Goal-oriented hp-Adaptive Discontinuous Galerkin Finite Element Methods for Elliptic Eigenvalue Problems

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Outline

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Model Problem

Given $\Omega \subset \mathbb{R}^2$, find (λ, u), with $\|u\|_{0,\Omega} = 1$, such that

$$-\nabla \cdot (\mathcal{A}\nabla u) + Vu \; = \; \lambda u \quad \text{in } \Omega, \qquad u = 0 \quad \text{on } \partial\Omega.$$

$$0 < \underline{a} \leq \xi^T \mathcal{A}(x)\xi \leq \overline{a} \quad \text{for all} \quad \xi \in \mathbb{R}^2 \quad \text{with} \quad |\xi| = 1 \quad \text{and all} \quad x \in \Omega \, .$$

$$0 < \underline{V} \leq V(x) \leq \overline{V} \quad \text{for all} \quad x \in \Omega.$$

S. G., L. Grubišić and J. S. Ovall
Benchmark results for testing adaptive finite element eigenvalue procedures
Applied Numerical Mathematics, Submitted, 2011

Laplace Eigenvalue Problem

Given a convex domain $\Omega \subset \mathbb{R}^2$, find (λ, u), with $\|u\|_{0,\Omega} = 1$, such that

$$-\Delta u = \lambda u \quad \text{in } \Omega, \qquad u = 0 \quad \text{on } \partial\Omega.$$

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$$S_{h,\underline{p}}(\mathcal{T}) = \{\, v \in L^2(\Omega) \,:\, v|_K \in \mathcal{Q}_{p_K}(K),\ K \in \mathcal{T} \,\}.$$

Interior Penalty Method: Find $(\lambda_h, u_h) \in \mathbf{R} \times S_{h,\underline{p}}(\mathcal{T})$ such that

$$\begin{aligned} A_h(u_h, v_h) := \int_\Omega \nabla_h u_h \cdot \nabla_h v_h \mathrm{d}\mathbf{x} - \int_{\mathcal{F}} [\![v_h]\!] \cdot \{\!\{ \nabla_h u_h \}\!\} \mathrm{d}s \\ - \int_{\mathcal{F}} [\![u_h]\!] \cdot \{\!\{ \nabla_h v_h \}\!\} \mathrm{d}s + \int_{\mathcal{F}} \mathbf{c} [\![u_h]\!] \cdot [\![v_h]\!] \mathrm{d}s \quad = \quad \lambda_h \int_\Omega u_h v_h \mathrm{d}\mathbf{x}. \end{aligned}$$

where

$\{\!\{\cdot\}\!\}$: Average Operator $\qquad [\![\cdot]\!]$: Jump Operator

$$\{\!\{ \nabla_h u_h \}\!\} = \frac{1}{2}(\nabla_h u_h|_F + \nabla_h u_h^{\mathrm{e}}|_F) \qquad [\![u_h]\!] = u_h|_F \ \underline{n}_K + u_h^{\mathrm{e}}|_F \ \underline{n}_{K^{\mathrm{e}}}.$$

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Measurement Problem

- Measurement Problem: Given a user–defined tolerance $\texttt{TOL} > 0$, can we efficiently design $S_{h,\underline{p}}$ such that

$$|J(\mathbf{u}) - J(\mathbf{u}_h)| \leq \texttt{TOL}.$$

Fluid dynamics:	drag and lift coefficients.
Electromagnetics:	far field pattern.
Elasticity theory:	stress intensity factor.
Stability analysis:	eigenvalue.
Other examples:	point value, flux, mean value, etc.

- Applications
  - Compressible (aerodynamic) flows.
    S. Giani (Nottingham), R. Hartmann (DLR, Braunschweig)
  - Stability/bifurcation structure of flows in pipes.
    K.A. Cliffe (Nottingham), E. Hall (Nottingham), T. Mullin (Manchester), E. Phipps (Sandia), A. Salinger (Sandia), J. Seddon (Manchester)
  - Neutron Transport Equation.
    R. Backhouse (Nottingham), D. Baker (Nottingham), K.A. Cliffe (Nottingham), P. Smith (Serco Assurance)

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Pros & Cons

Cons:

1. **Expensive:** a dual problem should be solved

Pros:

