Spectral method
Motivation
Framework
DiffGeoDansis
Non-isotropic
Darcy
resultsA

High order discretisation methods in CFD

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Spectral Methods

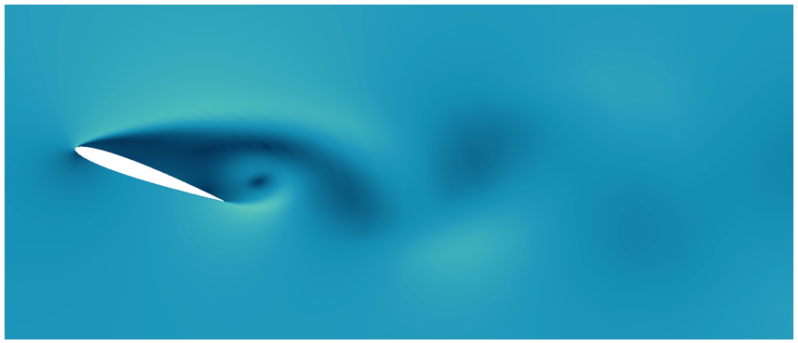
Motivation for high order discretisation.

1. Previously, we have mainly focused on either finite difference (collocation methods), finite element (Galerkin methods), or finite volume (sub-domain methods) for solving CFD problems.
2. In addition, we have concentrated on lower order discretization methods. First or second order Taylor expansions.
3. In todays seminar we will use high order discretization method where the unknowns are expanded in polynomials of an order higher than 3.

Spectral Methods

Motivation for high order discretisation continued.

- If we are interested in studying vortex interaction using e.g. a FV method, where we strive for 2nd order accuracy, the accuracy of the interaction of vortices is of zero order!



J Christensen & M Østerlund

Method of Weighted Residual

Let $u(x)$ be the solution of the problem

$$L[u] = f \text{ in } \Omega$$
$$B[u] = g \text{ on } \partial\Omega,$$

where L is a (non-linear) differential operator and B represents the boundary operator. The unknown solution function is approximated by a set of basis (also called expansion or trial functions) functions of the form

$$u^N(x) = \sum_{i=0}^{N} a_i \phi_i$$

where $u^N(x)$ is an approximate solution.

Method of Weighted Residual

The basis function are often chosen to linear independent function and the unknown expansion coefficients a_i are in general a function of the expansion order N. Substituting the expansion into the differential operator leaves an error function, the residual, $r(x)$,

$$r(x) = L[u^N] - f.$$

Having chosen a set of N basis functions we need N conditions to solve for the N expansion coefficients a_i. Introducing a test function $\psi_i(x)$, we force the inner product

$$\int_\Omega r(x)\psi_i(x)dx = (r, \psi_i)$$

Method of Weighted Residual

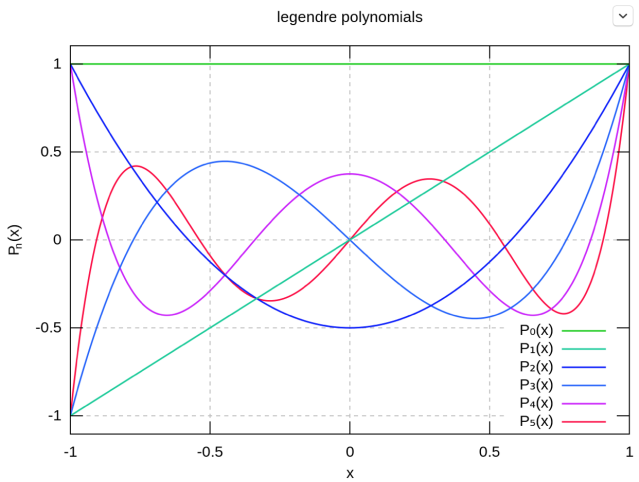
to vanish for $i = 0, 1, ..., N$. The error is set to zero in an average sence, $(r, \psi) = 0$ for $i = 0, 1, ..., N$. In choosing the $N + 1$ test functions we have $N + 1$ conditions to determine the $N + 1$ expansion coefficients.

1. The Galerkin method $\psi_i = \phi_i$
2. The collocation method $\psi_i = \delta(x - x_i)$
3. The Least Squares method $\psi_i = \frac{\partial r}{\partial a_i}$

Basis functions

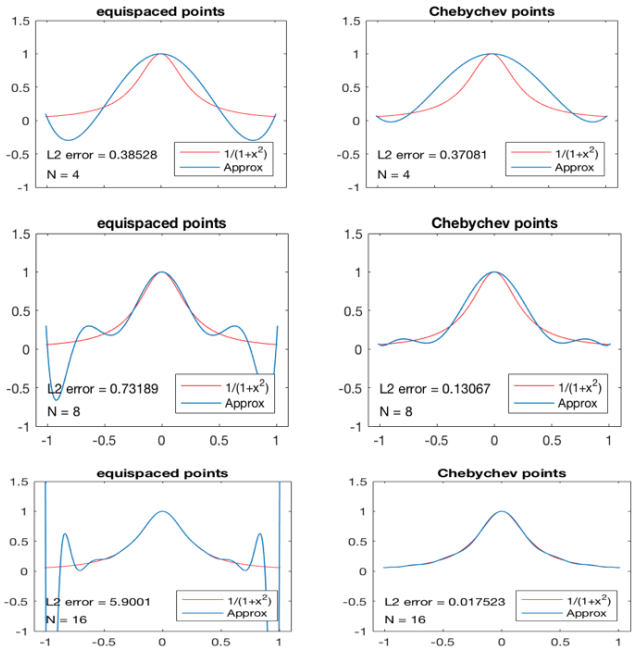
The most popular choice of basis functions are the eigenfunctions of the singular Sturm-Liouville problem and out of them we mainly use two sets of polynomials - the Chebychev and the Legendre polynomials.
The eigenfunctions, $\phi_i(x)$, are mutually orthogonal with respect to the positive weight function $w(x)$

$$\int_{-1}^{1} \phi_i(x)\phi_j(x)w(x)dx = 0 \text{ for } i \neq j$$



Spectral Methods

Approximation theory – Lagrange interpolation



$$f(x) = \frac{1}{1+x^2} = \sum_{i=0}^{N} f_i h_i(x) \Rightarrow f(x_j) = f_j$$

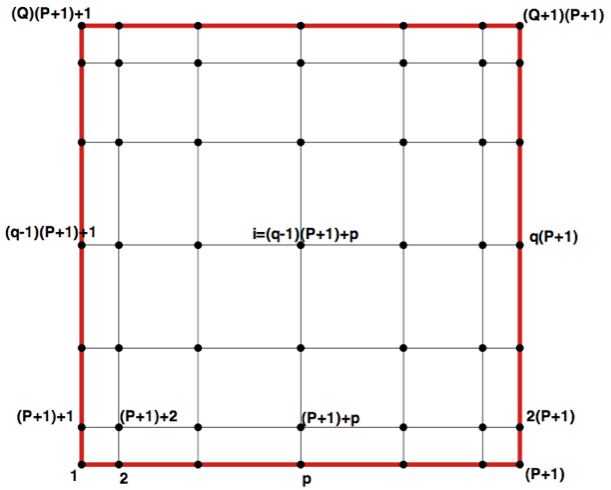
$$h_i(x_j) = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

