An adaptive hp-XFEM method for a Hardy problem featuring an inverse square point potential

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- For given parameter $\lambda \in \mathbb{R}$ and Lipschitz domain $\Omega \subset \mathbb{R}^d$ with $\partial\Omega = \Gamma_D \dot{\cup} \Gamma_N$, we seek for a solution framework of

$$\begin{aligned} -\Delta u - \lambda |\mathbf{x}|^{-2} u &= f \quad \text{in} \quad \Omega, \\ u &= g \quad \text{on} \quad \Gamma_D, \\ \partial_{\mathbf{n}} u &= h \quad \text{on} \quad \Gamma_N, \end{aligned}$$

- Choose a variational ansatz, *i.e.* closed solution space $H_0^1(\Omega) \subset U \subset H^1(\Omega)$.
- For $d = 2$, then necessary $u = 0$ at $\mathbf{x} = \mathbf{0}$ and $\mathbf{0} \notin \Omega$
- Force $\mathbf{0} \in \Gamma_D$ and by Dirichlet-lifting argument, consider the variational problem:

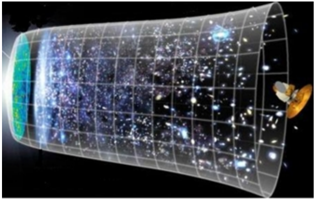
$$\text{Find } u \in U = H^1_{\Gamma_D}(\Omega), \text{ s.t. } \int_\Omega \nabla u \cdot \nabla v - \lambda \frac{uv}{|\mathbf{x}|^2} \,\mathrm{d}\mathbf{x} = \int_\Omega fv \,\mathrm{d}\mathbf{x} + \int_{\Gamma_N} hv \,\mathrm{d}S,$$

i.e. $f \in (H^1_{\Gamma_D})^*$, $h \in H_{00}^{1/2}(\Gamma_N)$ with associated bilinearform $a_\lambda : U \times U \to \mathbb{R}$.

Application:

- ▷ Quantum Cosmological models (via Wheeler-de-Witt equation)[1]
- ▷ Application in Linearization of Non-linear problems, e.g. combustion theory[2]

$$-\Delta u - \frac{\lambda}{|\mathbf{x}|^2} u = f, \quad \mathbf{0} \in \Gamma_D$$



source: http://www.pdl.cmu.edu/AstroDISC/DISC-Index.shtml

Mathematical features:

- ▷ $\frac{1}{|\mathbf{x}|^2} \notin L^p, p \in [1, \infty]$, but in $L^1_{\text{loc}}(\Omega)$
- ▷ in general **lack** of compactness

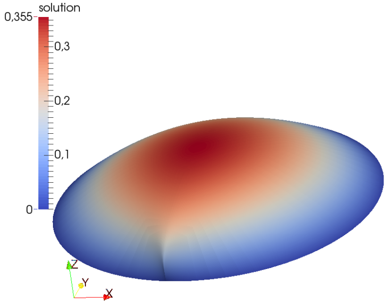
$$U \overset{c}{\not\hookrightarrow} L^2(\Omega, \mathrm{d}\mathbf{x}/|\mathbf{x}|^2) = \{u | u/|.| \in L^2(\Omega)\}$$

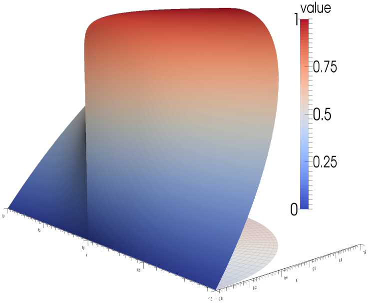
Goals:

- ▷ Ensure (Non-)Existence (via explicit Hardy-inequalities)
- ▷ Analyse regularity (via Kondrat'ev theory)
- ▷ Numerical treatment (Rayleigh-quotient, a-posterior analysis, extended *hp*-AFEM)

[1] Berestycki, H., Esteban, M., *Existence and Bifurcation of Solutions for an Elliptic Degenerate Problem*, Journal of differential equations, 1997

[2] Gel'fand, Izrail Moiseevich, *Some problems in the theory of quasi-linear equations*, Uspekhi Matematicheskikh Nauk, 1959





- Typical local situation: **arbitrary** strong singular behaviour depending on λ
- **slow** convergence rates of standard adaptive FEM strategies

1. Well-posedness of the boundary value problem
   - HARDY inequalities
   - Regularity in weighted spaces: Kondrat'ev and Babuška-Guo spaces
2. Numerical Treatment
   - Rayleight quotient approximation
   - adaptive *hp*- and *hp*-extended FEM
   - generalized Duffy transformation
3. Conclusion and perspectives

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Questions:

- Which properties of Ω and $\partial\Omega$ influence existence?
- What is the maximal range of λ to find unique weak solution?