1. **Flexible:** the quantity of interest can be chosen
2. **Sharp Bound:** the upper bound has constant 1

$$|J(\hat{u}) - J(\hat{u}_h)| \lesssim \sum_{K \in \mathcal{T}} |\eta_K(\hat{u}_h, \tilde{z}_h)| \, .$$

3. **Accurate:** it is possible to compute an accurate estimation of the error in the quantity of interest

$$J(\hat{u}) - J(\hat{u}_h) \approx \sum_{K \in \mathcal{T}} \eta_K(\hat{u}_h, \tilde{z}_h) \, ,$$

4. **Improved Accuracy:** it is possible to improve the accuracy of the quantity of interest

$$J(\hat{u}) \approx J(\hat{u}_h) + \sum_{K \in \mathcal{T}} \eta_K(\hat{u}_h, \tilde{z}_h) \, ,$$

Primal problem: Seek the eigenpair $\hat{u}_h := (\lambda_h, u_h) \in \mathbb{R} \times S_{h,\underline{p}}$

$$\mathcal{N}(\hat{u}_h, \hat{v}_h) := -A_h(u_h, v_h) + \lambda_h(u_h, v_h) + \delta_h(\|u_h\|_0^2 - 1) = 0 \ ,$$

for all $\hat{v}_h = (\delta_h, v_h) \in \mathbb{R} \times S_{h,\underline{p}}$.

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Fréchet derivative:

$$\begin{aligned} \bar{J}(\hat{u}, \hat{u}_h; \hat{u} - \hat{u}_h) &= J(\hat{u}) - J(\hat{u}_h) = \int_0^1 J'[\theta\hat{u} + (1-\theta)\hat{u}_h](\hat{u} - \hat{u}_h)\, d\theta \ , \\ \mathcal{M}(\hat{u}, \hat{u}_h; \hat{u} - \hat{u}_h, \hat{w}) &= \mathcal{N}(\hat{u}, \hat{w}) - \mathcal{N}(\hat{u}_h, \hat{w}) \\ &= \int_0^1 \mathcal{N}'[\theta\hat{u} + (1-\theta)\hat{u}_h](\hat{u} - \hat{u}_h, \hat{w})\, d\theta \ . \end{aligned}$$

Dual formal problem: Seek a solution $\hat{z} \in \mathbb{R} \times S$

$$\mathcal{M}(\hat{u}, \hat{u}_h; \hat{w}, \hat{z}) = \bar{J}(\hat{u}, \hat{u}_h; \hat{w}) \ , \quad \forall \hat{w} \in \mathbb{R} \times S \ .$$

Theorem

Let us denote by $\hat{z}_h$ the finite element approximation of $\hat{z}$ in $\mathbb{R} \times S_{h,\underline{p}}$. Then

$$J(\hat{u}) - J(\hat{u}_h) = -\mathcal{N}(\hat{u}_h, \hat{z} - \hat{z}_h) = \sum_{K \in \mathcal{T}} \eta_K(\hat{u}_h, \hat{z}) \ .$$

Goal-Oriented Error Estimator

Because $\hat{u}$ is unavailable, we introduce an auxiliary problem, which is an approximation of the formal dual problem.
Dual problem: Seek a solution $\hat{z} \in \mathbb{R} \times S$

$$\mathcal{N}'[\hat{u}_h](\hat{v}, \hat{z}) = J'[\hat{u}_h](\hat{v})$$

$$\mathcal{N}'[\hat{u}_h](\hat{v}, \hat{z}) := -A_h(v, z) + \lambda_h(v, z) + \delta(u_h, z) + 2\beta(u_h, v) \ ,$$

Seek $\hat{z} := (\beta, z) \in \mathbb{R} \times S$, such that

$$-A_h(v, z) + \lambda_h(v, z) + \delta(u_h, z) + 2\beta(u_h, v) = J'[\hat{u}_h](\hat{v}) \ ,$$

for all $(\delta, v) \in \mathbb{R} \times S$.