$$x_i = cos(\frac{i\pi}{N}) \quad i = 0, 1, ..., N$$

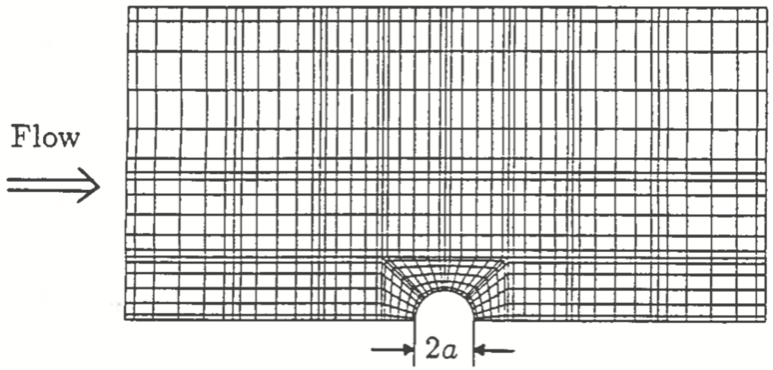
Spectral Methods

2D grids

N = 7, K = 1

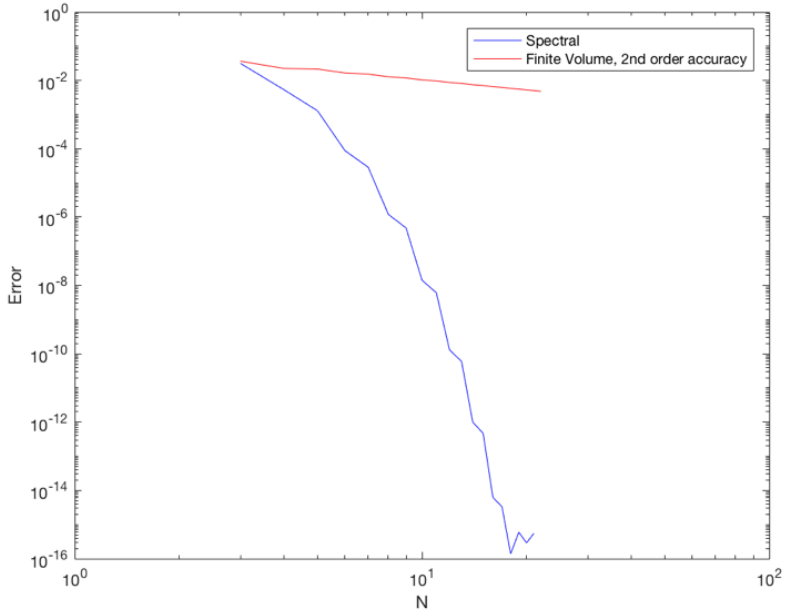


N = 6, K = 26



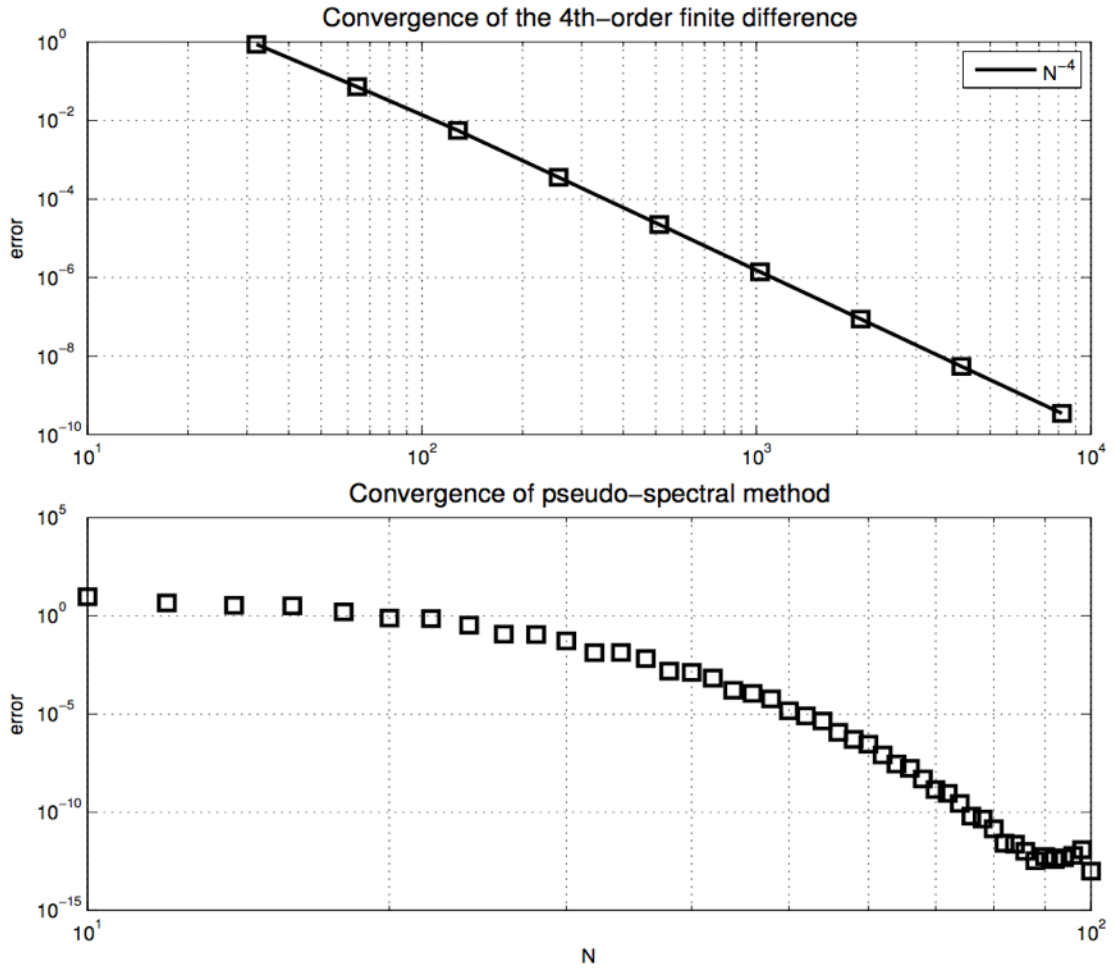
Spectral convergence for the 1D Poisson operator

$$\frac{d^2T}{dx^2} = sin(\pi x) \quad x \in [-1, 1]$$



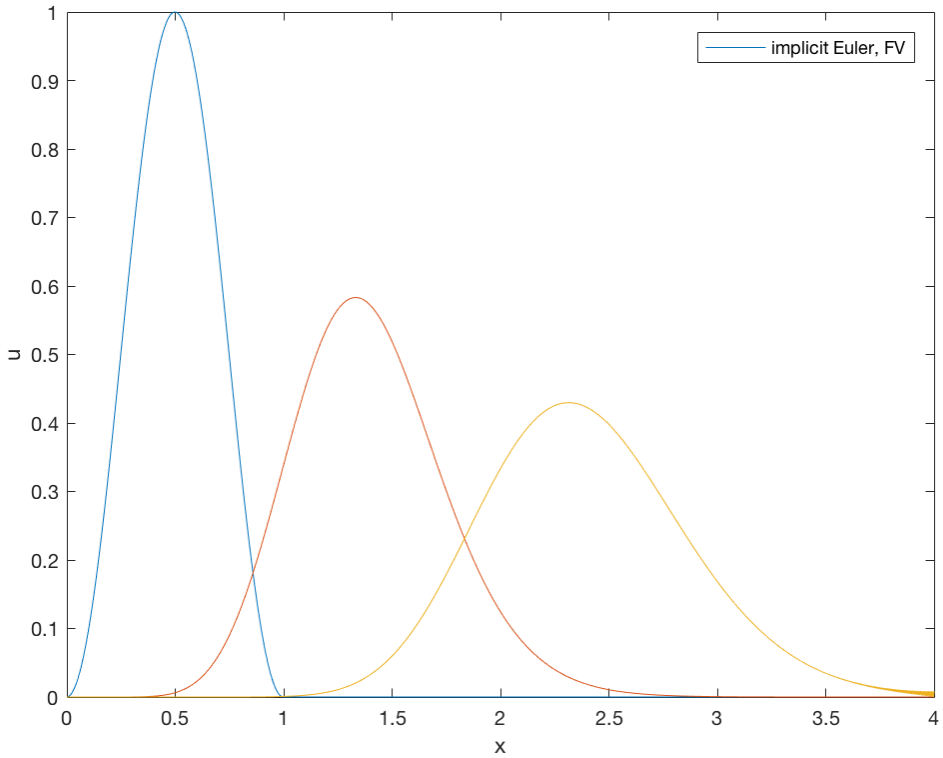
Spectral convergence for the 2D Poisson operator

$$u' = e^{\sin(2x)+\cos(3x)}$$



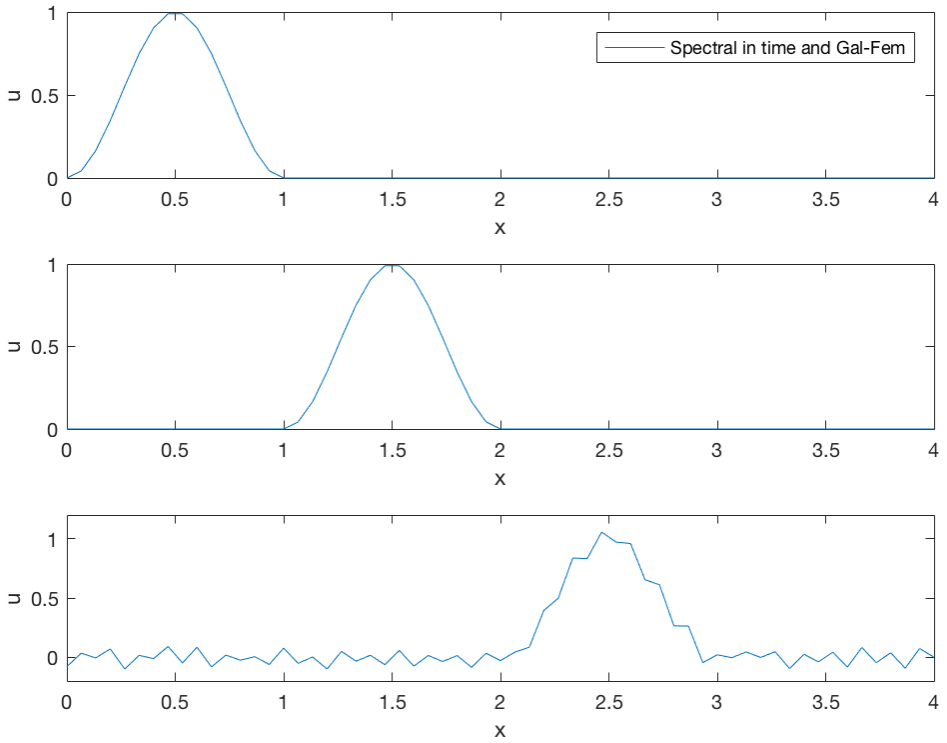
Spectral Methods - time-dependent hyperbolic problem

Solve the linear time dependent 1D convection equation $u_t + u_x = 0$ using an implicit Euler for time integration and FV for spatial discretisation. $u_0(x) = 0.5 * (1 - cos(2\pi x))$



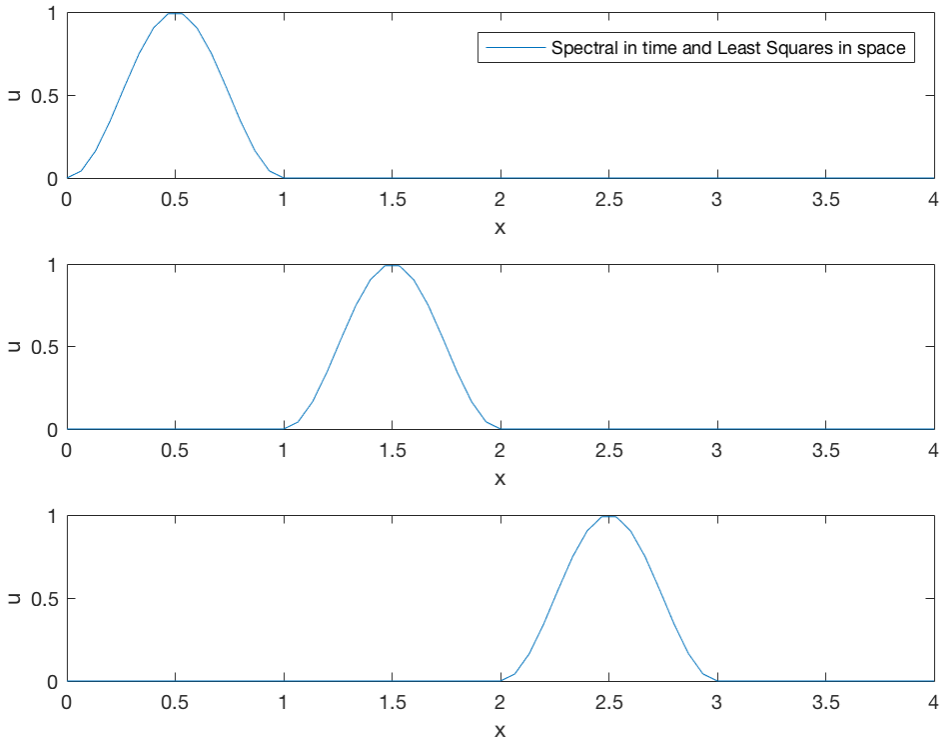
Spectral Methods - time-dependent hyperbolic problem

Solve the linear time dependent 1D convection equation $u_t + u_x = 0$ using spectral time integration and SEM for spatial discretisation. $u_0(x) = 0.5 * (1 - cos(2\pi x))$



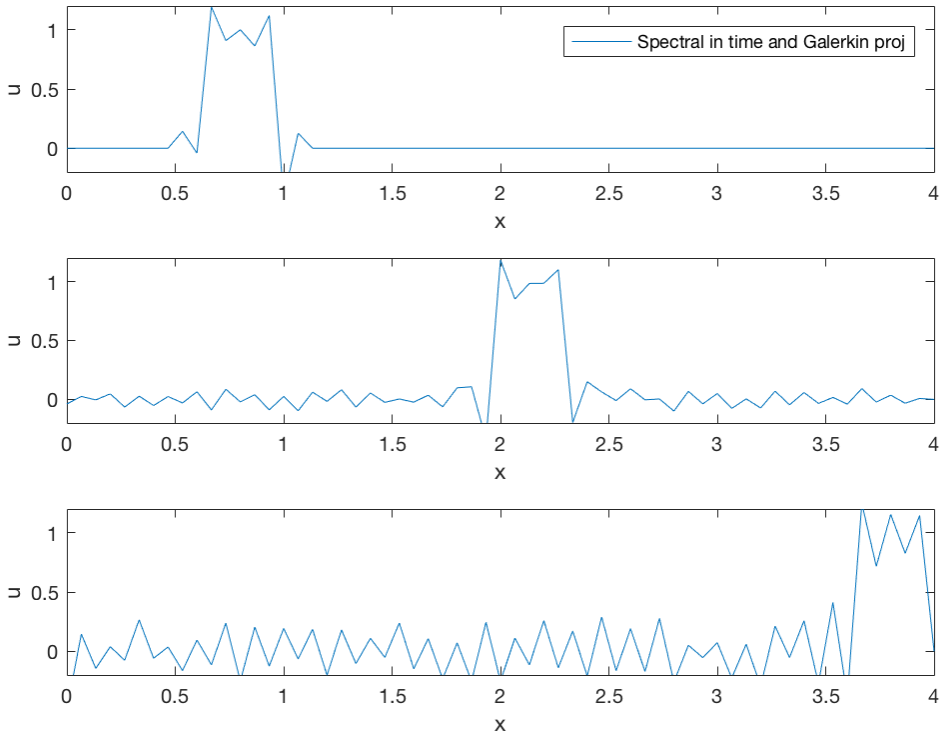
Spectral Methods - time-dependent hyperbolic problem