Answer via: **generalized Rayleigh quotient**

$$\Lambda = \Lambda(U) := \inf_{v \in U} \frac{\int_\Omega |\nabla v|^2 \,\mathrm{d}\mathbf{x}}{\int_\Omega \frac{u^2}{|\mathbf{x}|^2} \,\mathrm{d}\mathbf{x}}$$

- which yields an optimal HARDY type inequality with HARDY constant Λ

$$\int_\Omega |\nabla v|^2 \geq \Lambda \int_\Omega \frac{v^2}{|\mathbf{x}|^2}, \quad \forall v \in U.$$

Remark:

- Λ may be **not** attained in U ($\hat{=}$ lack of compactness).
- Λ may depend on the **whole** domain Ω.
- Above inequality may only can be improved by several **lower** order terms[3]

[3] e.g. For $U = H_0^1(\Omega)$ overview in *Functional inequalities: new perspectives and new applications by N. Ghoussoub and A. Moradifam*

Definition

- *A domain $\Omega \subset \mathbb{R}^2$ is* **admissable**[4] *if it allows for $\Lambda(H_0^1(\Omega)) > 0$.*
- *A boundary segment $\Gamma_N \subset \partial\Omega$ is* **admissable** *if $\Lambda(H^1_{\Gamma_D}) > 0$ and* **optimal** *if $\Lambda(H^1_{\Gamma_D}) = \Lambda(H^1_0) > 0$.*

- If Γ_N admissable $\Rightarrow$ Ω admissable.

Theorem (Existence and Uniqueness)

Let Γ_N be admissable, then for all $\lambda \in (-\infty, \Lambda)$ there exists a unique weak solution $u \in H^1_{\Gamma_D}(\Omega)$. The coercivity constant explodes for $\lambda \to \Lambda$.

- Question: Do such admissable sets exist? $\rightarrow$ **Yes!**

Remark: (Non-Existence)

- If $\lambda > \Lambda$ we do not even have ultra-weak solutions,
- If $\lambda = \Lambda$ there are scenarios of well-posedness

[4] Caldiroli, P. and Musina, R., *Stationary states for a two-dimensional singular Schrödinger equation*, Bollettino della Unione Matematica Italiana-B, 2001

Theorem (Hardy inequality on $H^1_{\Gamma_\mathbf{0}}$)

Let $d \geq 2$ and $\mathbf{0}$ lies in the interior of Γ_D, then

1. *Let Γ_D be smooth. Then there exists $C = C(\Gamma_\mathbf{0}, \Omega, d) > 0$, such that*

$$C \int_\Omega u^2 \,\mathrm{d}\mathbf{x} + \int_\Omega |\nabla u|^2 \,\mathrm{d}\mathbf{x} \geq \frac{d^2}{4} \int_\Omega \frac{u^2}{|\mathbf{x}|^2} \,\mathrm{d}\mathbf{x}, \quad \forall u \in H^1_{\Gamma_D}(\Omega).$$

2. *Let Ω locally coincide with a cone $\mathcal{C}_\Sigma = \{r\sigma | r > 0, \sigma \in \Sigma \subset \mathbb{S}^{d-1}$ Lipschitz$\}$, then there exists $C = C(\Gamma_\mathbf{0}, \Omega, d) > 0$, such that*

$$C \int_\Omega u^2 \,\mathrm{d}\mathbf{x} + \int_\Omega |\nabla u|^2 \,\mathrm{d}\mathbf{x} \geq \left(\frac{(d-2)^2}{4} + \Lambda_1(\Sigma) \right) \int_\Omega \frac{u^2}{|\mathbf{x}|^2} \,\mathrm{d}\mathbf{x}, \quad \forall u \in H^1_{\Gamma_D}(\Omega).$$

- If $d = 2$ for $\mathcal{C}_\Sigma = \mathcal{C}_\omega$, we find $\Lambda_1(\mathcal{C}_\omega) = \frac{\pi^2}{\omega^2}$.
- With the help of POINCARÉ inequality we find (non-optimal) HARDY constants > 0
- One may obtain optimal HARDY constants ($C = 0$), *e.g.* $\Omega \subset \mathbb{R}^2_+$ and Γ_N optimal

▷ A usefull tool for HARDY constants (if the L^1-trace is non-negative).