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seek $(\beta, \tilde{z}_h) \in \mathbb{R} \times \tilde{S}_{h,\underline{p}}$, such that

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Outline

Adaptivity

- Goal:

$$\left(\sum_{K\in\mathcal{T}^{(j)}}\eta_K^2\right)^{1/2}\leq \mathtt{Tol}.$$

- Automatic refinement algorithm:
  0. Start with initial (coarse) grid $\mathcal{T}^{(j=0)}$.
  1. Compute the numerical eigenpair $(\lambda_h^{(j)}, u_h^{(j)})$ on $\mathcal{T}^{(j)}$.
  2. Compute the dual space $\tilde{\mathcal{T}}_h^{(j)}, \tilde{S}_{h,\underline{p}}^{(j)}$ and the numerical eigenpair $(\beta_h^{(j)}, \tilde{z}_h^{(j)})$ on $\mathcal{T}^{(j)}$.
  3. Compute the local error indicators $\eta_K(u_h^{(j)}, \tilde{z}_h^{(j)})$.
  4. If $\left(\sum_{K\in\mathcal{T}^{(j)}}\eta_K^2\right)^{1/2}\leq \mathtt{Tol} \rightarrow$ stop. Otherwise, adapt $\mathcal{T}^{(j)}$, $S_{h,\underline{p}}$.
  5. $j=j+1$, and go to step (1).

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Outline

$$\begin{cases} -\triangle u = \lambda u, & \text{in } \Omega \ , \\ u = 0 \ , & \text{on } \partial\Omega \ . \end{cases}$$

n	DOFs	dDOFs	elements	$\vert\lambda - \lambda_h\vert$	$\sum_{K\in\mathcal{T}} \eta_K$	effectivity
1	192	320	32	5.030e-02	4.984e-02	0.99
2	224	360	32	2.658e-02	2.605e-02	0.98
3	264	410	32	1.728e-02	1.690e-02	0.98
4	320	480	32	6.080e-04	6.032e-04	0.99
5	360	528	32	3.067e-04	3.020e-04	0.98
6	420	600	32	1.480e-04	1.444e-04	0.98
7	480	672	32	4.596e-06	4.574e-06	1.00
8	528	728	32	2.361e-06	2.338e-06	0.99
9	588	798	32	1.684e-06	1.665e-06	0.99
10	672	896	32	2.363e-08	2.355e-08	1.00
11	728	960	32	1.189e-08	1.180e-08	0.99
12	812	1056	32	3.043e-09	2.989e-09	0.98

Table: Results for the *hp*-adaptive method on the first eigenvalue $\lambda = 2\pi^2$.

n	DOFs	dDOFs	elements	$\|\lambda - \lambda_h\|$	$\sum_{K \in \mathcal{T}} \eta_K$	effectivity
1	48	108	12	1.748e-01	2.072e-01	1.19
2	84	189	21	1.019e-01	1.158e-01	1.14
3	130	284	30	7.600e-02	8.084e-02	1.06
4	210	425	39	3.096e-02	2.983e-02	0.96
5	337	616	45	1.464e-02	1.276e-02	0.87
6	555	902	45	7.641e-03	7.455e-03	0.98
7	902	1339	45	4.903e-03	4.642e-03	0.95
8	1674	2045	54	1.945e-03	1.841e-03	0.95
9	2269	2688	63	7.718e-04	7.306e-04	0.95
10	3045	3437	72	3.063e-04	2.899e-04	0.95
11	3794	4411	81	1.215e-04	1.151e-04	0.95
12	4581	5434	90	4.824e-05	4.566e-05	0.95
13	5535	6575	99	1.914e-05	1.812e-05	0.95
14	6868	7862	108	7.597e-06	7.192e-06	0.95
15	8213	9670	117	3.015e-06	2.854e-06	0.95
16	10077	11548	126	1.195e-06	1.133e-06	0.95

Table: Results for the *hp*-adaptive method on the first eigenvalue.

