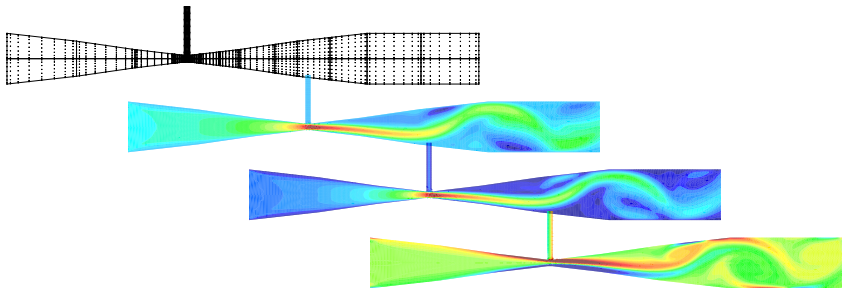


Spectral Element Methods

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Spectral (Element) Methods - S(E)M

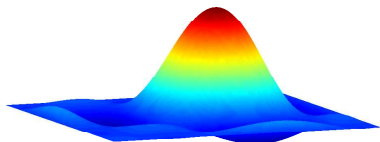
- **S(E)M** are **high-order** numerical methods to solve boundary value problems
- they are alternative to low-order FEM, but you can combine them with FEM (e.g., through a MORTAR approach)
- historically they were designed on quadrilaterals (**quads**)
- they have been extended to **simplices** more recently
- in SEM, **continuity** at interface elements is imposed (otherwise one speaks about DG-SEM)
- SEM are also known as either spectral/*hp* or *hp*-FEM

Nomenclature

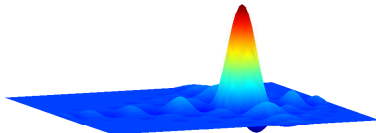
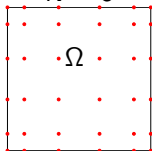
Gottlieb & Orszag (1977),
Canuto, Hussaini, Quarteroni, & Zang (1988),
Bernardi & Maday (1992)

Spectral Methods: one quad element Ω and global support of the polynomial basis functions on Ω .

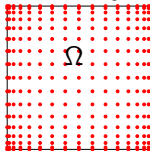
One parameter: $N = \text{polynomial degree}$ (\nearrow)



$N = 5$



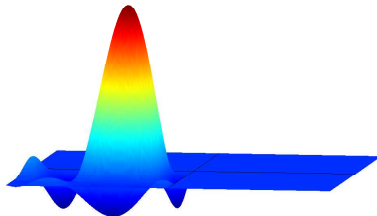
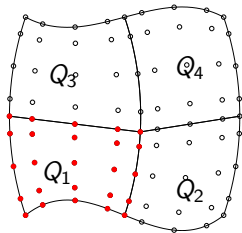
$N = 16$



Spectral Element Methods: conformal partition of quads in Ω , global C^0 basis functions (local polynomials) with local support.

Two parameters: $N = \text{pol. degree}$ (\nearrow)

$h = \text{mesh size (=elements diameter)}$ ($\searrow 0$)

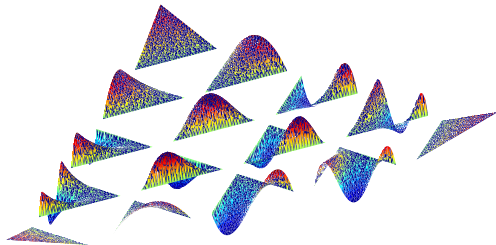
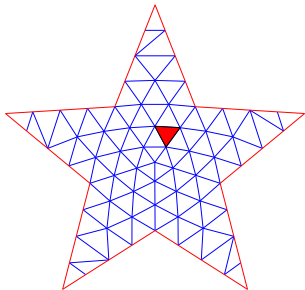


Nomenclature

Patera (1984) for SEM on quads,
Dubiner (1991), Sherwin & Karniadakis (1995) for SEM on simplices

spectral/*hp* conformal partition of quads/simplices in Ω ,
global C^0 basis functions (local polynomials) with local support.

Two parameters: $p(=N) = \text{pol. degree}$ (\nearrow)
 $h = \text{mesh size (=elements diameter)}$ ($\searrow 0$)



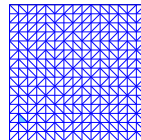
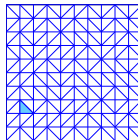
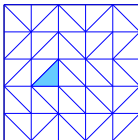
Nomenclature

h -FEM: fixed low degree
refinement in h
(simplices and quads)

One parameter:

h = mesh size

(the same on quads)

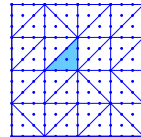
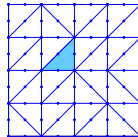
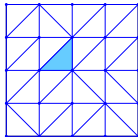


p -FEM: fixed h
refinement in p
(simplices and quads)

One parameter:

p = pol. degree

(the same on quads)



hp -FEM: refinement in both h and p (simplices and quads)

Two parameters: p = pol. degree (\nearrow)

h = mesh size (=elements diameter) ($\searrow 0$)

The borderline between spectral/ hp and hp -FEM seems invisible

Spectral Elements on quads

Spectral Element Methods on quads

Strong points (of the most used form nowadays)

- 1 **nodal** (Lagrange) basis
- 2 the **interpolation** nodes are the Legendre Gauss Lobatto (**LGL**) nodes
- 3 when **Numerical Integration** is used (**SEM-GNI**) then the **quadrature nodes** are exactly the **interpolation nodes** and Lagrange **basis is orthogonal** w.r.t. the discrete L^2 inner product (induced by quadrature) \implies **diagonal mass matrices** (in \mathbb{R}^d , $d \geq 1$)
- 4 **tensorial structure** of the basis functions in \mathbb{R}^d (with $d \geq 2$) \implies high computational efficiency

The reference problem

Given $\nu(\mathbf{x}) \geq \nu_0 > 0$ and $\gamma(\mathbf{x}) \geq 0$ in $L^\infty(\Omega)$; $f \in L^2(\Omega)$

look for $u : \Omega \subset \mathbb{R}^d \rightarrow \mathbb{R}$:

$$\text{strong form} \quad \begin{cases} -\nabla \cdot (\nu \nabla u) + \gamma u = f & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

By setting $V = H_0^1(\Omega)$, $a(u, v) = \int_{\Omega} \nu \nabla u \cdot \nabla v d\Omega + \int_{\Omega} \gamma u v d\Omega$,

$$(f, v) = \int_{\Omega} f v d\Omega$$

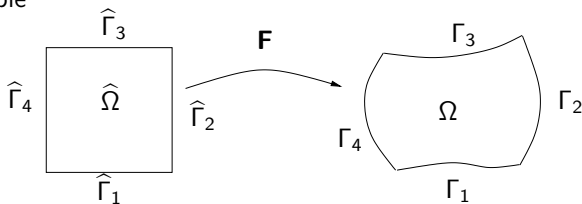
$$\text{weak form} \quad ?u \in V : \quad a(u, v) = (f, v) \quad \forall v \in V$$

The computational domain $\Omega \subset \mathbb{R}^d$, ($d \geq 2$)

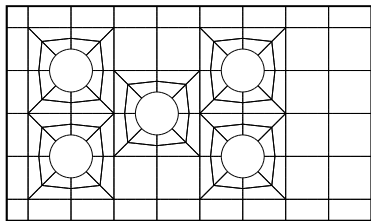
Historically SM are designed on quads

Reference domain: $\widehat{\Omega} = (-1, 1)^d$.