Solve the linear time dependent 1D convection equation $u_t + u_x = 0$ using spectral time integration and spectral Least Squares for spatial discretisation. $u_0(x) = 0.5 * (1 - cos(2\pi x))$



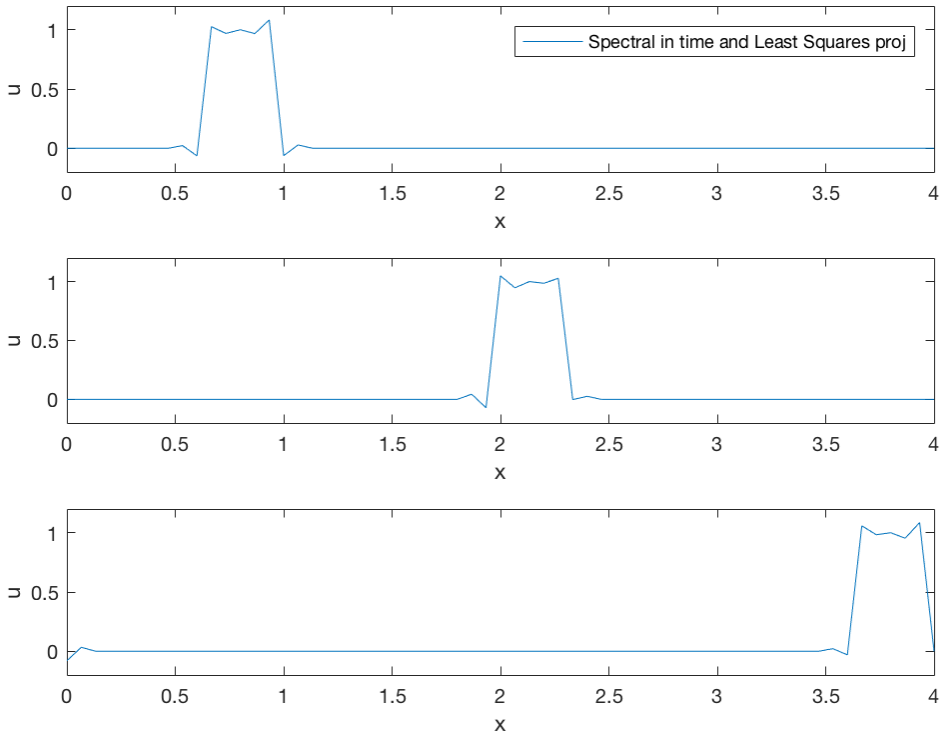
Spectral Methods - time-dependent hyperbolic problem

Solve the linear time dependent 1D convection equation $u_t + u_x = 0$ using spectral time integration and SEM for spatial discretisation. u_0: square wave.



Spectral Methods - time-dependent hyperbolic problem

Solve the linear time dependent 1D convection equation $u_t + u_x = 0$ using spectral time integration and spectral least squares for spatial discretisation. u_0: square wave.



The use of a mimetic method

- Also called structure preserving
- Mimics the nature of the problem (preserves its structure)

A physical model typically consists of two kinds of relations:

- Topological (e.g. conservation and equilibrium laws)
- Constitutive (e.g. relations between stress and strains etc.)

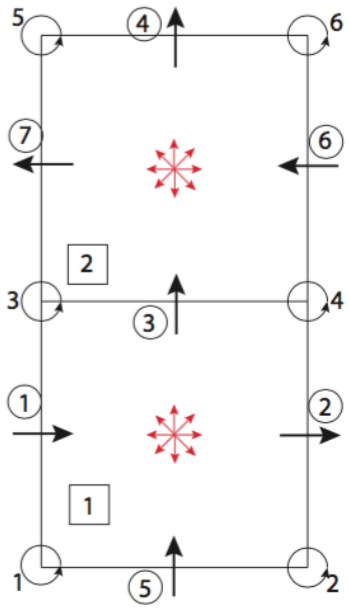
Topological relations ought to be exact, but typical numerical schemes only satisfies this when the element size approaches zero.

Numerical approximations are located in the discretisation of the constitutive equations, just as in the physical world.

Simple grid

- Consider the 2D grid shown on the right.
- Number all the vertices in the mesh
- Number all edges in the mesh
- Number all volumes in the mesh

- Give the vertices a default orientation
- Give a default orientation to all edges
- Give default orientation to the volumes



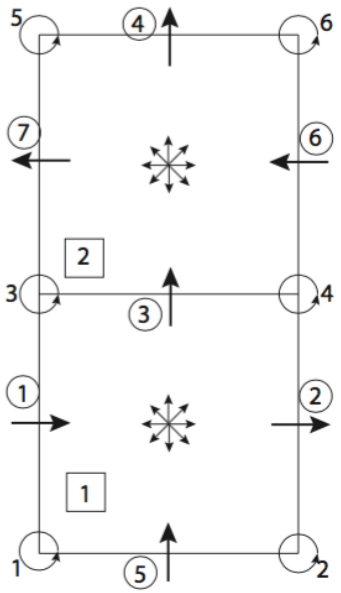
Incidense matrices

$$\mathbb{E}^{1,0} = \begin{pmatrix} -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 \\ 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & 0 & -1 & 0 \end{pmatrix}$$

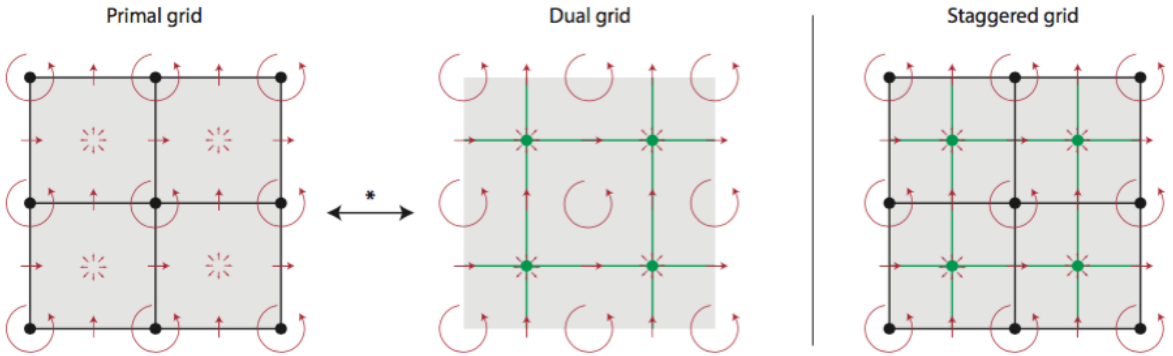
$$\mathbb{E}^{2,1} = \begin{pmatrix} -1 & 1 & 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & -1 & 1 \end{pmatrix}$$

The matrices $\mathbb{E}^{1,0}$ and $\mathbb{E}^{2,1}$ are called incidence matrices. The incidence matrices only contain entries -1, 0 and 1.

The incidence matrices are independent of the shape and coarseness of the grid



Staggered grid



$$H(curl;\Omega) \qquad H_0(div;\Omega)$$
$$\downarrow \qquad\qquad \uparrow$$
$$H(div;\Omega) \qquad H_0(curl;\Omega)$$
$$\downarrow \qquad\qquad \uparrow$$
$$L^2(\Omega) \qquad H_0^1(\Omega)$$

De Rham complex

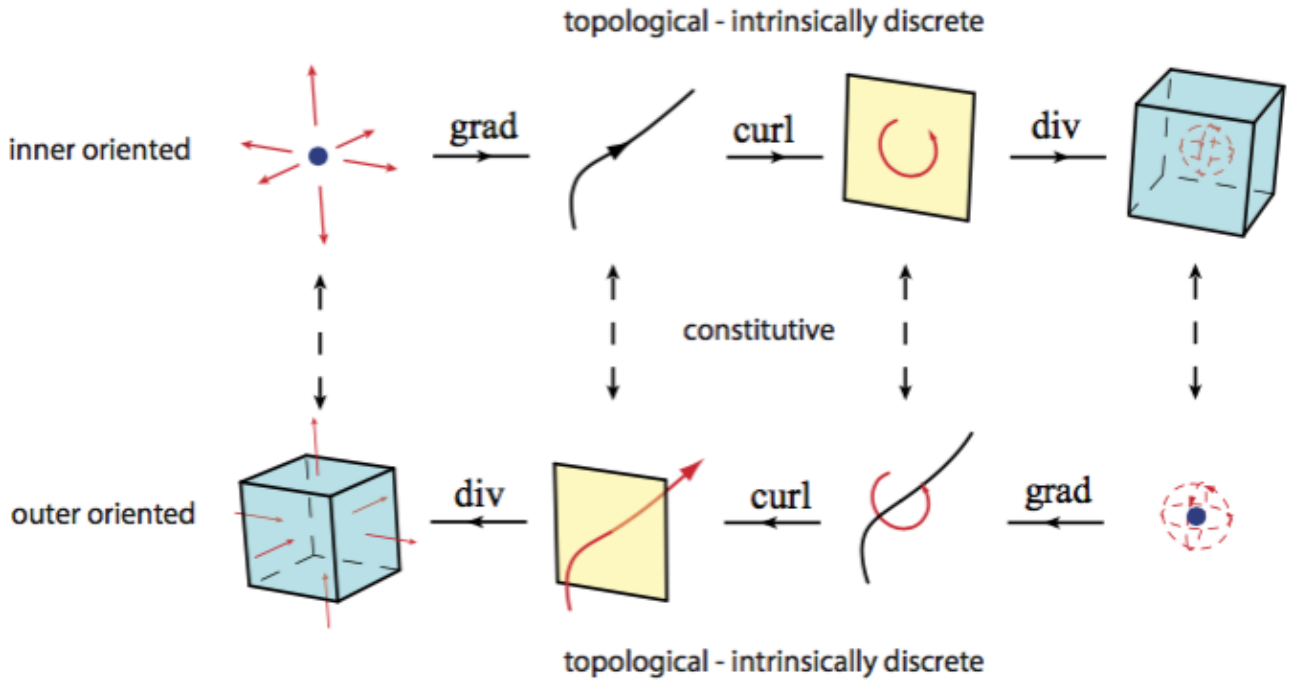
We have in 3D

$$\mathbb{R} \longrightarrow H_P \xrightarrow{\mathbb{E}^{1,0}} H_E \xrightarrow{\mathbb{E}^{2,1}} H_S \xrightarrow{\mathbb{E}^{3,2}} H_V \longrightarrow 0$$

$$0 \longleftarrow H_{\tilde{V}} \xleftarrow{\mathbb{E}^{1,0^T}} H_{\tilde{S}} \xleftarrow{\mathbb{E}^{2,1^T}} H_{\tilde{E}} \xleftarrow{\mathbb{E}^{3,2^T}} H_{\tilde{P}} \longleftarrow \mathbb{R}$$

and on the dual grid

De Rham complex continues



Differential forms

A PDE (e.g. NS) can be solved using differential geometry. This allows us to rephrase differential equations in such a way that its conserved quantity is preserved. This ensures that for example the continuity equation is conserved independent of the grid.
The main building blocks in differential geometry are differential forms, which are anti-symmetric k-tensors acting on vector fields.
Or they are object underneath an integration sign.
In R^3 we can write forms as:

$$\begin{aligned}
\alpha^{(0)} &= f(x,y,z) \\
\beta^{(1)} &= A(x,y,z)dx + B(x,y,z)dy + C(x,y,z)dz \\
\gamma^{(2)} &= P(x,y,z)dydz + Q(x,y,z)dzdx + R(x,y,z)dxdy \\
\omega^{(3)} &= g(x,y,z)dxdydz
\end{aligned}$$

Why differential forms?