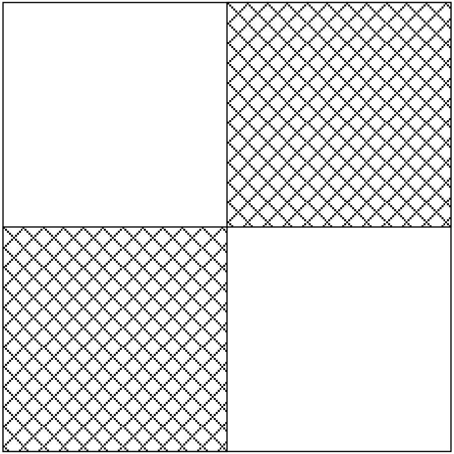
L-Shaped Domain

n	λ_h	$\lvert\lambda - \lambda_h\rvert$	$\lvert\lambda - \lambda_h - \sum_{K\in\mathcal{T}} \eta_K\rvert$
1	38.73368195	1.748e-01	3.240e-02
2	38.66081840	1.019e-01	1.386e-02
3	38.63489499	7.600e-02	4.845e-03
4	38.58985563	3.096e-02	1.135e-03
5	38.57353627	1.464e-02	1.876e-03
6	38.56653588	7.641e-03	1.856e-04
7	38.56379818	4.903e-03	2.612e-04
8	38.56083998	1.945e-03	1.037e-04
9	38.55966714	7.718e-04	4.116e-05
10	38.55920165	3.063e-04	1.633e-05
11	38.55901692	1.215e-04	6.482e-06
12	38.55894361	4.824e-05	2.572e-06
13	38.55891452	1.914e-05	1.021e-06
14	38.55890297	7.597e-06	4.051e-07
15	38.55889839	3.015e-06	1.607e-07
16	38.55889657	1.195e-06	6.381e-08

Table: Improved accuracy for the first eigenvalue of the L-shaped domain.

Asymptotic doubling of the multiplicity

$$-\triangle\psi + \kappa V_{MD} \cdot \psi = \lambda\psi, \quad \psi \in H_0^1([-1,1]^2), \|\psi\|_0 = 1.$$



λ	N	DOFs	dDOFs	elements	CPU time
5.42471651467	13	1684	2028	16	13.061
12.47333477067	15	5652	9121	445	23.624
13.19367701575	14	5076	8155	391	18.367
20.22822122972	13	1776	2512	64	7.400
25.16706773416	15	14891	24075	1162	63.759
25.18999056233	15	4931	6521	112	38.258
32.43757892927	14	12609	19757	862	49.056
32.69700326366	14	11843	18810	865	45.874
42.39525913789	18	48695	62361	904	352.948
42.51072321200	19	53145	67045	862	302.182

Table: Results for the *hp*-adaptive on the first 10 eigenvalues with $\kappa = 1$.

Asymptotic doubling of the multiplicity

According to the theory, as $\kappa \to \infty$ we have that the two smallest eigenvalues — denoted by λ_1^κ and λ_2^κ — are distinct for any finite κ and both converge to the double eigenvalue $2\pi^2$ of the Dirichlet Laplace eigenvalue problem posed in the domain consisting of the two unit white squares. Additionally, it holds that

$$\frac{|\lambda_1^\kappa - 2\pi^2|}{2\pi^2} = O\left(\kappa^{-\alpha}\right), \qquad \frac{|\lambda_2^\kappa - 2\pi^2|}{2\pi^2} = O\left(\kappa^{-\alpha}\right) .$$

We will estimate $0 < \alpha \leq 1$ by fitting the computed error estimates. The theory does not cover this case, but we formally expect that $\alpha = 1/2$.

κ	α
1.0e+01	-
1.0e+02	0.469
1.0e+03	0.486
1.0e+04	0.488
1.0e+05	0.496
1.0e+06	0.499
1.0e+07	0.500

(a)

κ	α
1.0e+01	-
1.0e+02	0.276
1.0e+03	0.447
1.0e+04	0.486
1.0e+05	0.496
1.0e+06	0.499
1.0e+07	0.500
1.0e+08	0.500

(b)

AptoFEM

- Non-conforming Discontinuous Galerkin finite element methods.
- Standard conforming finite element methods.
- Dimension independent data structures.
- 2D/3D unstructured hybrid grids consisting of triangles, quadrilaterals, hexahedra, tetrahedra, prisms, pyramids.
- Local isotropic and anisotropic mesh adaptation.
- Arbitrary high-order hp-FEM
- A posteriori error estimation (explicit and implicit)
- Mesh partition with METIS on parallel machines
- Matrix assembly in parallel
- Interfaces to a variety of third party linear algebra packages.
    - MUMPS
    - PETSc
    - Hypre
    - Pardiso
    - ...