FEM for a modified Schrödinger operator

Joint work with

Hengguang Li

Finite Element Circus, Cornell, Ithaca, October 2007

Victor Nistor, Penn State U.

www.math.psu.eadu/nistor/
This work was supported in part by NSF

The problem

Ω is a curvilinear *polygonal* domain.

Let $r = \sqrt{x^2 + y^2}$ be the distance to the origin.

Problem: To approximate the solution of

$$-\Delta u + \delta r^{-2} u = f \in H^{m-1}(\Omega)$$

with *mixed boundary conditions*, $\delta > 0$.

The origin $O \in \overline{\Omega}$.

More generally,

$$-\Delta u + V u = f \in H^{m-1}(\Omega), \ \ \delta > 0,$$

with V a potential with the same type of singularities.

Motivation: Schrödinger equations with centrifugal potentials and fluid dynamics (Mazzucato–Taylor) ...

Disjoint decomposition $\partial\Omega = \partial_D\Omega \cup \partial_N\Omega$.

Study the *Finite Element approximations* of the solutions of the mixed boundary value problem

$$\begin{cases} -\Delta u + Vu = f & \text{in } \Omega, \\ \partial_\nu u = 0 & \text{on } \partial_N\Omega, \text{ and} \\ u = 0 & \text{on } \partial_D\Omega, \end{cases}$$

The solution u will have singularities due to

- corners;
- change of boundary conditions;
- singularities of coefficients.

The analytic form of the singularities is *the same*.

A similar numerical treatment is possible.

The numerical treatment of the corner singularities was extensively studied: **Arnold, Babuška, Bacuta, Bramble, Brenner, Costabel, Dauge, Falk, Guo, Kellogg, Osborn, Raugel, Schatz, Schwab, Wahlbin, Xu, Zikatanov**, and many others.

The effect of change of boundary conditions was less studied, and the effect of coefficients singularities even less (see **Hengguang Li**'s talk (transmission and Neumann problems) and, also, **Yunrong Zhu**).

The theoretical justification in the case of *coefficients singularities* requires new ideas.

Difficulty similar to the ones in the (pure) Neumann problem.

Additional difficulty: *quadrature* (GFEM: Babuška, Banerjee, Osborn, ...).

Weak formulation and discretization

Let $\vartheta(x)$ be the distance from x to the subset of $\overline{\Omega}$ consisting of:

– the vertices of Ω,
– to the points where the boundary conditions change,
– to the *singularities* of the potential V.

Our weak formulation is in the space

$$\mathcal{W} := \{u,\ \int_\Omega |u/\vartheta|^2 dx + \int_\Omega |\nabla u|^2 dx < \infty, \\ u = 0 \text{ on } \partial_D \Omega\}.$$

Then the *weak formulation* of $-\Delta u + Vu = f$ with mixed boundary conditions is:

Weak formulation. *Find $u \in \mathcal{W}$ such that*

$$a(u,v) := (\nabla u, \nabla v)_{L^2} + (Vu, v)_{L^2} = (f, v)_{L^2},$$

for all $v \in \mathcal{W}$.

The discrete solution $u_S \in S \subset \mathcal{W}$ of our problem is defined, as usual, by analogy:

Discrete solution. *Find* $u_S \in S$ *such that*

$$a(u_S, v_S) = (f, v_S)_{L^2},$$

for all $v_S \in S$*.*

where $a(u_S, v_S) := (\nabla u_S, \nabla v_S)_{L^2} + (V u_S, v_S)_{L^2}$.

The space $\mathcal{W}$ is closely related to the *weighted Sobolev spaces*

$$\mathcal{K}_a^m(\Omega) := \{u : \Omega \to \mathbb{R},\ \vartheta^{i+j-a} \partial_x^i \partial_y^j u \in L^2(\Omega)\},$$

for all $i + j \leq m$.

$$\mathcal{W} = \mathcal{K}_1^1(\Omega) \cap \{u|_{\partial_D \Omega} = 0\}.$$

Theorem. (Hengguang Li-Mazzucato-N.) There is $\eta > 0$ such that the map

$$\Delta : \mathcal{K}_{a+1}^{m+1}(\Omega) \cap \{u|_{\partial_D \Omega} = 0,\ \partial_\nu u|_{\partial_N \Omega} = 0\} \to \mathcal{K}_{a-1}^{m-1}(\Omega)$$

is an isomorphism for $|a| < \eta$ and all m.

