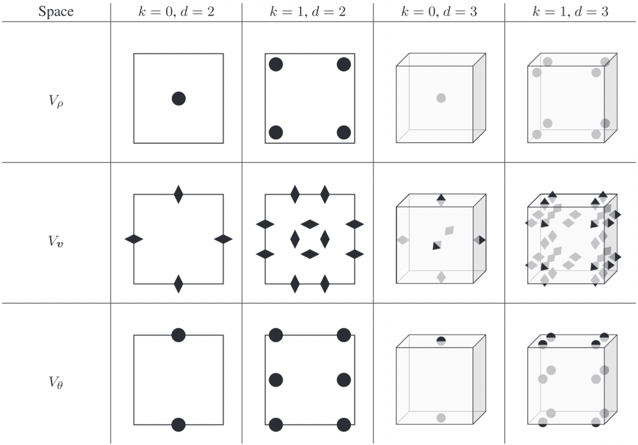
1. Energy and mass conservation
2. No spurious modes from pressure or inertia terms,
3. Geostrophic modes are exactly steady.

We additionally get:

1. No orthogonality constraints on mesh.
2. Flexibility to change pressure/velocity DOF ratios to avoid spurious mode branches.

See: C. Cotter and J. Shipton, JCP (2012).

What about in 3D?



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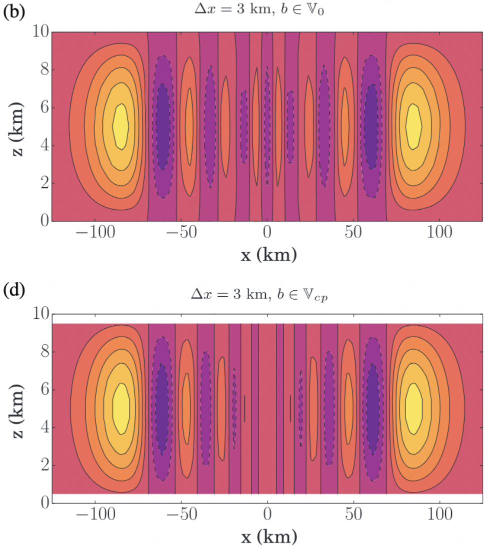

Melvin, T., et al. "Choice of function spaces for thermodynamic variables in mixed finite-element methods." QJRMS (2018)

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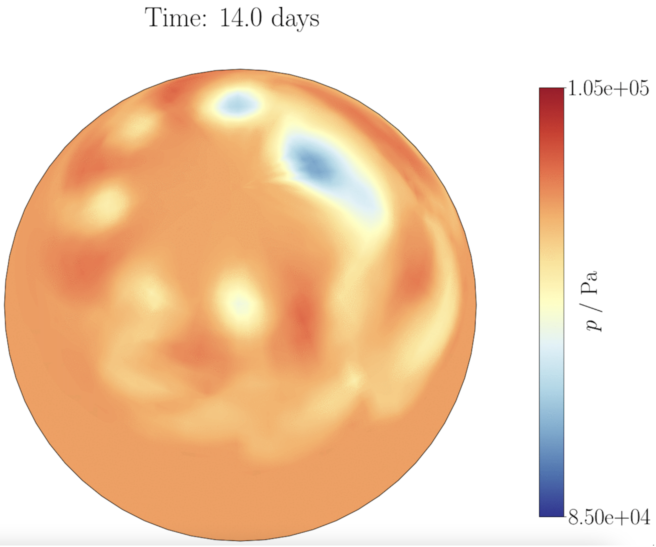

Very new result from Thomas Bendall and Daniel Witt!

Research directions

- Physics-dynamics coupling
- Higher order methods
- Faster solvers for the matrix-vector equations
- Adaptive meshes
- Exponential timestepping methods
- Parallel timestepping methods