Lipschitz bounded domain $\Omega \in \mathbb{R}^d$: $\exists \mathbf{F} : \widehat{\Omega} \rightarrow \Omega$ bijective and differentiable



SEM (or *hp*-fem) on quads. $\mathcal{T} = \{Q_k\}_{k=1}^{Ne}$ is a conforming partition of Ω : $\Omega = \cup_{k=1}^{Ne} Q_k$ and $\exists \mathbf{F}_k : \widehat{\Omega} \rightarrow Q_k$ bij and diff (for any $k = 1, \dots, Ne$)



How to design mappings F_k

Conformal mappings preserve orthogonality, the divergence and the gradient (Milne-Thomson 1966, Israeli 1981, Trefethen 1980, Gordon-Hall 1973)

The simplest ones are linear blending mappings

In \mathbb{R}^2 , given the maps $\pi_\ell^{(k)} : [-1, 1] \rightarrow \Gamma_\ell$ (arcs in \mathbb{R}^2) for $\ell = 1, \dots, 4$, $F_k : \hat{\Omega} \rightarrow Q_k$ is defined as

$$\begin{aligned} \begin{bmatrix} x \\ y \end{bmatrix} = F_k \left(\begin{bmatrix} \hat{x} \\ \hat{y} \end{bmatrix} \right) &= \frac{1 - \hat{y}}{2} \pi_1^{(k)}(\hat{x}) + \frac{1 + \hat{y}}{2} \pi_3^{(k)}(\hat{x}) \\ &+ \frac{1 - \hat{x}}{2} \left[\pi_4^{(k)}(\hat{y}) - \frac{1 + \hat{y}}{2} \pi_4^{(k)}(1) - \frac{1 - \hat{y}}{2} \pi_4^{(k)}(-1) \right] \\ &+ \frac{1 + \hat{x}}{2} \left[\pi_2^{(k)}(\hat{y}) - \frac{1 + \hat{y}}{2} \pi_2^{(k)}(1) - \frac{1 - \hat{y}}{2} \pi_2^{(k)}(-1) \right] \end{aligned}$$

Similar construction in 3D, now $\pi_\ell : [-1, 1]^2 \rightarrow \Sigma_\ell$ (faces in \mathbb{R}^3) for $\ell = 1, \dots, 6$.

Finite dimensional spaces

Let $p \geq 1$ integer and \mathbb{Q}_p the space of polynomials of degree $\leq p$ w.r.t. each variable x_1, \dots, x_d .

Set

$$\mathcal{X}_\delta = \{v \in C^0(\overline{\Omega}) : v|_{Q_k} = \hat{v} \circ \mathbf{F}_k^{-1}, \text{ with } \hat{v} \in \mathbb{Q}_p(\hat{\Omega}), \forall Q_k \in \mathcal{T}\}$$

mesh size $h = \max_k h_k$, $h_k = \text{diam}(Q_k)$, polynomial degree p

$$\Rightarrow \delta = (h, p)$$

Set $V_\delta = \mathcal{X}_\delta \cap V$

Galerkin
SEM

$$? u_\delta \in V_\delta : a(u_\delta, v_\delta) = (f, v_\delta) \quad \forall v_\delta \in V_\delta$$

At element interface, u_δ is merely continuous. The continuity of the flux at interfaces is ensured only in the limit $p \rightarrow \infty$.

Attention: large computational effort in evaluating integrals

\Rightarrow Galerkin with Numerical Integration (SEM-GNI)

Numerical Integration

$$\int_{-1}^1 f(\hat{x}) d\hat{x} \simeq \sum_{\ell=0}^p f(\hat{\xi}_\ell) \hat{w}_\ell$$

$\hat{\xi}_\ell$ and \hat{w}_ℓ ($\ell = 0, \dots, p$) **Legendre Gauss Lobatto (LGL)** quadrature nodes and weights

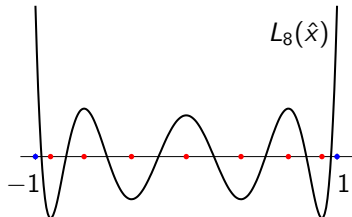
Degree of exactness = $2p - 1$ when $(p + 1)$ nodes are used.

$L_p(\hat{x}) \in \mathbb{P}_p$ Legendre pol

$$\hat{x}_0 = -1, \quad \hat{x}_p = 1$$

$\hat{x}_{1, \dots, p-1} =$ zeros of $L'_p(\hat{x})$

$$\hat{w}_j = \frac{2}{p(p+1)} \frac{1}{[L'_p(\hat{x}_j)]^2}$$

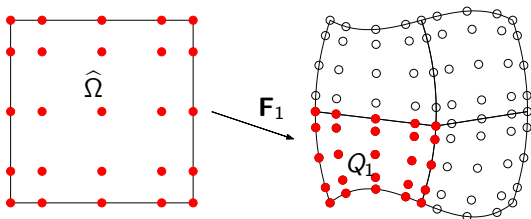


$$\int_a^b f(x) dx \simeq \sum_{\ell=0}^p f(\xi_\ell) w_\ell, \quad \xi_\ell = \frac{b-a}{2} \hat{\xi}_\ell + \frac{a+b}{2}, \quad w_\ell = \hat{w}_\ell \frac{b-a}{2}$$

Numerical integration ($\Omega \subset \mathbb{R}^2$)

$$\mathbf{F}_k : \hat{\mathbf{x}} \rightarrow \mathbf{x}$$

$$J_k = \left[\frac{\partial x_i}{\partial \hat{x}_j} \right]_{i,j=1}^d$$



Local: LGL quadrature

$$\int_{Q_k} u(\mathbf{x})v(\mathbf{v})d\mathbf{x} \simeq (u, v)_{\delta, Q_k} = \sum_{q,r=0}^p u(\xi_q, \xi_r)v(\xi_q, \xi_r)w_q w_r |\det(J_k(\xi_q, \xi_r))|$$

Global: composite LGL quadrature

$$\int_{\Omega} u(\mathbf{x})v(\mathbf{v})d\mathbf{x} \simeq \sum_{k=1}^{Ne} (u, v)_{\delta, Q_k} = (u, v)_{\delta, \Omega}$$

Quadrature error: $\exists c = c(\Omega) > 0 : \forall f \in H^s(\hat{\Omega}), s \geq 1, v_p \in \mathbb{Q}_p$

$$\left| \int_{\hat{\Omega}} f v_p - (f, v_p)_{\delta, \hat{\Omega}} \right| \leq c p^{-s} \|f\|_{H^s(\hat{\Omega})} \|v_p\|_{L^2(\hat{\Omega})}$$

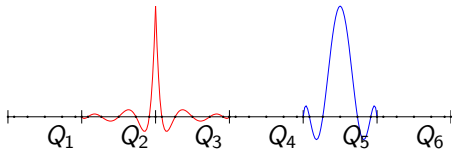
How to represent $v_\delta \in V_\delta$

N_p = total number of nodes in Ω

Nodal Lagrange basis functions $\{\varphi_i\}_{i=1}^{N_p}$ w.r.t. the LGL nodes ξ_i
 φ_i are globally continuous in $\bar{\Omega}$, and locally polynomials of degree p w.r.t. each variable x_1, \dots, x_d .

$$d = 1,$$

$$\varphi_i(x) = \varphi_i^{(1)}(x)$$



$$d = 2,$$

$$\varphi_i(\mathbf{x}) = \varphi_{i1}^{(1)}(x_1)\varphi_{i2}^{(1)}(x_2),$$

$$d = 3,$$

$$\varphi_i(\mathbf{x}) = \varphi_{i1}^{(1)}(x_1)\varphi_{i2}^{(1)}(x_2)\varphi_{i3}^{(1)}(x_3)$$

$$v_\delta(\mathbf{x}) = \sum_{i=1}^{N_p} v_\delta(\xi_i)\varphi_i(\mathbf{x}) \quad \forall v_\delta \in V_\delta$$

Interpolation error at LGL nodes:

$$\|u - I_p u\|_{H^k(-1,1)} \leq C(s)p^{k-s}\|u\|_{H^s(-1,1)}, \quad s \geq 1, k = 0, 1$$

SEM-GNI formulation

$$\text{SEM-GNI} \quad ?u_\delta \in V_\delta : \quad a_\delta(u_\delta, v_\delta) = (f, v_\delta)_\delta \quad \forall v_\delta \in V_\delta$$

At element interface, u_δ is merely continuous

The continuity of the flux at interfaces is ensured only in the limit $\rho \rightarrow \infty$.