Approximation

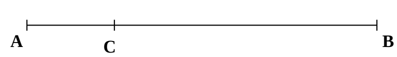
Let us explain the mesh refinement for $V = \delta r^{-2}$.

From now on we shall ignore all singularities except the ones coming from the coefficient δr^{-2}*.*

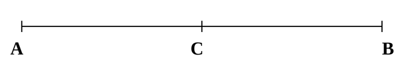
One can show that $u \in H^{1+\sqrt{\delta}-\epsilon}(\Omega)$ (close to the origin), but not better ($\delta > 0$).

Our mesh refinement is given in terms of a parameter $\kappa \in (0, 1/2]$, leading to the κ*–refinement* technique

Definition:



If $A = O$, $|AC| = \kappa|AB|$.



If $A, B \neq O$, $|AC| = |AB|$.

We have $\kappa = 2^{-1/(ma)}$, where m is the degree of the polynomials used in the approximation and $0 < a < \sqrt{\delta}$.

Start with an initial mesh.

Refine using the "κ–refinement" technique.

Sequence of FEM spaces $S_n \in \mathcal{W}$ (piecewise degree m polynomials).

$u \in S_n$ is zero on $\partial_D \Omega$ and at the singularities of V.

$u_n = u_{S_n} \in S_n$ are the associated *discrete* solutions.

Theorem. (Hengguang Li-Mazzucato-N.) Assume $f \in H^{m-1}(\Omega)$. The "κ–refinement" technique leads to *a sequence of meshes* S_n that yields quasi-optimal rate of convergence

$$\|u - u_n\|_{\mathcal{K}_1^1} \leq C \,\mathrm{dim}(S_n)^{-m/2} \|f\|_{H^{m-1}}.$$

Numerical tests

In our implementation, $m = 1$, so

$$\kappa = 2^{-1/a},$$

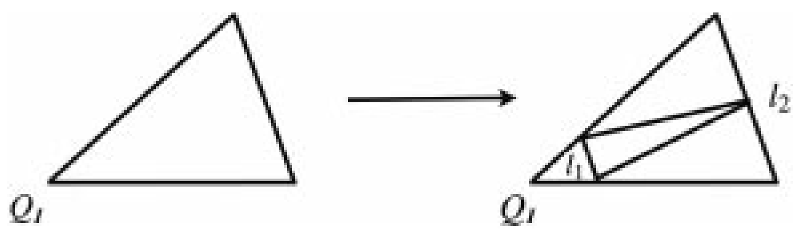
with $0 < a < \sqrt{\delta}$.

We list the *estimated rate of convergence*

$$e = \log_2 \frac{|u_j - u_{j-1}|_{\mathcal{K}_1^1}}{|u_{j+1} - u_j|_{\mathcal{K}_1^1}}.$$

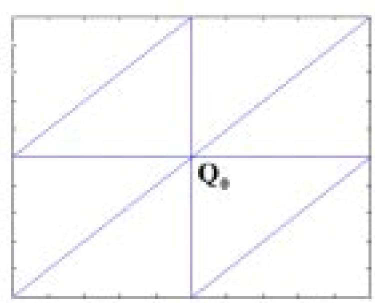
Model cases: square and L-shaped domain.

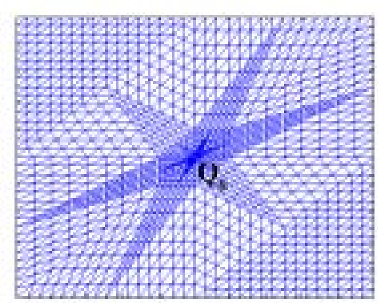
We first consider the square $\Omega = (-1, 1) \times (-1, 1)$.