1. Many operators become metric-free when represented by differential forms;
2. Discrete analogue in terms of chains and cochains from algebraic topology;
3. Closer connection with physics

Differential forms

How do differential forms differ from scalar and vector fields:

1. point scalar field - zero-form
2. curve vector field - 1-form
3. surface vector field - 2-form
4. volume scalar field - 3-form

$$\beta^{(1)} = A(x,y,z)dx + B(x,y,z)dy + C(x,y,z)dz$$

A 1-form can be integrated over one-dimensional, smooth curves C to give:

$$\int_C \beta^{(1)} = \int_C A(x,y,z)dx + B(x,y,z)dy + C(x,y,z)dz$$

This is denoted the pairing between the 1-form and the associated geometric one-dimensional curve C.

$$(\beta^{(1)}, C) := \int_C \beta^{(1)}$$

Classical vector calculus only works with the coefficients A, B, C, which forms the vector proxy of 1-forms, and ignores the basis vectors dx, dy, dz. Geometrically we associate one-forms with curves.

Differential forms

A 2-form can be integrated over two-dimensional, smooth surfaces S to give:

$$\int_S \gamma^{(2)} = \int_S P(x,y,z)dydz + Q(x,y,z)dzdx + R(x,y,z)dxdy$$

or

$$(\gamma^{(2)}, S) := \int_S \gamma^{(2)}$$

This is the duality pairing between a 2-form and the associated geometric two-dimensional surface S. The vector proxy P, Q, R also represents a vector in normal vector calculus. But the distinction between 1-forms and 2-forms is lost.
A 3-form can be integrated over volumes V to give:

$$\int_V \omega^{(3)} = \int_V g(x,y,z)dxdydz$$

or

$$(\omega^{(3)}, V) := \int_V \omega^{(3)}$$

Here we associate the duality pairing between the 3-form and the three-dimensional object.
A 0-form is a normal scalar function and can be integrated over points:

$$\int_{P_1,\ldots,P_k} \alpha^{(0)} = \sum_{i=1}^{k} f(P_k)$$

A differential form

The exterior derivative, d, is an operation on k-form, which maps k-forms into $(k+1)$-forms:

$$d\alpha^{(0)} = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy + \frac{\partial f}{\partial z}dz$$

Here the vector proxy of $d\alpha^{(0)}$ is $\boldsymbol{grad}\, f$.

$$d\beta^{(1)} = (\frac{\partial C}{\partial y} - \frac{\partial B}{\partial z})dydz + (\frac{\partial A}{\partial z} - \frac{\partial C}{\partial x})dzdx + (\frac{\partial B}{\partial x} - \frac{\partial A}{\partial y})dxdy$$

If $\boldsymbol{u} = (A, B, C)$ the vector proxy of $d\beta^{(1)}$ is $\boldsymbol{curl}\, \boldsymbol{u}$.

$$d\gamma^{(2)} = (\frac{\partial P}{\partial x} + \frac{\partial Q}{\partial y} + \frac{\partial R}{\partial z})dxdydz$$

If $\boldsymbol{v} = (P, Q, R)$ the vector proxy of $d\gamma^{(2)}$ is $\boldsymbol{div}\, \boldsymbol{v}$.

A differential form

Let's consider the Poisson equation $\Delta\phi = f$ as a first order system:

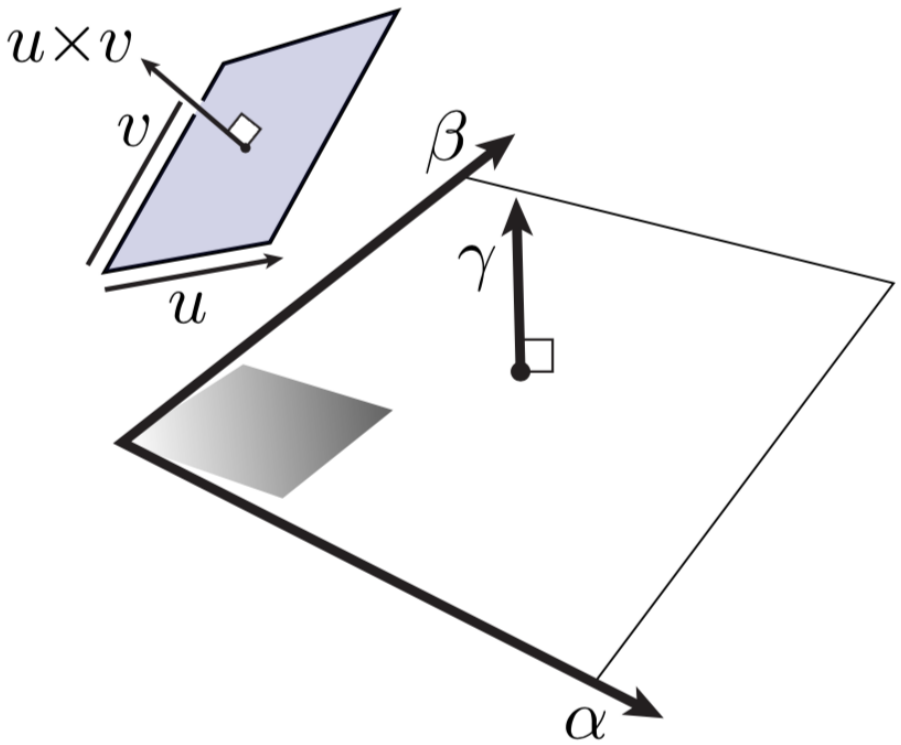
$$\begin{aligned} \boldsymbol{div}\, \boldsymbol{q} &= f \\ \boldsymbol{grad}\, \phi &= u \\ \boldsymbol{u} &= \boldsymbol{q} \end{aligned}$$

We can now rewrite the above system using differential geometry to obtain:

$$\begin{aligned} dq^{(2)} &= f^{(3)} \\ d\phi^{(0)} &= u^{(1)} \\ u^{(1)} &= q^{(2)} \quad !!! \end{aligned}$$

A differential form

Solution: The Hodge-$\star$ operator. It maps k-forms onto $(n-k)$-forms, where n is the dimension of the ambient space. The Hodge-$\star$ operator does not alter the scalar field or the vector field, but changes the geometric object with which these fields are associated. Geometrically we can illustrate it with the way we represent a surface. We could either use the normal vector γ or the two vectors in the plane α and β.



Representation of physical quantities: geometric origin

Fundamental theorem of calculus

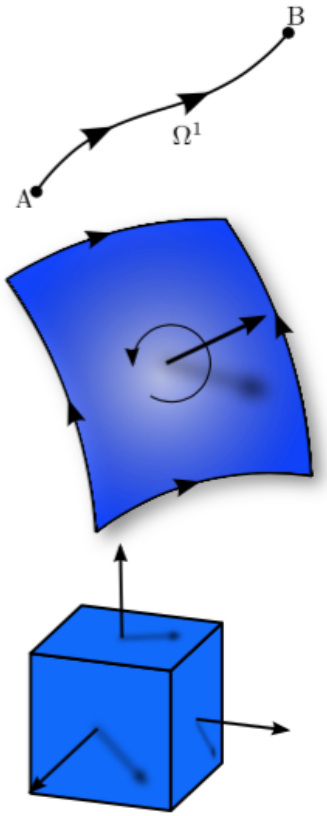
$$\int_{\Omega^1} \nabla\varphi \cdot d\vec{l} = \varphi(\Omega^1_B) - \varphi(\Omega^1_A)$$

Kelvin-Stokes theorem

$$\int_{\Omega^2} (\nabla \times \vec{v}) \cdot \vec{n} dS = \int_{\partial\Omega^2} \vec{v} \cdot d\vec{l}$$

Gauss theorem

$$\int_{\Omega^3} (\nabla \cdot \vec{v}) dV = \int_{\partial\Omega^3} \vec{v} \cdot \vec{n} dS$$



The non-isotropic diffusion problem

We present a discretisation of the non-isotropic diffusion problem based on a spectral multi-scale method. In fluid dynamics these problems are known as the Darcy flow problem, which model single phase, incompressible flow in porous media. These types of flows appear among others in groundwater dynamics, petroleum engineering and CO_2 storage.
The stationary non-isotropic diffusion problem can take the form:

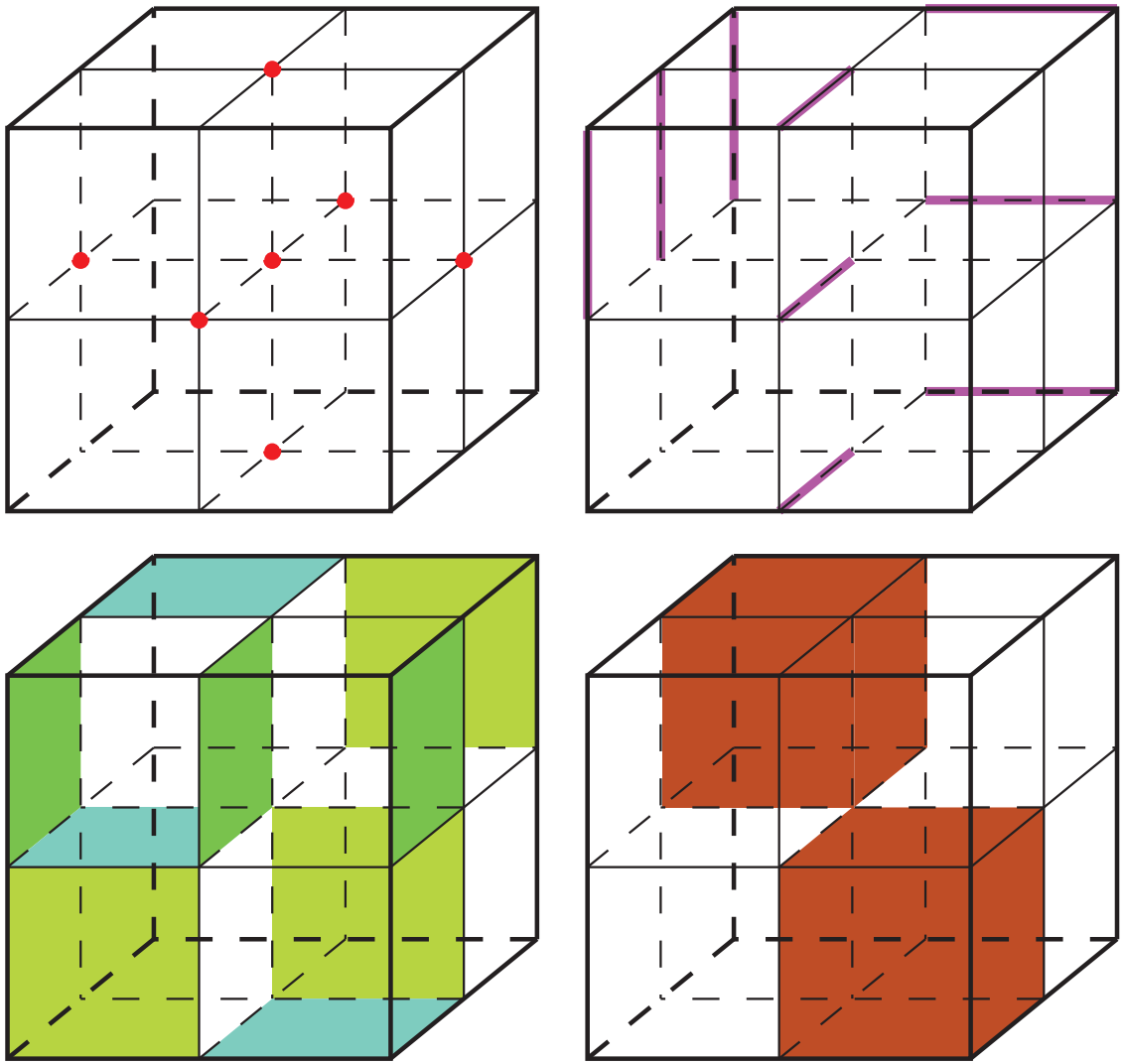
$$u = -K\nabla p$$
$$\nabla \cdot u = f$$

Matrix K is a symmetric, positive definite tensor, representing the material permeability divided by the fluid kinematic viscosity.