Expand u_δ w.r.t. the Lagrange basis: $u_\delta(\mathbf{x}) = \sum_{i=1}^{Np} u_\delta(\mathbf{x}_i) \varphi_i(\mathbf{x})$

and choose $v_\delta(\mathbf{x}) = \varphi_i(\mathbf{x})$ for any $i = 1, \dots, Np$.

SEM-GNI reads:

look for $\mathbf{u} = [u_\delta(\mathbf{x}_j)]_{j=1}^{Np}$:

$$\sum_{j=1}^{Np} a_\delta(\varphi_j, \varphi_i) \mathbf{u}_j = (f, \varphi_i)_\delta \quad \text{for any } i = 1, \dots, Np$$

where $a_\delta(\varphi_j, \varphi_i) = (\nu \nabla \varphi_j, \nabla \varphi_i)_\delta + (\gamma \varphi_j, \varphi_i)_\delta$.

How to evaluate derivatives $\nabla \varphi_i$ efficiently

Derivatives computation (let us work on $\hat{\Omega}$)

$$(\nu \nabla \varphi_j, \nabla \varphi_i)_{\delta, \hat{\Omega}} = \sum_{q,r=0}^p \nu(\hat{\xi}_q, \hat{\xi}_r) \nabla \varphi_j(\hat{\xi}_q, \hat{\xi}_r) \cdot \nabla \varphi_i(\hat{\xi}_q, \hat{\xi}_r) \hat{w}_q \hat{w}_r$$

We need to know **derivatives at quadrature nodes (=interpolation nodes)**, then (recalling that $\varphi_j(\mathbf{x}) = \varphi_{j1}^{(1)}(x_1)\varphi_{j2}^{(1)}(x_2)$)

$$\begin{aligned} \frac{\partial \varphi_j}{\partial \hat{x}_1}(\hat{\xi}_q, \hat{\xi}_r) &= \frac{\partial \varphi_{j1}^{(1)}}{\partial \hat{x}_1}(\hat{\xi}_q) \varphi_{j2}^{(1)}(\hat{\xi}_r) = D_{q,j1} \delta_{r,j2} \\ \frac{\partial \varphi_j}{\partial \hat{x}_2}(\hat{\xi}_q, \hat{\xi}_r) &= \varphi_{j1}^{(1)}(\hat{\xi}_q) \frac{\partial \varphi_{j2}^{(1)}}{\partial \hat{x}_2}(\hat{\xi}_r) = \delta_{q,j1} D_{r,j2} \end{aligned}$$

spectral derivative matrix

$$D_{ij} = \left[\begin{array}{c|c|c} \dots & \varphi_j'(\hat{\xi}_i) & \dots \\ \hline & & \end{array} \right]$$

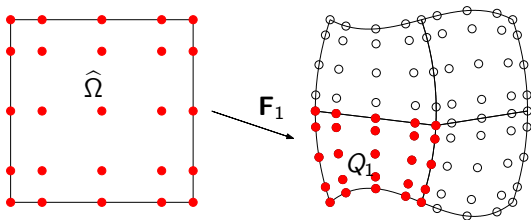
$$\varphi_j(\xi) = -\frac{1}{\rho(\rho+1)} \frac{(1-\xi^2)}{\xi-\xi_j} \frac{L'_\rho(\xi)}{L_\rho(\xi_j)}$$

$$D_{ij} = \begin{cases} \frac{L_\rho(\hat{\xi}_j)}{L_\rho(\hat{\xi}_i)} \frac{1}{\hat{\xi}_j - \hat{\xi}_i} & j \neq i \\ -\frac{\rho(\rho+1)}{4} & j = i = 0 \\ \frac{\rho(\rho+1)}{4} & j = i = \rho \\ 0 & \text{otherwise} \end{cases}$$

Derivatives on $Q_k = \mathbf{F}_k(\hat{\Omega})$

Standard arguments:

$$\mathbf{F}_k : \hat{\mathbf{x}} \rightarrow \mathbf{x}$$
$$J_k = \left[\frac{\partial x_i}{\partial \hat{x}_j} \right]_{i,j=1}^d$$



$$(\varphi_j(\mathbf{x}) = \hat{\varphi}_j(\hat{\mathbf{x}}))$$

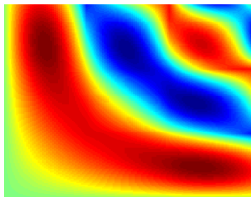
$$\begin{bmatrix} \frac{\partial \varphi_j}{\partial x_1}(\xi_i) \\ \frac{\partial \varphi_j}{\partial x_2}(\xi_i) \end{bmatrix} = \frac{1}{\det J_k(\hat{\xi}_i)} \begin{bmatrix} \frac{\partial x_2}{\partial \hat{x}_2}(\hat{\xi}_i) & -\frac{\partial x_2}{\partial \hat{x}_1}(\hat{\xi}_i) \\ -\frac{\partial x_1}{\partial \hat{x}_2}(\hat{\xi}_i) & \frac{\partial x_1}{\partial \hat{x}_1}(\hat{\xi}_i) \end{bmatrix} \begin{bmatrix} \frac{\partial \hat{\varphi}_j}{\partial \hat{x}_1}(\hat{\xi}_i) \\ \frac{\partial \hat{\varphi}_j}{\partial \hat{x}_2}(\hat{\xi}_i) \end{bmatrix}$$

Convergence analysis for SEM-GNI

$$? u_\delta \in V_\delta : a_\delta(u_\delta, v_\delta) = (f, v_\delta)_\delta \quad \forall v_\delta \in V_\delta$$

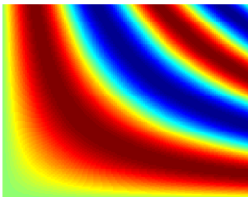
u_δ converges with spectral accuracy (with respect to p) to the exact solution when the latter and f are smooth:

$$\|u - u_\delta\|_{H^1(\Omega)} \leq C_1(s) \left(h^{\min(p+1,s)-1} p^{1-s} \|u\|_{H^s(\Omega)} + h^{\min(p+1,r)} p^{-r} \|f\|_{H^r(\Omega)} \right)$$



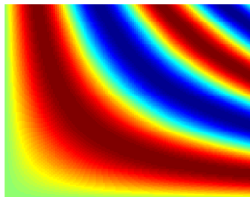
$$h = 2/3, \quad p = 2$$

$$e_{H1} \simeq 3.77e^{-01}$$



$$h = 2/3, \quad p = 6$$

$$e_{H1} \simeq 8.80e^{-04}$$



$$h = 2/3, \quad p = 16$$

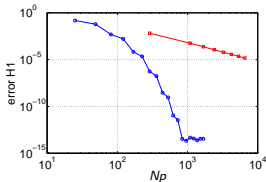
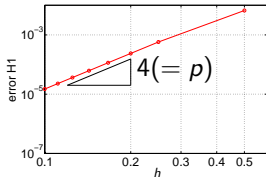
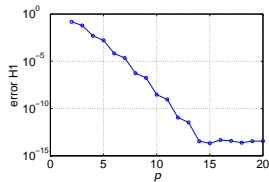
$$e_{H1} \simeq 3.64e^{-14}$$

Convergence rate

1. s, r large ($s, r > p + 1$)

$$\|u - u_\delta\|_{H^1(\Omega)} \leq C_1(s)(h^p p^{1-s} \|u\|_{H^s(\Omega)} + h^p p^{1-r} \|f\|_{H^r(\Omega)})$$

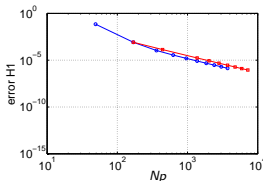
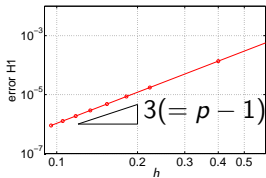
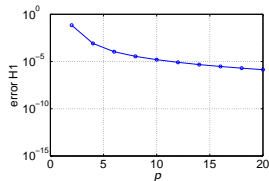
$s, r = \infty$



2. s small ($s \leq p + 1$)

$$\|u - u_\delta\|_{H^1(\Omega)} \leq C_1(s) \left(\frac{h}{p}\right)^{s-1} \|u\|_{H^s(\Omega)}$$