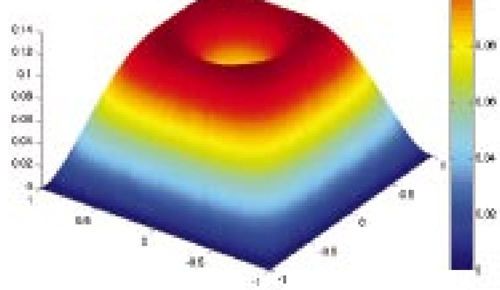
$\kappa = l_1/l_2$

Refinement of a triangle with vertex $Q_I = O$.





Initial triangulation   Four refinements, $\kappa = 0.2$



$\delta = 1/2$ on the square $\Omega := (-1, 1) \times (-1, 1)$:

$$-\Delta u + \frac{1}{2} r^{-2} u = 1.$$

The origin O is an interior point.

We have $u \in H^{1+s}$ for $s < \eta = \sqrt{1/2} \approx 0.707$.

The solution is not in H^2.

We take $\kappa = 2^{-1/a} < 2^{-1/\eta} \approx 0.375$.

$j \backslash \kappa$	$e : 0.1$	$e : 0.2$	$e : 0.3$	$e : 0.4$	$e : 0.5$
3	0.885	0.907	0.896	0.840	0.754
4	0.945	0.953	0.922	0.828	0.691
5	0.973	0.972	0.926	0.798	0.626
6	0.987	0.981	0.924	0.767	0.578
7	0.994	0.986	0.921	0.740	0.548
8	0.998	0.990	0.917	0.720	0.531
9	0.999	0.992	0.914	0.705	0.521

$\delta = 2$, keep Ω the unit square.

The origin O is an interior point.

$u \in H^{1+s}$ for $s < \eta = \sqrt{0.5} \approx 1.414 > 1$.

The solution is in H^2, and hence no graded mesh is necessary for piecewise linear functions.

$j \backslash \kappa$	e : 0.1	e : 0.2	e : 0.3	e : 0.4	e : 0.5
3	0.899	0.920	0.938	0.947	0.918
4	0.961	0.971	0.978	0.982	0.958
5	0.987	0.991	0.993	0.994	0.976
6	0.996	0.997	0.998	0.998	0.985
7	0.999	0.999	0.999	0.999	0.990
8	1.000	1.000	1.000	1.000	0.994
9	1.000	1.000	1.000	1.000	0.996

$-\Delta u + .15 r^{-2} u = 1$ on an L shaped domain.

The origin O is the reentrant corner.

Change of boundary conditions at O.

We have $u \in H^{1+s}$ for $s < \eta \approx 0.511$

($\eta := \sqrt{\delta + (\pi/2\alpha)^2} = \sqrt{0.15 + 1/9}$, $\alpha = 3\pi/2$.)

The solution is not in H^2.

$\eta \approx 0.511$ gives $\kappa < 0.258$.

$j \backslash \kappa$	$e : 0.1$	$e : 0.2$	$e : 0.3$	$e : 0.4$	$e : 0.5$
3	0.885	0.907	0.896	0.840	0.754
4	0.945	0.953	0.922	0.828	0.691
5	0.973	0.972	0.926	0.798	0.626
6	0.987	0.981	0.924	0.767	0.578
7	0.994	0.986	0.921	0.740	0.548
8	0.998	0.990	0.917	0.720	0.531
9	0.999	0.992	0.914	0.705	0.521

Conclusions

We have studied the Finite Element solutions of

$$-\Delta u + \delta r^{-2} u = f$$

with *mixed boundary conditions*.

A "κ–graded mesh refinement" for suitable κ yields a sequence of meshes that exhibit quasi-optimal rates of convergence.

The theoretical justification is based on a regularity and isomorphism theorem (well-posedness) in *weighted Sobolev spaces*.

Our numerical test confirm our results.

Open problem: to account theoretically for the effect of numerical integration (quadrature).