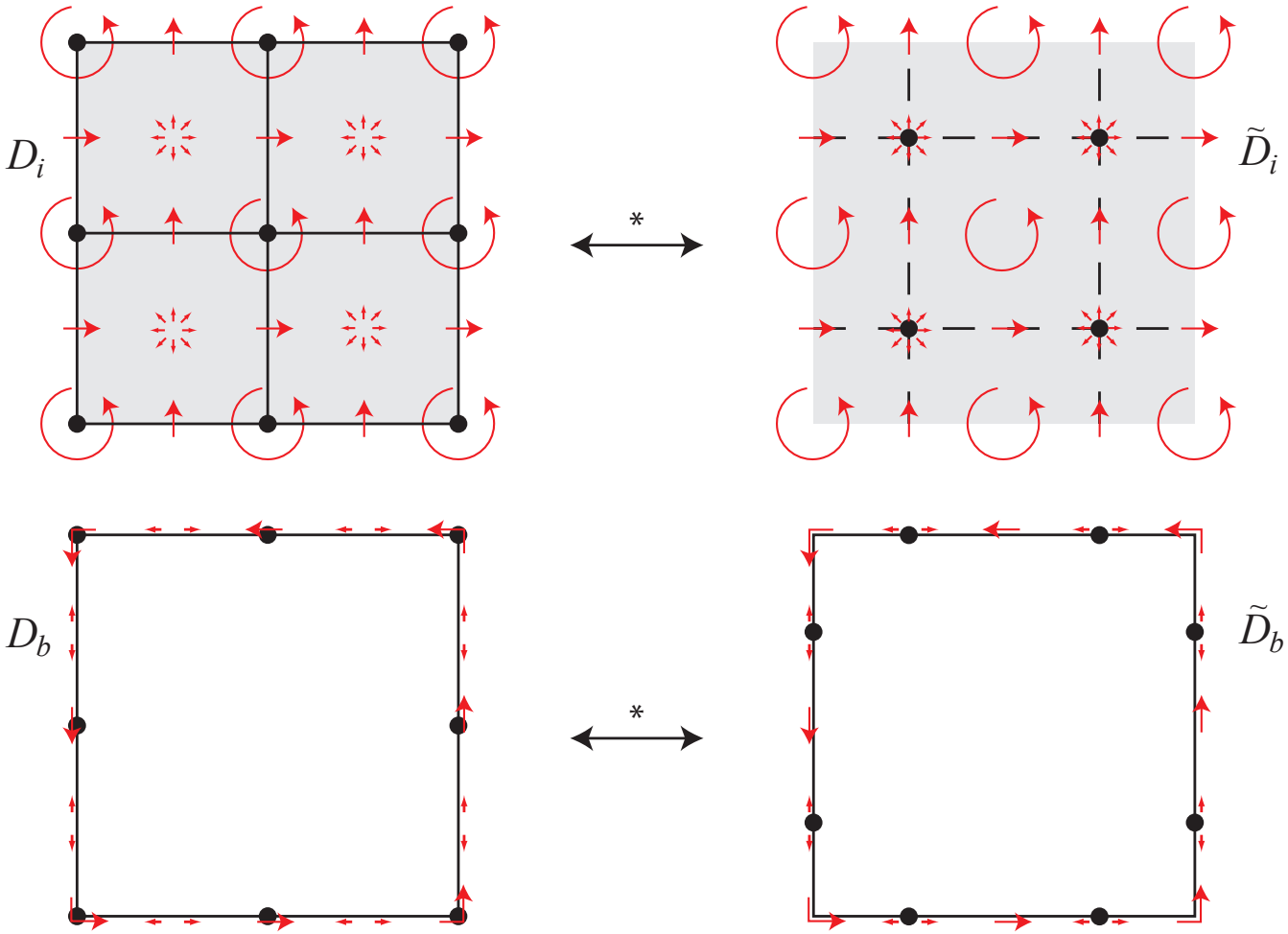
The tools

- Differential geometry $\rightarrow$ Algebraic topology;
- Discrete De Rham complex;
- Dual cell complex;
- Discrete topological conservation laws using coboundary operator;
- Approximate constitutive relations

Geometric structure/cell complex



Geometric structure/cell complex



Geometrical associations

The objective is:
Associate each discrete physical quantity such that they are consistent in the topological equations.

The conservation law we are looking at is the continuity equation:

$$\nabla \cdot \boldsymbol{u} = f$$

and the kinematic equation relating the flux $\vec{u}$ to the gradient of pressure p weighted with a material coefficient tensor K representing the material permeability divided by the fluid kinematic viscosity:

$$u = -K\nabla p$$

Darcy's model using differential forms

In terms of differential forms Darcy's model is given as:
The conservation law, which in this case is the continuity equation takes the form:

$$du^{(n-1)} = f^{(n)}$$

and the constitutive equation we can write as:

$$u^{(n-1)} = -Kdp^{(0)}$$

where n is the dimension of the problem.
Since u in the first equation is outer oriented and inner oriented in the second equation we need to use the Hodge star operator and we can rewrite the second equation as:

$$\star u^{(n-1)} = -Kdp^{(0)}$$

Darcy's model using differential forms in 2D

In 2D we can write Darcy's model:

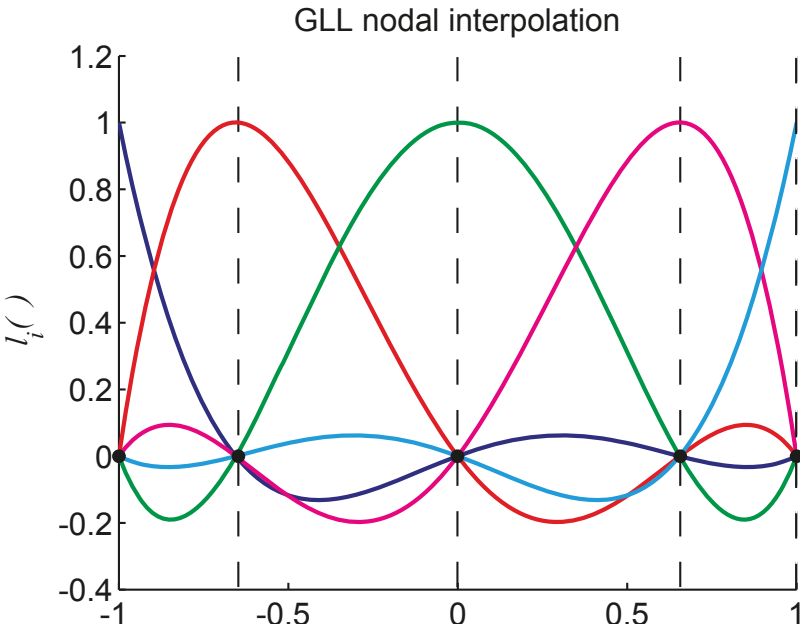
$$du^{(1)} = f^{(2)}$$

$$\star u^{(1)} = -Kdp^{(0)}$$

Expansions

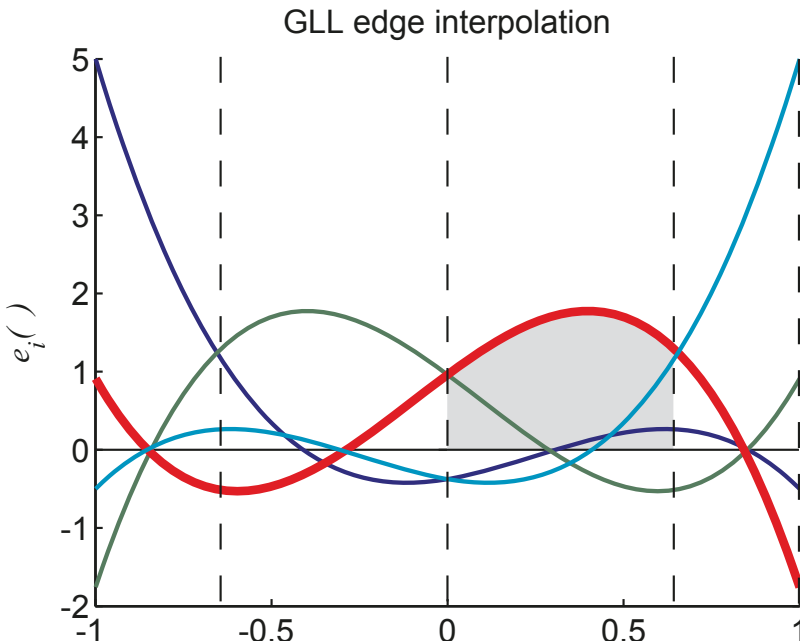
The expansions of the different quantities are performed using Lagrange and edge polynomials.

Lagrange polynomials



$$l_i^{(0)}(x_p) = \begin{cases} 1 & \text{if} \quad i = p \\ 0 & \text{if} \quad i \neq p \end{cases}$$

Edge polynomials



$$\int_{x_p}^{x_{p+1}} e_i^{(p)}(x) = \begin{cases} 1 & \text{if} \quad i = p \\ 0 & \text{if} \quad i \neq p \end{cases}$$

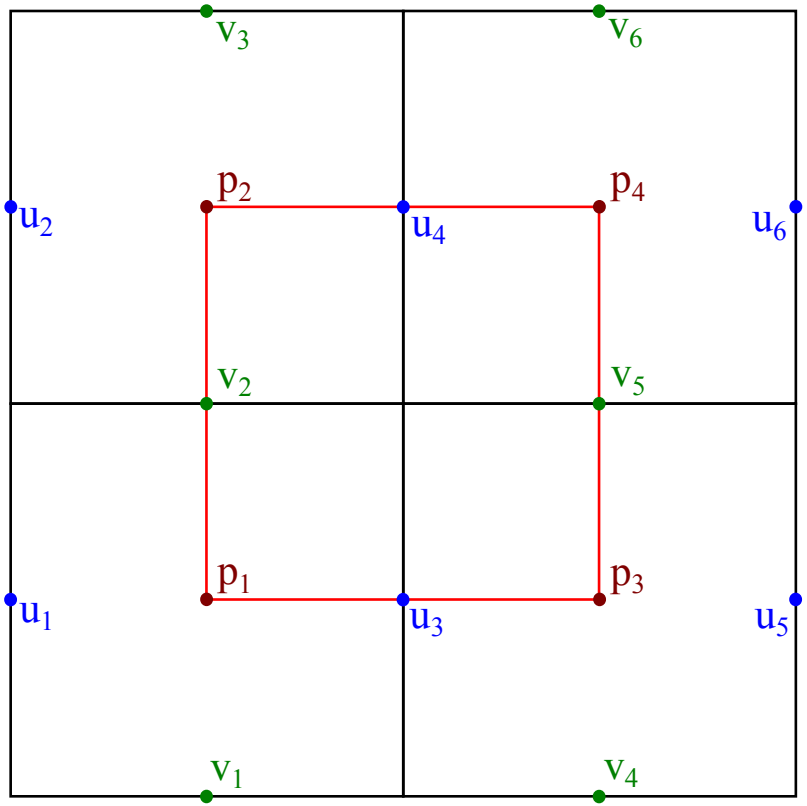
[1] Edge Functions for Spectral Element Methods, M Gerritsma, 2009.