$s = 4, r = 2, f$ composite \mathbb{Q}_2 , null quadrature error on f , when $p > 2$



Algebraic aspects of SEM-GNI

Recall that $a_\delta(\varphi_j, \varphi_i) = (\nu \nabla \varphi_j, \nabla \varphi_i)_\delta + (\gamma \varphi_j, \varphi_i)_\delta$

$$A \in \mathbb{R}^{N_p \times N_p} : a_\delta(\varphi_j, \varphi_i)$$

$$M \in \mathbb{R}^{N_p \times N_p} : M_{ij} = (\varphi_j, \varphi_i)_\delta \quad \text{mass matrix}$$

$$K \in \mathbb{R}^{N_p \times N_p} : K_{ij} = (\nabla \varphi_j, \nabla \varphi_i)_\delta \quad \text{stiffness matrix}$$

Let us define the **Spectral condition number**

$$\text{cond}(A) := \frac{\max_j |\lambda_j(A)|}{\min_j |\lambda_j(A)|} \quad \forall A \in \mathbb{R}^{n \times n} \text{ non-singular}$$

It is responsible for Conjugate-Gradient (in general Krylov) iterations:

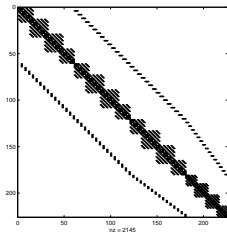
$$\#it \simeq \sqrt{\text{cond}(A)}$$

Mass matrix M

- diagonal for any $d \geq 1$
- $M_{ij} > 0$
- $\lambda_{\min}(M) = \mathcal{O}(p^{-2d} h^d)$, $\lambda_{\max}(M) = \mathcal{O}(p^{-d} h^d)$
- $\text{cond}(M) = \mathcal{O}(p^d)$ (Bernardi, Maday '92)
- $\tilde{M} = [(\gamma\varphi_j, \varphi_i)_\delta]_{i,j=1}^{Np}$ is diagonal even when $\gamma = \gamma(\mathbf{x})$.

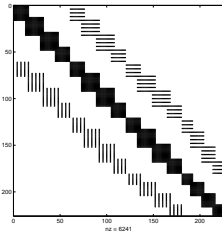
Stiffness matrix K

$$\Omega = (-1, 1)^2$$



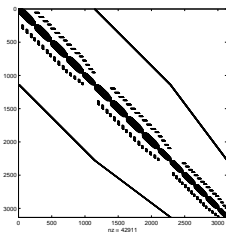
$p = 4$
 4×4 elem

$$\Omega \text{ skew quadrilateral}$$



$p = 4$
 4×4 elem

$$\Omega = (-1, 1)^3$$



$p = 4$
 $3 \times 4 \times 5$ elem

Sparsity

• s.p.d. 4%

12%

0.4%

• $\lambda_{\min}(K) = \mathcal{O}(p^{-d} h^d)$, $\lambda_{\max}(K) = \mathcal{O}(p^{3-d} h^{d-2})$

• $cond(K) = \mathcal{O}(p^3 h^{-2})$

(Bernardi, Maday '92 for Dir. b.c.,
 Melenk 2002 for Neu. b.c.)

Bank, Scott '89 procedure for regular meshes)

• pattern of A is like that of K , even when $\nu = \nu(\mathbf{x})$



SEM-GNI Algebraic System

Let us consider the **differential problem**

$$\begin{cases} -\Delta u = f & \text{in } \Omega \subset \mathbb{R}^d, \quad (d = 2, 3) \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

SEM-GNI:

$$? \mathbf{u} = [u_\delta(\mathbf{x}_j)]_{j=1}^{Np} : \sum_{j=1}^{Np} a_\delta(\varphi_j, \varphi_i) \mathbf{u}_j = (f, \varphi_i)_\delta \quad i = 1, \dots, Np$$

Since $A = K$, by setting $\mathbf{f} = [f(\mathbf{x}_j)]_{j=1}^{Np}$,
the **algebraic system** reads

$$K\mathbf{u} = M\mathbf{f} \quad \text{weak form}$$

or equivalently

$$M^{-1}K\mathbf{u} = \mathbf{f} \quad \text{strong (or collocation) form}$$

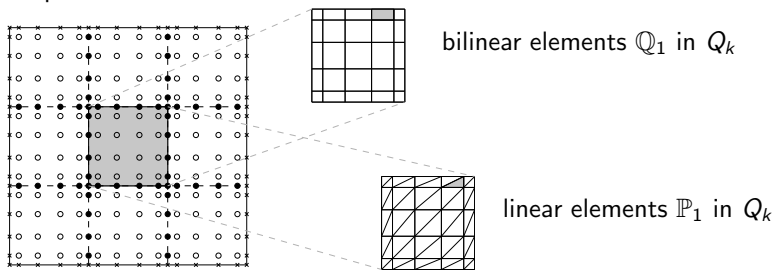
$$\text{cond}(K) \simeq c_1 p^3 h^{-2}$$

$$\text{cond}(M^{-1}K) \simeq c_2 p^4 h^{-2}$$

Preconditioning on quads by low-order FEM

Preconditioning by low-order Finite Element Matrices

The LGL nodes in each spectral element Q_k induce a mesh of simplicial or quadrilateral elements.



Quadrilaterals: Q_1 (exact integration or high order LGL q.f.)
 $Q_{1,N}$ (trapezoidal quadrature formula)

Simplices: P_1 (exact integration or high order LGL q.f.)

FEM Matrices

Quadrilaterals/Hexahedra:

Q_1 (exact integration)

$Q_{1,N}$ (trapezoidal quadrature formula)

Triangles/Tetrahedra:

P_1 (exact integration)

Different mass and stiffness matrices for any choice

$$d = 1. \quad K_{Q_1} = K_{P_1} = K_{Q_{1,N}}; \\ M_{Q_1} = M_{P_1} \neq M_{Q_{1,N}}$$

$$d = 2. \quad K_{Q_1} \neq K_{P_1} = K_{Q_{1,N}}; \\ M_{Q_1} \neq M_{P_1} \neq M_{Q_{1,N}}$$

$$d = 3. \quad K_{Q_1} \neq K_{P_1} \neq K_{Q_{1,N}}; \\ M_{Q_1} \neq M_{P_1} \neq M_{Q_{1,N}}$$

$M_{Q_{1,N}}$ is diagonal and

$$M_{Q_{1,N}}^{-1} K_{Q_{1,N}} = L_{FD} \quad (=2\text{nd order, centered finite difference matrix})$$

Finite Element (Left) Preconditioners

Orszag '80, Canuto-Quarteroni '85, Deville-Mund '85, Quarteroni-Zampieri '92,
Parter-Rothman '95, Parter '01, Canuto-G-Quarteroni '10

Strong form

$$M^{-1}Ku = f$$

$$A = M^{-1}K$$

strong- Q_1

$$P = M_{Q_1}^{-1}K_{Q_1}$$

strong- $Q_{1,Nl}$ - **FD**

$$P = M_{Q_{1,Nl}}^{-1}K_{Q_{1,Nl}}$$

strong- P_1

$$P = M_{P_1}^{-1}K_{P_1}$$

$$Au = b$$

$$P^{-1}Au = P^{-1}b$$

Q_1

$Q_{1,Nl}$

P_1

Weak form

$$Ku = Mf$$

$$A = K$$

weak- Q_1

$$P = K_{Q_1}^{-1}$$

weak- $Q_{1,Nl}$

$$P = K_{Q_{1,Nl}}$$

weak- P_1

$$P = K_{P_1}^{-1}$$

Questions:

1. Which is **the best preconditioner** from both **theoretical** and **computational** points of view?

- analysis of the condition number of $P^{-1}A$ in simple cases
numerical test on more complex cases
- CPU-time measurements

2. How to **solve** the system $Pz^{(k)} = r^{(k)}$ **efficiently**?

- ad-hoc direct and iterative solvers

$cond(P^{-1}A)$. $\Omega = (-1, 1)^d$, $d = 1 : 3$, one element in Ω

Theorem. $\exists c_1, \dots, c_4 > 0$ const. indep. of both p and d :

weak forms

$$cond(K_{Q_1}^{-1}K) \leq c_1(3c_2)^{d-1}$$

$$cond(K_{Q_1,NI}^{-1}K) \leq c_1c_2^{d-1}$$

$$cond(K_{P_1}^{-1}K) \leq c_1c_2^{d-1}\sigma_d, \quad \sigma_1 = \sigma_2 = 1, \sigma_3 = 2$$

strong forms

$$cond((M_{Q_1}^{-1}K_{Q_1})^{-1}M^{-1}K) \leq c_3$$

$$cond((M_{Q_1,NI}^{-1}K_{Q_1,NI})^{-1}M^{-1}K) \leq c_4.$$

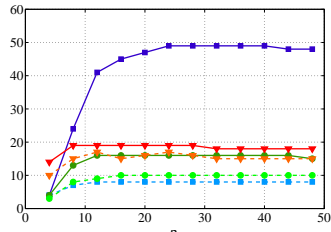
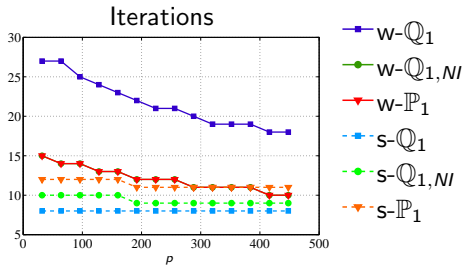
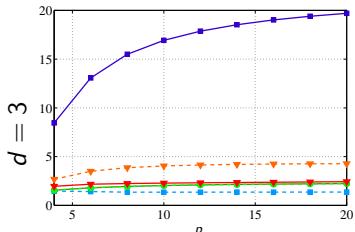
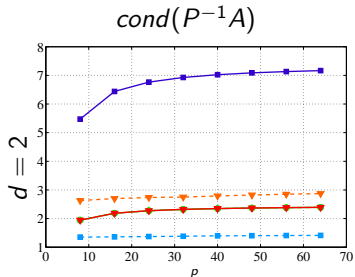
Numerically, $c_1 \leq 2.5$, $c_2 \leq 1.00245$, $c_3 \leq 1.5$, $c_4 \leq 2.5$.

No proof for the **strong- \mathbb{P}_1** formulation, numerical results show that $\exists c_5 = c_5(d)$ independent of p , but depending on d s.t.

$$cond((M_{P_1}^{-1}K_{P_1})^{-1}M^{-1}K) \leq c_5(d)$$

Single domain

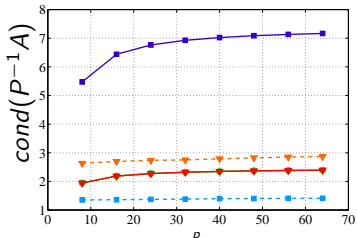
Problem: $Lu = -\Delta u$, in $\Omega = (-1, 1)^d$, $u = 0$ on $\partial\Omega$
Algebraic Solver: CG (weak forms) and Bi-CGStab (strong forms)
Initial guess $\mathbf{u}^{(0)} = \mathbf{0}$, stopping test: $\|\mathbf{r}^{(k)}\|_{P-1} / \|\mathbf{r}^{(0)}\|_{P-1} < 10^{-14}$



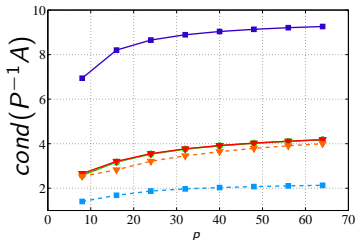
- w- Q_1
- w- Q_1,NI
- ▼ w- P_1
- s- Q_1
- s- Q_1,NI
- ▼ s- P_1

$cond(P^{-1}A)$. $d = 2$. Single domain

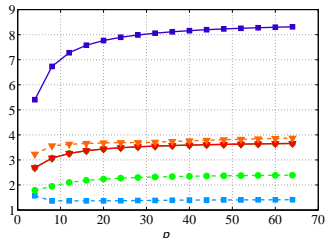
$Lu = -\Delta u$, $\Omega = (-1, 1)^2$
Dirichlet b.c.



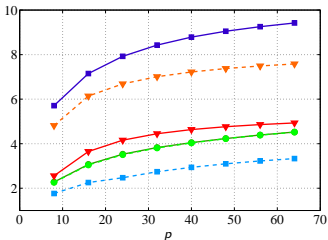
$Lu = -\nabla \cdot ((1 + 3x^2y^2)\nabla u)$,
 $\Omega = (-1, 1)^2$, Dirichlet b.c.



$Lu = -\Delta u$, $\Omega = (-1, 1)^2$
Dirichlet / Neumann b.c.



$Lu = -\Delta u$, skew Ω
Dirichlet b.c.



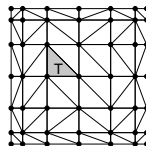
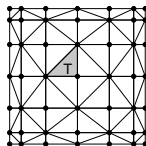
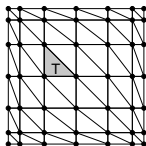
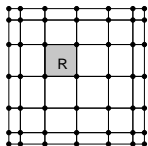
- $w-Q_1$
- $w-Q_{1,N1}$
- ▼ $w-P_1$
- $s-Q_1$
- $s-Q_{1,N1}$
- ▼ $s-P_1$

Ω



The induced Finite Element Mesh

Quadrilateral or triangular 2D-mesh induced by the LGL nodes in Ω :

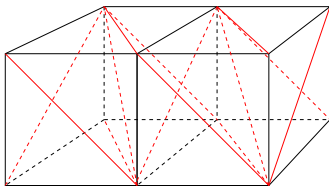


oriented

alternating

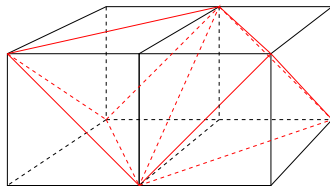
random

hexahedral or tetrahedral 3D-mesh.



6 tetra in each hexa

oriented



5 tetra in each hexa

alternating

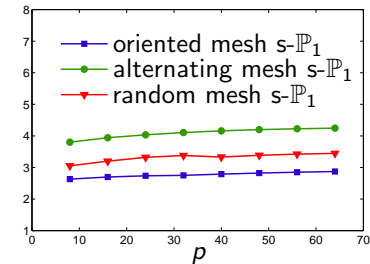
$cond(P^{-1}A)$. Single domain

$$Lu = -\Delta u, \text{ in } \Omega = (-1, 1)^d, \quad u = 0 \text{ on } \partial\Omega$$

$$d = 2$$

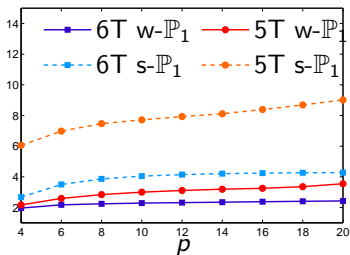
$cond(K_{\mathbb{P}_1}^{-1}K)$ is independent of the mesh orientation

$cond((M_{\mathbb{P}_1}^{-1}K_{\mathbb{P}_1})^{-1}M^{-1}K)$ mildly depends on the mesh:



$$d = 3$$

$P = K_{\mathbb{P}_1}^{-1}$ on 6 tetrahedra is the best one



First conclusions (single domain)

$$Lu = -\Delta u \quad \text{in } \Omega = (-1, 1)^d, \quad u = 0 \quad \text{on } \partial\Omega$$

● The **best** preconditioner for the *strong form* (by analysing the iterative condition number and the Bi-CGstab iterations) is that based on \mathbb{Q}_1 :

$$\text{cond}(P^{-1}A) \leq 1.5 \quad \forall p, d = 1, 2, 3$$

● The **best** preconditioner for the *weak form* (by analysing the iterative condition number and the CG iterations) is that based on $\mathbb{Q}_{1,N1}$ ($= \mathbb{P}_1$, for $d = 2$) :

$$\text{cond}(P^{-1}A) \leq 2.5 \quad \forall p, \text{ for } d = 1, 2, 3$$

Comparison in terms of CPU-time

Computational cost analysis (versus p)