Expansions - velocity

$$u_h^{(1)} = \sum_{i=1}^{N+1} \sum_{j=1}^{N} u_{ij} h_i(x) e_j(y) + \sum_{i=1}^{N} \sum_{j=1}^{N+1} v_{ij} e_i(x) h_j(y)$$

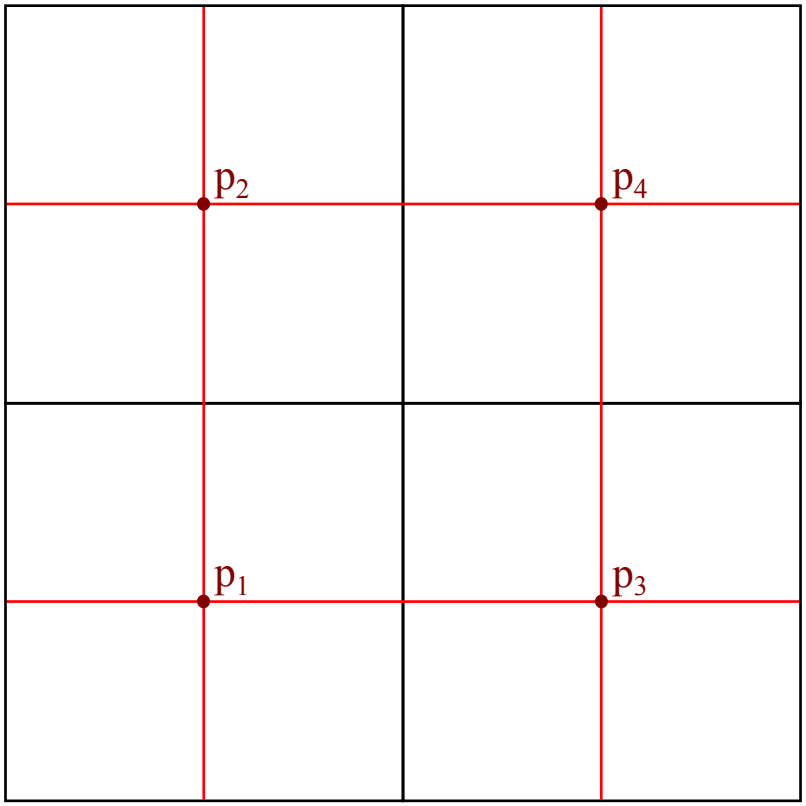
h_i: Lagrange polynomials based on Gauss-Lobatto-Legendre

e_i: Edge polynomials based on Gauss-Lobatto-Legendre



Expansions - pressure

$$p_h^{(0)} = \sum_{i=1}^{N} \sum_{j=1}^{N} p_{ij} \tilde{h}_i(x) \tilde{h}_j(y)$$



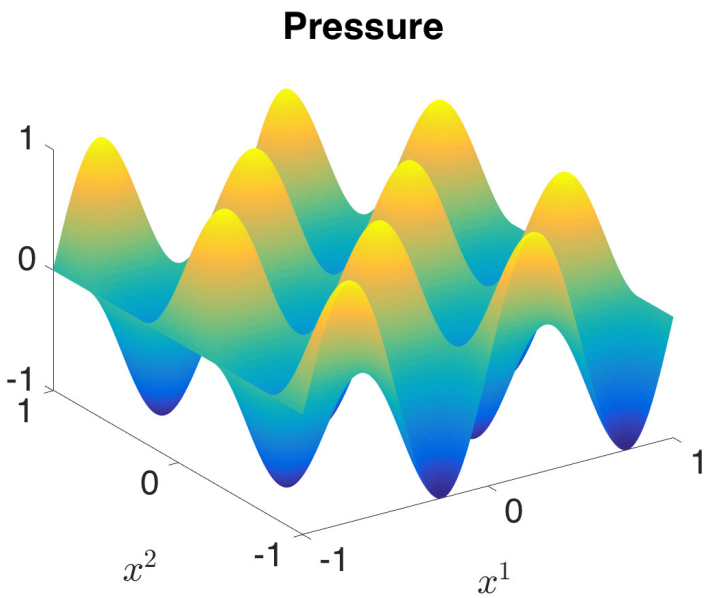
System of equations

Galerkin:

$$\langle du^{(1)}, p^{(0)} \rangle = \langle f^{(2)}, p^{(0)} \rangle$$

$$\langle dp^{(0)}, u^{(1)} \rangle = (\frac{1}{K} \star u^{(1)}, u^{(1)})$$

Results



$$u = -K\nabla p \quad K = 1$$

$$\nabla \cdot u = f$$

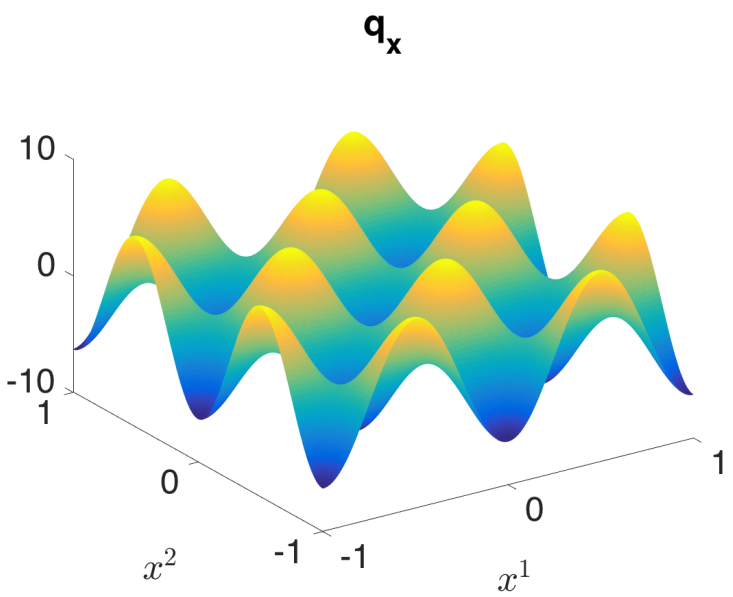
$$P(x, y) = sin(2\pi x)sin(2\pi y)$$

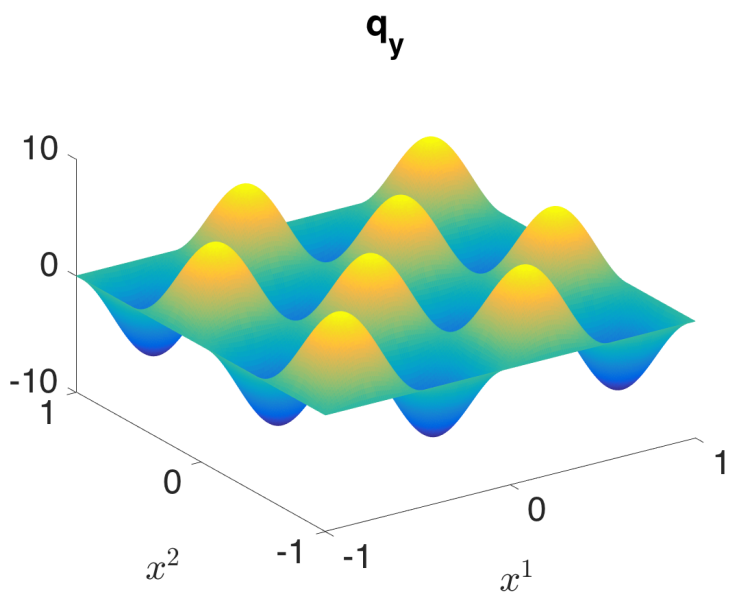
$$u_x = -2\pi cos(2\pi x)sin(2\pi y)$$

$$u_y = -2\pi sin(2\pi x)cos(2\pi y)$$

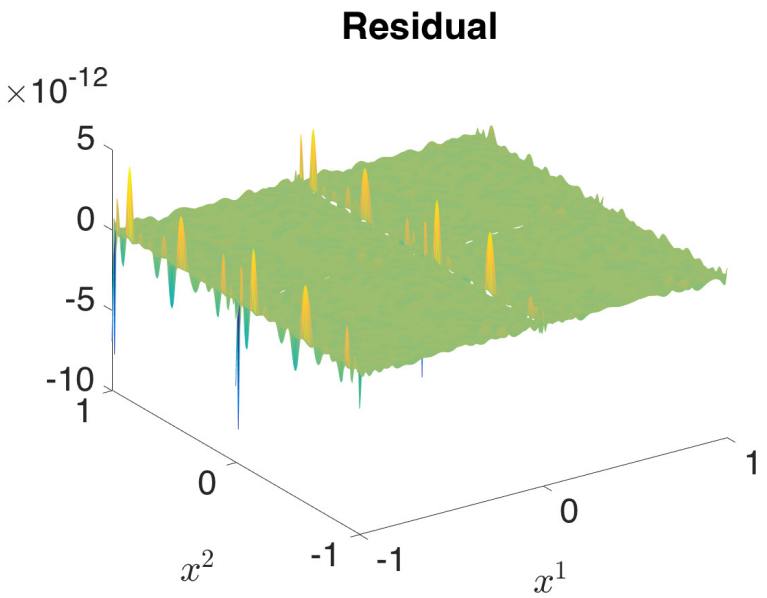
$$f = 8\pi sin(2\pi x)sin(2\pi y)$$

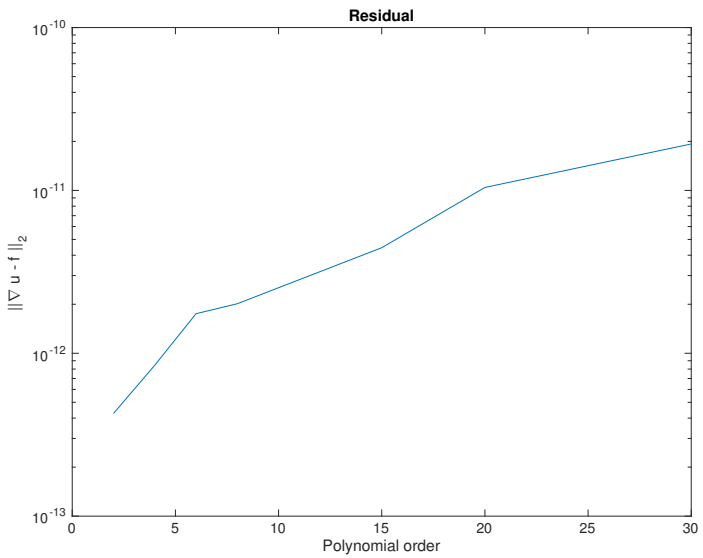
Results



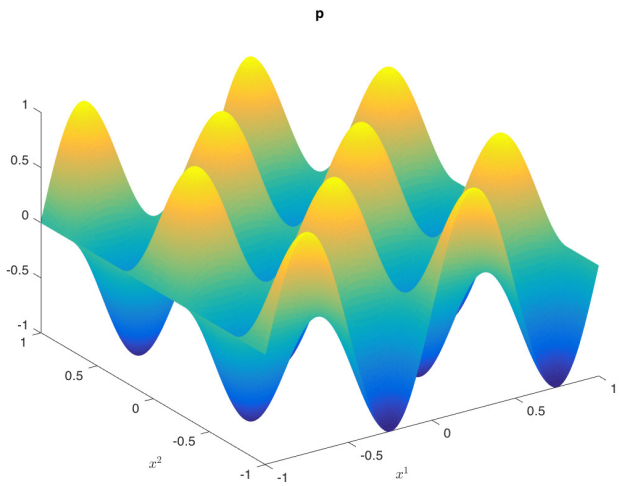


Results


Residual
×10^-12
5
0
-5
-10
1
0
-1
x^2
-1
0
1
x^1


Residual
10^-10
10^-11
10^-12
10^-13
‖∇ u - f ‖_2
0
5
10
15
20
25
30
Polynomial order