- **Preprocessing:** assemble and factorize the FEM preconditioner

- **CG:**

for $k = 1, \dots$ until convergence

- spectral residual computation $\mathbf{r}^{(k)} = M\mathbf{f} - K\mathbf{u}^{(k)}$ ($\mathcal{O}(p^{d+1})$)

- solve $P\mathbf{z}^{(k)} = \mathbf{r}^{(k)}$, ($P = K_{FE}$ stiffness Finite Elements) with one of the following strategies:

- **CHOL:** *Cholesky factorization* for banded matrices
- **ND-MF:** *Nested Dissection - Multi Frontal*
- **RIC(0)-CG:** PCG with *Incomplete Cholesky factorization* of K_{FE} , *relaxed row-sum equivalence* and *zero fill-in*

Global costs:

CHOL: $\mathcal{O}(p^{3d-2})$, ND-MF: $\mathcal{O}(p^{3d-3})$ RIC(0)-CG: $\mathcal{O}(p^{d+1})$

Oss. Each Bi-CGstab iteration $\simeq 2$ CG iterations (flops).

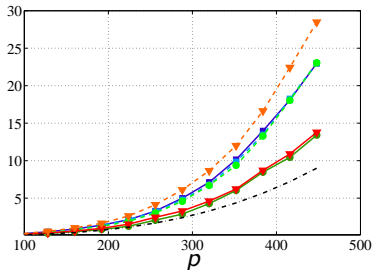
The system $P\mathbf{z}^{(k)} = \mathbf{r}^{(k)}$ is solved by symmetric solvers: the mass matrix M_{FE} is moved at r.h.s. (only matrix-vector products by M_{FE}).

CPU-time. $d = 2$

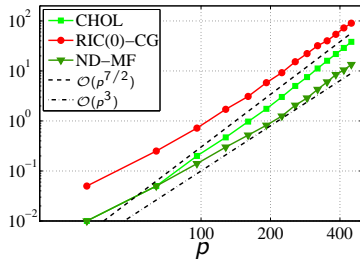
$$\begin{aligned} -\Delta u &= 1 & \text{in } \Omega &= (-1, 1)^2 \\ u &= 0 & \text{on } \partial\Omega & \end{aligned}$$

The most efficient solver: ND-MF.
 CPU-time $\simeq \mathcal{O}(p^3) = \mathcal{O}((Np)^{3/2})$
 # d.o.f. = $Np = (p-1)^2$

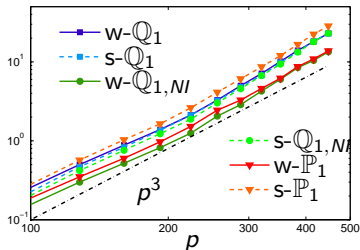
ND-MF solver



Weak- $Q_{1,Nl}$ preconditioner



ND-MF solver



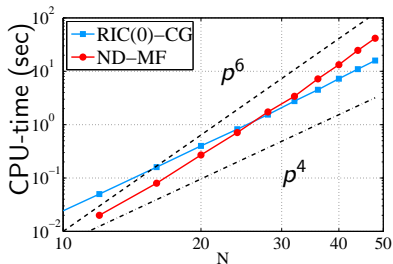
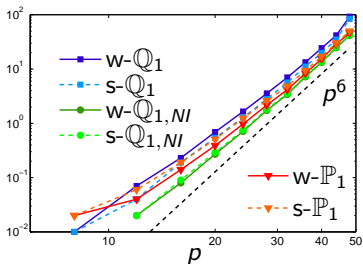
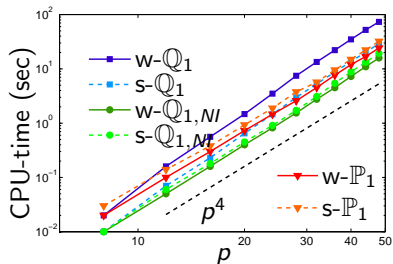
The most efficient preconditioner: weak- $Q_{1,Nl}$ (= weak- P_1)

CPU-time. $d = 3$

$-\Delta u = 1$ in $\Omega = (-1, 1)^3$, $u = 0$ on $\partial\Omega$

RIC(0)-CG

ND-MF



Most efficient solver:

ND-MF when $p \lesssim 25$,

$$\text{CPU-time} = \mathcal{O}((Np)^2)$$

RIC(0)-CG when $p \gtrsim 25$,

$$\text{CPU-time} = \mathcal{O}((Np)^{4/3})$$

$$\# \text{ d.o.f.} = Np = (p-1)^3$$

The most efficient preconditioner
is weak- $Q_{1,NI}$

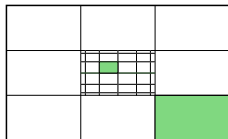


$\text{cond}(P^{-1}A)$: $d = 2$, SEM-GNI

$$\Omega = (-1, 1)^2$$

Total number of spectral elements = $Ne \times Ne$.

$$\text{Dof} = (p \cdot Ne - 1)^2.$$



best weak form:

$$Q_{1,NI} = \mathbb{P}_1$$

p	$Ne = 1$	$Ne = 2$	$Ne = 4$	$Ne = 8$
4	1.55	2.69	2.69	2.70
8	1.95	3.07	3.07	3.07
12	2.10	3.26	3.26	3.26

best strong form:

$$Q_1$$

p	$Ne = 1$	$Ne = 2$	$Ne = 4$	$Ne = 8$
4	1.46	1.59	1.59	1.59
8	1.35	1.38	1.38	1.38
12	1.35	1.37	1.37	1.37

The condition number is bounded independently of both p and Ne

$cond(P^{-1}A)$: $d = 3$, SEM-GNI

$$-\Delta u = 1 \quad \text{in } \Omega = (-1, 1)^3, \quad u = 0 \quad \text{on } \partial\Omega$$

Total number of spectral elements = $Ne \times Ne \times Ne$.

$$\text{Dof} = (p \cdot Ne - 1)^3.$$

best weak form:

$Q_{1,Nl}$

p	$Ne = 1$	$Ne = 2$	$Ne = 4$
4	1.46	1.59	1.59
6	1.41	1.47	1.47
8	1.35	1.38	1.38

best strong form:

Q_1

p	$Ne = 1$	$Ne = 2$	$Ne = 4$
4	1.55	4.97	5.00
6	1.80	5.34	5.35
8	1.95	5.60	5.60

SEM on triangles

What happens on triangles

We recall the **strong points of SEM-GNI on quads**:

- 1 **nodal** (Lagrange) basis
- 2 the **interpolation** nodes are the Legendre Gauss Lobatto (**LGL**) nodes
- 3 the **quadrature nodes** are exactly the **interpolation nodes** and Lagrange **basis is orthogonal** w.r.t. the discrete L^2 inner product (induced by quadrature) \implies **diagonal mass matrices** (in \mathbb{R}^d , $d \geq 1$)
- 4 **tensorial structure** of the basis functions in \mathbb{R}^d (with $d \geq 2$) \implies high computational efficiency

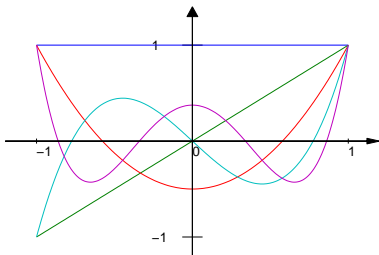
Unfortunately, it is not possible to preserve simultaneously all these upsides on simplices

Nodal basis and tensorial structure are incompatible in T, then two alternatives are possible:

1. preserve **tensorization** and use the modal basis
- or
2. preserve **nodal basis** and lose tensorization

1D Modal basis

Let $L_k(x) \in \mathbb{P}_k$ the orthogonal Legendre polynomials in $[-1, 1]$



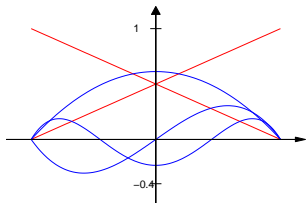
Any polynomial $u_p \in \mathbb{P}_p$ has the **modal expansion**

$$u_p(x) = \sum_{k=0}^p \hat{u}_k L_k(x), \quad \hat{u}_k \text{ are the modes}$$

Remark: this orthogonal basis is not useful to impose Dirichlet boundary conditions and the continuity at the interfaces of spectral elements.

The Legendre basis is adapted to the boundary

$$\begin{aligned}\varphi_0(\xi) &= \frac{1}{2}(L_0(\xi) - L_1(\xi)) = \frac{1 - \xi}{2} \\ \varphi_p(\xi) &= \frac{1}{2}(L_0(\xi) + L_1(\xi)) = \frac{1 + \xi}{2} \\ \varphi_k(\xi) &= \frac{1}{2(2k - 1)}(L_{k-2}(\xi) - L_k(\xi)) \\ &\text{for } k = 1, \dots, p - 1, \quad -1 \leq \xi \leq 1\end{aligned}$$



boundary adapted modal basis (or **modified C^0 basis**) and

$$u_p(\xi) = \sum_{k=0}^p \tilde{u}_k \varphi_k(\xi), \quad \text{for any } u_p \in \mathbb{P}_p$$

Remark: Now we can easily impose Dirichlet b.c. (and continuity at interfaces) but **we lose orthogonality**.

The **mass matrix** $M_{ij} = (\varphi_j, \varphi_i)_{L^2(-1,1)}$ is a **pentadiagonal** matrix.

The expansion with the **modal** basis instead of the **nodal** one is very easy to implement in one-dimensional SEM

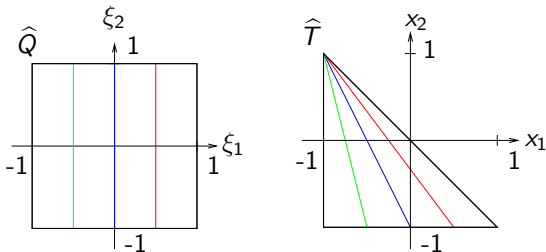
How to set up an adapted modal basis functions on triangles in order to exploit tensorization?

- 1 Collapsed Cartesian coordinates
- 2 Warped tensorial basis functions

Collapsed Cartesian coordinates

First,

collapse the reference square into the reference triangle by the map $\widehat{\mathbf{F}}$:



$\widehat{Q} = \{(\xi_1, \xi_2) \in \mathbb{R}^2 : -1 < \xi_1, \xi_2 < 1\}$ is the reference square

$\widehat{T} = \{(x_1, x_2) \in \mathbb{R}^2 : -1 < x_1, x_2 ; x_1 + x_2 < 0\}$ is the reference triangle

$$\widehat{\mathbf{F}} \left(\begin{bmatrix} \xi_1 \\ \xi_2 \end{bmatrix} \right) = \begin{bmatrix} \frac{1}{2}(1 + \xi_1)(1 - \xi_2) - 1 \\ \xi_2 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

is a bijective map, **singular at the upper vertex** of the triangle.
Nevertheless it stays bounded as one approaches the vertex.

Warped tensorial basis

- Given the polynomial degree p , let $\mathbb{P}_p(\widehat{T})$ be the space of polynomials of global degree p , $\dim(\mathbb{P}_p(\widehat{T})) = \frac{(p+1)(p+2)}{2} = nb$.
- $\varphi_{k_1}^{(1)}(\xi_1)$, for $-1 \leq \xi_1 \leq 1$ and $k_1 = 0, \dots, p$, are the boundary adapted 1D basis functions along the 1st coordinate
- $\varphi_{k_1, k_2}^{(2)}(\xi_2)$, for $-1 \leq \xi_2 \leq 1$ are the boundary adapted 1D basis functions along the 2nd coordinate. Each polynomial depends on the index k_2 , but also on k_1 .

$$\varphi_{k_1, k_2}^{(2)}(\xi_2) = \begin{cases} \varphi_{k_2}^{(1)}(\xi_2) & k_1 = 0, 0 \leq k_2 \leq p \\ \left(\frac{1-\xi_2}{2}\right)^{k_1+1} & 1 \leq k_1 \leq p-1, k_2 = 0 \\ \left(\frac{1-\xi_2}{2}\right)^{k_1+1} \left(\frac{1+\xi_2}{2}\right) P_{k_2-1}^{(2k_1+1, 1)}(\xi_2) & 1 \leq k_1 \leq p-1, \text{ and} \\ & 1 \leq k_2 \leq p-k_1-1 \\ \varphi_{k_2}^{(1)}(\xi_2) & k_1 = p, 0 \leq k_2 \leq p-1 \end{cases}$$

where $P_k^{(\alpha, \beta)}$ is the Jacoby polynomial of degree k .

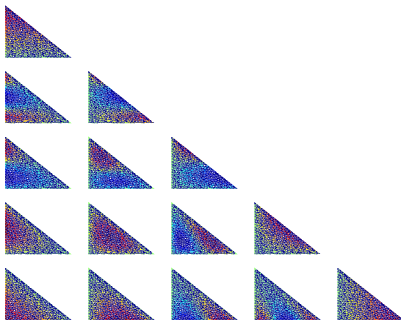
Warped tensorial basis

Let $k = (k_1, k_2)$ a bijection to use 1-index ordering. The **boundary adapted modal basis in 2d on \hat{T}** (also named **modified C^0 modal expansion**) reads

$$\phi_k(x_1, x_2) = \varphi_k(\xi_1, \xi_2) = \varphi_{k_1}^{(1)}(\xi_1)\varphi_{k_1, k_2}^{(2)}(\xi_2)$$

where $(x_1, x_2) = \hat{\mathbf{F}}(\xi_1, \xi_2)$, $-1 \leq \xi_1, \xi_2 \leq 1$.

but at the corner point $V_3(-1, 1)$: $\phi_3(x_1, x_2) = \varphi_3(\xi_1, \xi_2) = \frac{1+\xi_2}{2}$

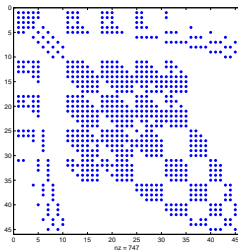


Mass matrix on one triangle

You can exploit the tensorial structure of the basis functions:

$$M_{ij} = \int_{\hat{T}} \phi_j \phi_i d\hat{T} = \int_{-1}^1 \varphi_{j1}^{(1)}(\xi_1) \varphi_{i1}^{(1)}(\xi_1) d\xi_1 \cdot \int_{-1}^1 \varphi_{j1,j2}^{(2)}(\xi_2) \varphi_{i1,i2}^{(2)}(\xi_2) \frac{1-\xi_2}{2} d\xi_2$$

(recall that $\varphi_3(\xi_1, \xi_2) = \frac{1+\xi_2}{2}$)



Quadrature formulas with $(p + 1)$ nodes in $[-1, 1]$:

	degree of exactness	at the end-points
Legendre-Gauss	$2p + 1$	open – open
Legendre-Gauss-Radau	$2p$	closed – open
Legendre-Gauss-Lobatto	$2p - 1$	closed – closed

Set the nodes and weights in \hat{Q} and collapse them on \hat{T} by $\hat{\mathbf{F}}$.