Results



$$u = -K\nabla p$$

$$K11 = 4 \quad K12 = 3 \quad K21 = 3 \quad K12 = 20$$

$$\nabla \cdot u = f$$

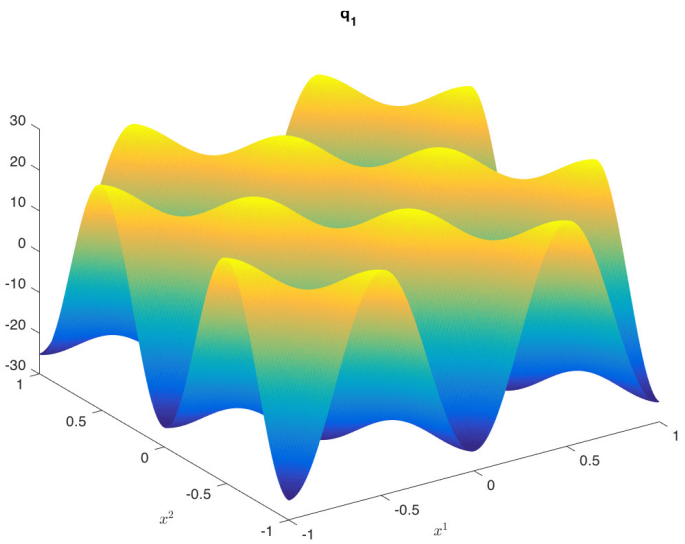
$$P(x, y) = sin(2\pi x)sin(2\pi y)$$

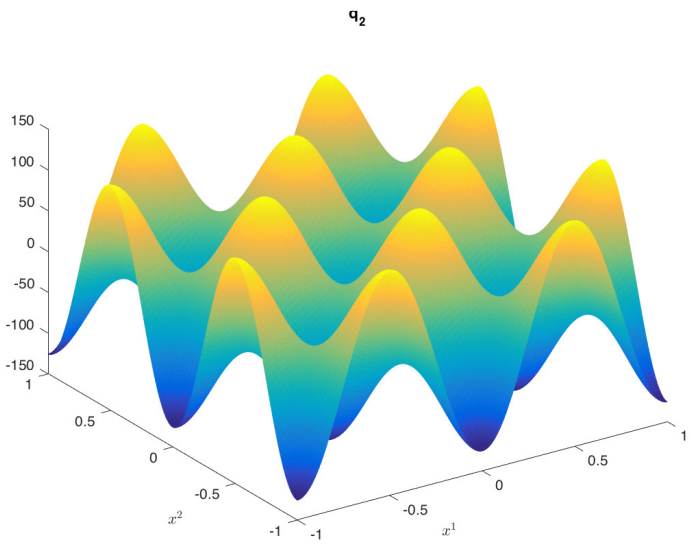
$$u_x = -2\pi k11 cos(2\pi x)cos(2\pi y) + 2\pi k12 sin(2\pi x)sin(2\pi y)$$

$$u_y = -2\pi k21 cos(2\pi x)cos(2\pi y) + 2\pi k22 sin(2\pi x)sin(2\pi y)$$

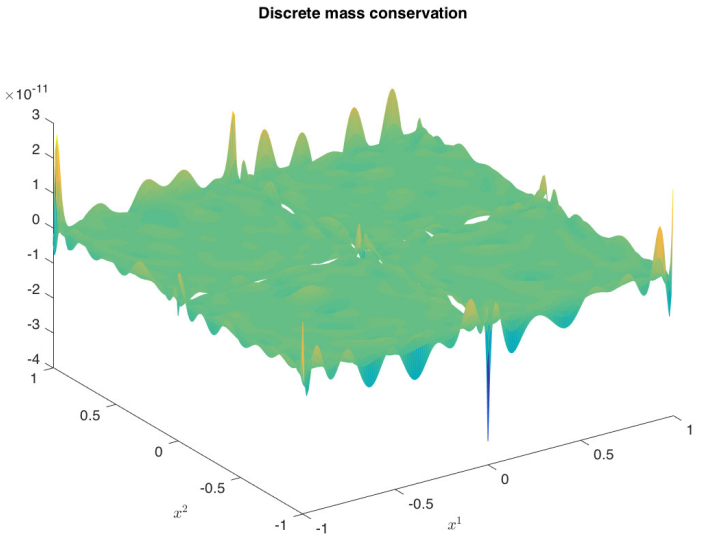
$$f = 4\pi^2((k11 + k22)sin(2\pi x)cos(2\pi y) + (k12 + k21)cos(2\pi x)sin(2\pi y))$$

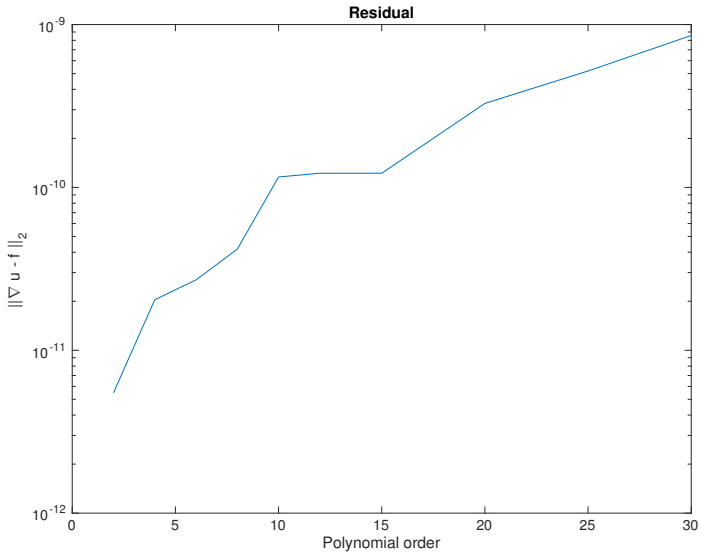
Results


q_1
30
20
10
0
-10
-20
-30
1
0.5
0
-0.5
-1
x^2
-1
-0.5
0
0.5
1
x^1

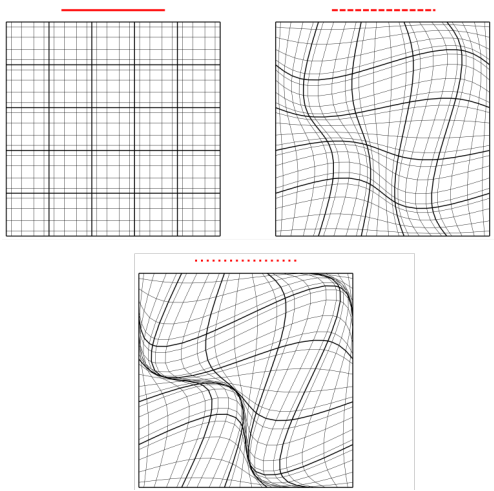

q_2
150
100
50
0
-50
-100
-150
1
0.5
0
-0.5
-1
x^2
-1
-0.5
0
0.5
1
x^1

Results


Discrete mass conservation
×10^-11
3
2
1
0
-1
-2
-3
-4
1
0.5
0
-0.5
-1
x^2
-1
-0.5
0
0.5
1
x^1


Residual
10^-9
10^-10
10^-11
10^-12
|| ∇ u - f ||_2
0
5
10
15
20
25
30
Polynomial order

Results



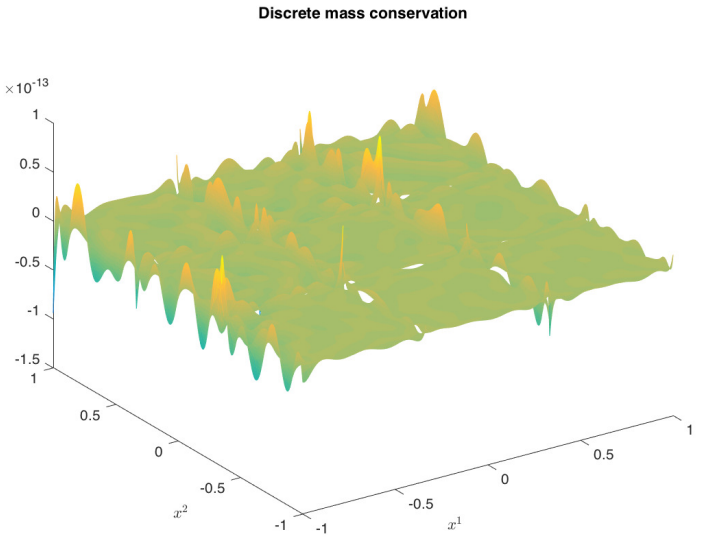
$$K11 = (1, 2, 3, 4, 5, 6, 7, 8, 9)$$

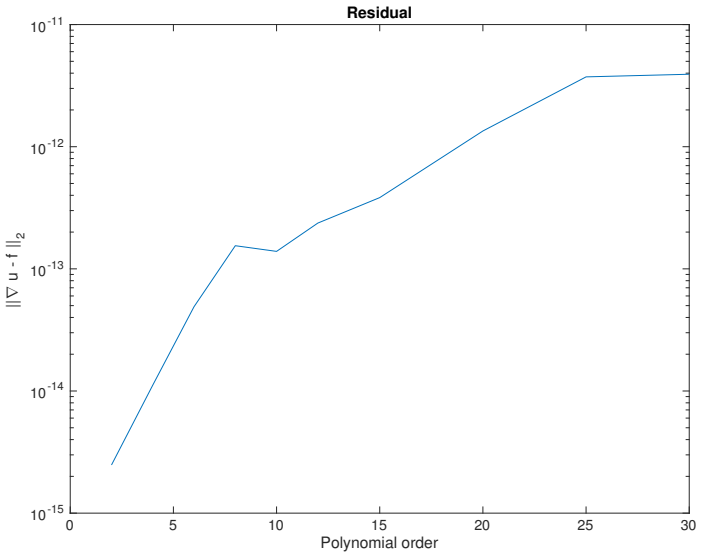
$$K12 = (0.25, 0.5, 0.75, 1, 0.5, 1, 0.5, 1, 0.5)$$

$$K21 = (0.25, 0.5, 0.75, 1, 0.5, 1, 0.5, 1, 0.5)$$

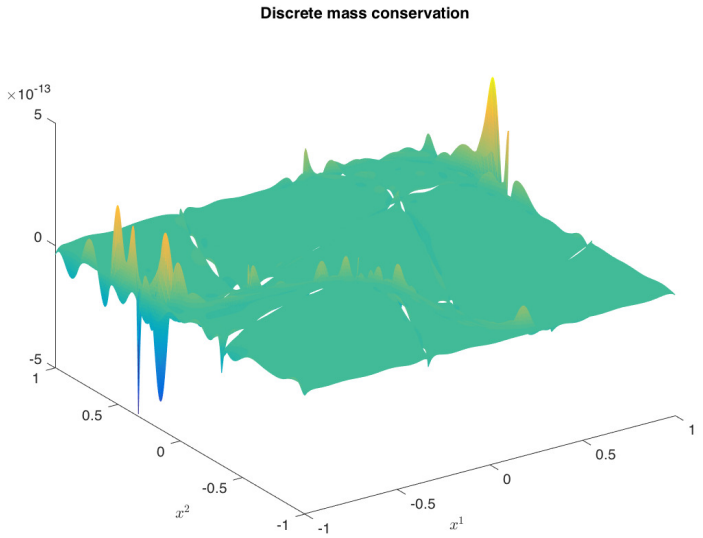
$$K22 = (9, 8, 7, 6, 5, 4, 3, 2, 1)$$

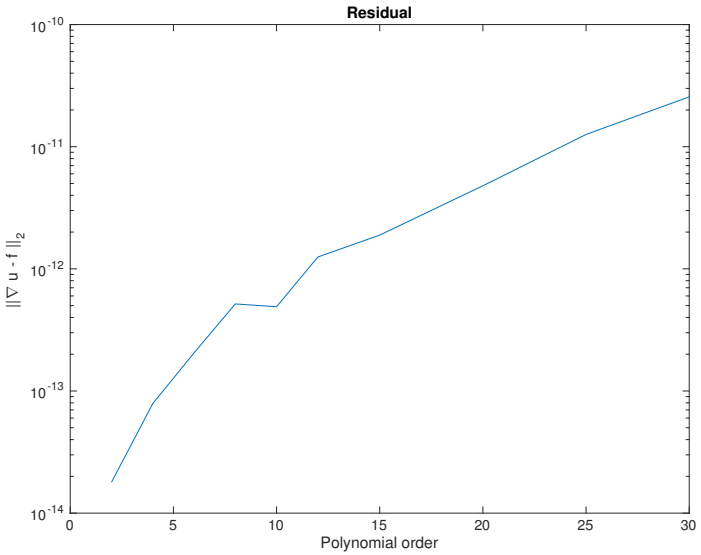
Results


Discrete mass conservation
×10^-13
1
0.5
0
-0.5
-1
-1.5
1
0.5
0
-0.5
-1
x^2
-1
-0.5
0
0.5
1
x^1


Residual
10^-11
10^-12
10^-13
10^-14
10^-15
|| ∇ u - f ||_2
0
5
10
15
20
25
30
Polynomial order

Results


Discrete mass conservation
×10^-13
5
0
-5
1
0.5
0
-0.5
-1
x^2
-1
-0.5
0
0.5
1
x^1


Residual
10^-10
10^-11
10^-12
10^-13
10^-14
||∇ u - f ||_2
0
5
10
15
20
25
30
Polynomial order

Euler equations

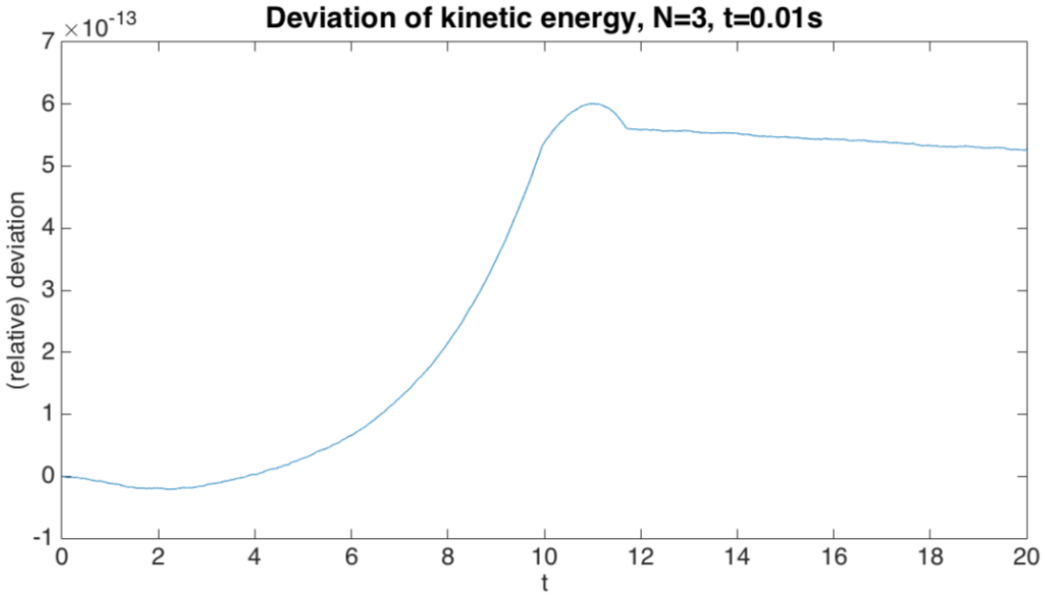
For the Euler equations

$$\frac{\partial v}{\partial t} + (v \cdot \nabla)v + \frac{1}{\rho}\nabla p = 0$$
$$\nabla \cdot v = 0$$

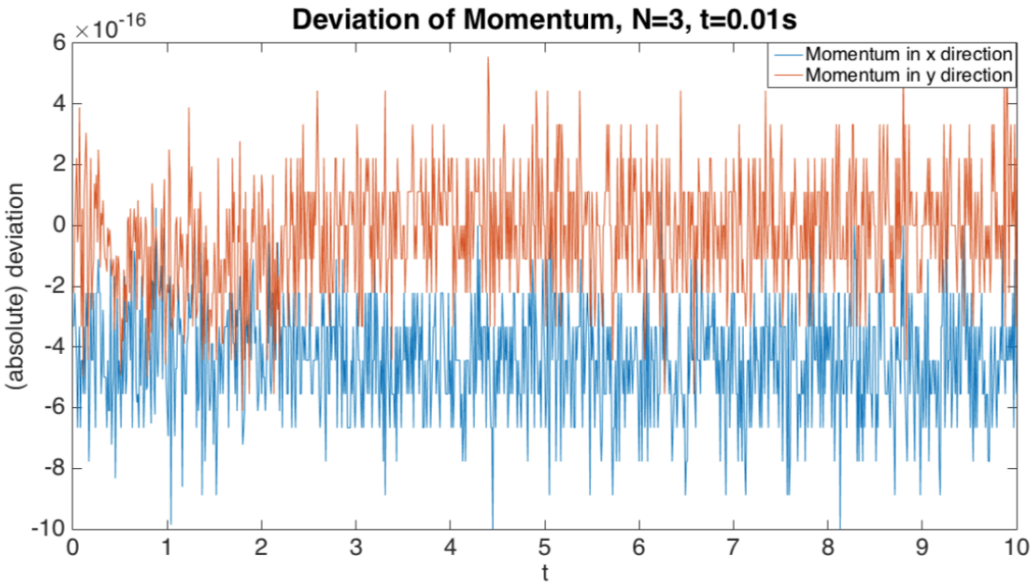
we have four invariant quantities:

$$K = \int_\Omega \frac{1}{2} v^2 d\Omega$$
$$M = \int_\Omega v d\Omega$$
$$V = \int_\Omega \omega d\Omega$$
$$E = \int_\Omega \frac{1}{2} \omega^2 d\Omega$$

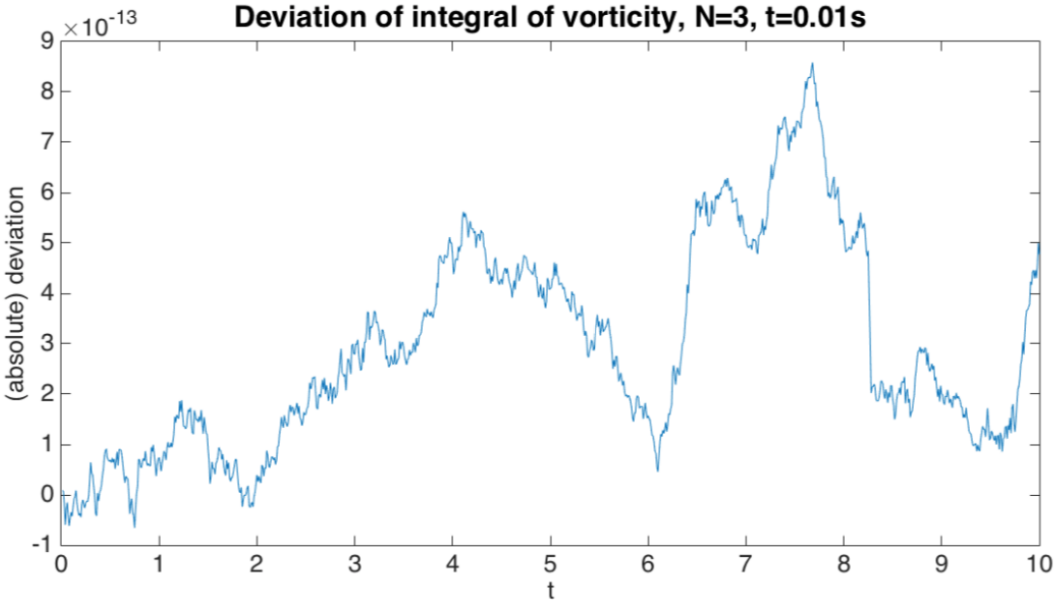
Euler equations



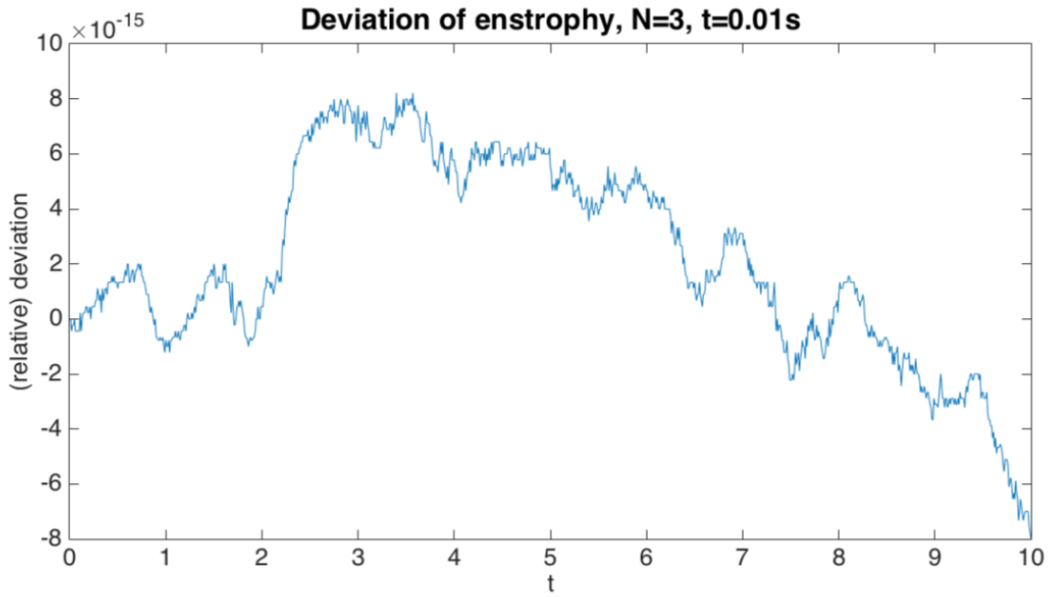
Euler equations



Euler equations



Euler equations



Thank you