Stiffness matrix on one triangle

You can exploit the tensorial structure of the basis functions to compute derivatives, **but not to compute integrals for a generic triangle.**

$$\frac{\partial \varphi_j}{\partial x_1}(x_1, x_2) = \frac{\partial \varphi_{j1}^{(1)}}{\partial x_1}(x_1) \varphi_{j1, j2}^{(2)}(x_2) \quad \frac{\partial \varphi_j}{\partial x_2}(x_1, x_2) = \varphi_{j1}^{(1)}(x_1) \frac{\partial \varphi_{j1, j2}^{(2)}}{\partial x_2}(x_2)$$

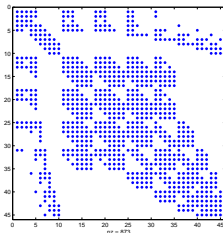
and, as usual,

$$K_{ij} = \int_{\hat{T}} \nabla \phi_j \cdot \nabla \phi_i d\hat{T} = \int_{\hat{Q}} \left(\frac{J^{cof}}{\det J_F} \nabla \varphi_j \right) \cdot \left(\frac{J^{cof}}{\det J_F} \nabla \varphi_i \right) \det J_F d\hat{Q}$$

$\det J_F = 0$ at $V_3(-1, 1)$, thus you can use:

Legendre-Gauss-Lobatto along x - direction
(quadrature nodes are in $[-1, 1]$)

Legendre-Gauss-Radau along y - direction
(quadrature nodes are in $[-1, 1]$)



Dirichlet boundary conditions or global C^0

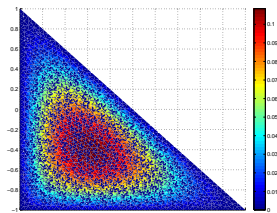
To impose Dirichlet b.c. or the continuity across adjacent elements, replace the $3p$ equations associated to the boundary modes with

$$\mathbb{P}_p \ni u_p(\mathbf{x}_\ell) = \sum_{k=1}^{nb} \tilde{u}_k \phi_k(\mathbf{x}_\ell) = g(\mathbf{x}_\ell) \quad \ell = 1, \dots, 3p$$

where g is a known function and \mathbf{x}_ℓ on each edge are the image, through $\widehat{\mathbf{F}}$, of the $p+1$ Legendre-Gauss-Lobatto nodes.

$$\begin{cases} -\Delta u + u = 1 & \text{in } \Omega = \widehat{T} \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

$A = K + M$, $\mathbf{f} = [(1, \phi_i)_{L^2(\Omega)}]_{i=1}^{nb}$
Modify $3p$ equations to impose Dir b.c. and solve $A\tilde{\mathbf{u}} = \mathbf{f}$.



The numerical solution is $u_p(\mathbf{x}) = \sum_{k=1}^{nb} \tilde{u}_k \phi_k(\mathbf{x})$

For a general partition, standard arguments for assembling matrices and ordering the modes/nodes can be applied.

Triangular SEM with boundary adapted modal basis

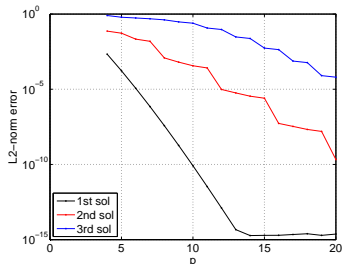
Condition number of the stiffness matrix (Laplace operator) is
 $cond(A) = \mathcal{O}(p^3 h^{-2})$

Preconditioners designed by Babuska et al. (1991) for \mathbb{P}_p can be used:
coarse \mathbb{P}_1 , and coarse average.

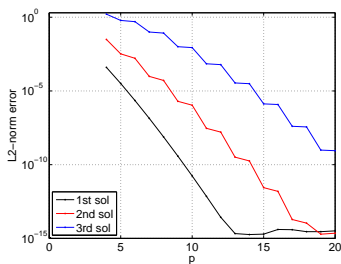
For both: $cond(P^{-1}A) = \mathcal{O}(\log^2 p)$, independently of h , but it does depend on the interior angles and aspect ratios of the elements.

Convergence analysis: spectral accuracy in both L^2 - and H^1 -norm versus p :

$$u(x, y) = e^{-x-y}, \quad u(x, y) = \sin(\pi xy) + 1, \quad u(x, y) = \sin(2\pi x) \cos(2\pi y)$$



Triangular SEM on $\Omega = \hat{T}$



Quad SEM on $\Omega = \hat{Q}$

Triangular SEM with nodal basis

Given p , $\mathbb{P}_p(\hat{T})$, $\dim(\mathbb{P}_p(\hat{T})) = \frac{(p+1)(p+2)}{2} = nb$.

- **Nodal Lagrange basis** $\{\varphi_i(\mathbf{x})\}$ (on \hat{T}) associated with a set of interpolation nodes $\{\mathbf{x}_i\}$ (on \hat{T}): $\varphi_j(\mathbf{x}_i) = \delta_{ij}$
- choose the set of **interpolation nodes** $\{\mathbf{x}_i\}$ so that:
 - it includes LGL nodes on the edges (to use triangles in conjunction with quads)
 - the interpolation is stable (small Lebesgue constant)
 \implies **electrostatic points** (Hesthaven (1998)),
Fekete points (Bos (1983), Chen & Babuska (1995), Taylor et al. (2000))Both sets are not known explicitly, but computable by suitable algorithms. **They provide very poor quadrature formulas.**
- choose a **set of quadrature nodes and weights**.
A good choice: Gaussian quadrature formulas on \hat{Q} and collapse the nodes on \hat{T} by $\hat{\mathbf{F}}$

Lagrange basis on \hat{T}

While the Lagrange polynomials have an explicit form in $[-1, 1]$

$$\varphi_j(\xi) = -\frac{1}{p(p+1)} \frac{(1-\xi^2) L'_p(\xi)}{\xi - \xi_j L_p(\xi_j)}$$

and this is the keypoint to compute efficiently derivatives,

there is not a closed-form expression for the Lagrange polynomials associated with an arbitrary set of points in T .

\implies **express** the Lagrange polynomials in terms of another polynomial basis, e.g. the **orthogonal modal basis** (Dubiner) polynomials $\{\psi_k(\xi)\}$ in \hat{Q} and, if $\xi_j = \hat{\mathbf{F}}^{-1}(\mathbf{x}_j)$ (nb interpolation nodes),

$$\psi_k(\xi) = \sum_{j=1}^{nb} \underbrace{\psi_k(\xi_j)}_{V_{jk}} \varphi_j(\xi), \quad \varphi_j(\xi) = \sum_{k=1}^{nb} (V^{-1})_{kj} \psi_k(\xi) \quad j, k = 1, \dots, nb$$

V is the matrix of basis change, also known as **generalized Vandermonde matrix**.



Triangular SEM with nodal basis

Derivatives: V and V^{-1} are used to compute derivatives of basis functions.

Analogous matrices are used for **Quadrature:**

$$\tilde{V}_{\ell,k} = \psi_k(\boldsymbol{\eta}_\ell), \quad k = 1, \dots, nb, \quad \ell = 1, \dots, nq$$

In general $nq \geq nb$ and \tilde{V} is rectangular

Condition number. V and \tilde{V} affect the condition number of both mass and stiffness matrices.

Numerical results show that $\text{cond}(A) = C(h)(p^4)$ when A is the stiffness matrix of the Laplace operator. (Pasquetti & Rapetti (2004)).

Preconditioning: \mathbb{P}_1 FEM stiffness matrix (induced by either Fekete and electrostatic meshes) is not an optimal preconditioner, contrary to what happens for quads. $\text{cond}(P^{-1}A) = \mathcal{O}(p)$ (independent of h) (Warburton, Pavarino, & Hesthaven (2000))

Convergence rate: numerical results show spectral accuracy, only if quadrature formulas are adequate. (Warburton & Pavarino & Hesthaven (2000), Pasquetti & Rapetti (2004), (2006), (2010))

To finish (today) and to begin (tomorrow)

Essential bibliography (books)

- BM** C. Bernardi, Y. Maday. *Approximations Spectrales de Problèmes aux Limites Elliptiques*. Springer Verlag (1992)
- KS** G.E. Karniadakis, S.J. Sherwin. *Spectral/hp Element Methods for Computational Fluid Dynamics*, 2nd ed. Oxford University Press (2005)
- CHQZ2** C. Canuto, M.Y. Hussaini, A. Quarteroni, T. Zang. *Spectral Methods. Fundamentals in Single Domains*. Springer (2006)
- CHQZ3** C. Canuto, M.Y. Hussaini, A. Quarteroni, T. Zang. *Spectral Methods. Evolution to Complex Geometries and Applications to Fluid Dynamics*. Springer (2007)
-

A simple matlab library for spectral methods:

paola-gervasio.unibs.it/CHQZ_lib