Lemma

Let $\mathbf{x}_0, \ldots, \mathbf{x}_m \in \overline{\Omega}$, $\Phi \in \mathcal{C}^2(\Omega \setminus \{\mathbf{x}_0, \ldots, \mathbf{x}_m\})$ *and* $\Phi > 0$ *in* $\Omega \setminus \{\mathbf{x}_0, \ldots, \mathbf{x}_m\}$ *allowing for a* L^1*-trace* $\mathbf{n} \cdot \nabla\Phi/\Phi$ *on* Γ_N. *Then for all* $u \in H^1_{\Gamma_0}(\Omega)$

$$\int_\Omega \left(|\nabla u|^2 + \frac{\Delta\Phi}{\Phi} u^2 \right) \mathrm{d}\mathbf{x} = \int_\Omega \Phi^2 \left| \nabla \left(\frac{u}{\Phi} \right) \right|^2 \mathrm{d}\mathbf{x} + \int_{\Gamma_N} u^2 \left[\frac{\mathbf{n} \cdot \nabla\Phi}{\Phi} \right] \mathrm{d}s,$$

In particular if $-\frac{\Delta\Phi}{\Phi} \geq C \frac{1}{|\mathbf{x}|^2}$, *then*

$$\int_\Omega |\nabla u|^2 \geq C \int_\Omega \frac{u^2}{|\mathbf{x}|^2} \mathrm{d}\mathbf{x} + \int_{\Gamma_N} \left[\frac{\mathbf{n} \cdot \nabla\Phi}{\Phi} \right] u^2 \, \mathrm{d}s.$$

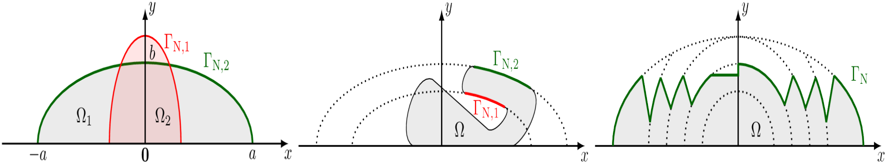
Remark: Also applies for $-\Delta + V(x)$ operators, enforcing $-\Delta\Phi/\Phi \geq CV(x)$

Theorem (Existence of optimal boundaries)

Let up to rotation $\Omega \subset \mathbb{R}^2_+$ be smooth around the origin and $\Gamma_N \subset \partial\Omega$ with outer normal $\mathbf{n} \in S^1$.

- *Let $\Gamma_N \subset \mathcal{E}_r^{a,b}$ be ellipsoid formed with $\mathbf{n} \in S^1_+$ (resp. $\mathbf{n} \in S^1_-$), then Γ_N is optimal if $b \leq a$ (resp. $a \leq b$).*
- *If $\Gamma_N \subset \mathcal{V}_{g_\pm}$ is valley-formed with $\mathbf{n} \in S^1_+$, then it conserves optimality with respect to Ω.*
- *The x_2-axis is optimal for $x_2 > 0$.*

Moreover any finite union of these is optimal.



- **only** green segment is optimal, **only** red may not be optimal

Storyline: for Ω locally conical and $d = 2$

- $1/|.|^2 \notin L^\infty(\Omega)$ is of same order as Δ, **standard** elliptic regularity theory **does not** apply
- Regularity **depends on** λ, i.e. for $\lambda \to \Lambda$ we have $u \in H^{1+\epsilon}(\Omega)$ with $\epsilon \to 0$

Decomposition:

- With the help of Kondrat'ev spaces (following[5]) we find

$$u = u_{\text{reg}} + u_{\text{sing}}, \quad u_{\text{sing}}(r,\theta) = \sum_{n=1}^{N} c_n r^{\lambda_n} \Phi_n(\theta).$$

- (λ_n, Φ_n) are the first eigenpairs of the corresponding operator Pencil induced by **Mellin** transformation of $-\Delta - \lambda/|\mathbf{x}|^2$
  - Example: $\lambda_n = \sqrt{\frac{\pi^2}{\omega^2} n^2 - \lambda}$ for DD b.c., $\lambda_n = \sqrt{\frac{\pi^2}{4\omega^2} n^2 - \lambda}$ for DN b.c.
- If $\lambda \to \Lambda = \frac{\pi^2}{\omega^2}$ or $\frac{\pi^2}{4\omega^2}$, then $\lambda_1 \to 0$

Remark: We note a similarity to Poisson problem in polygonal domains, *e.g.* shifting

[5] Kozlov, V. A. and Maz′ya, V. G. and Rossmann, J., *Elliptic boundary value problems in domains with point singularities*, Mathematical Surveys and Monographs, American Mathematical Society, Providence, RI, 1997

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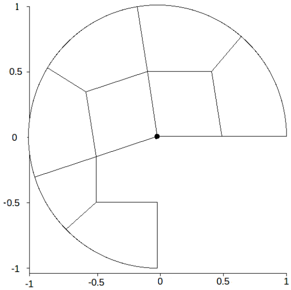
- ▷ HARDY constant Λ not known in general, but existence strongly depends on $\lambda : \Lambda$ ratio

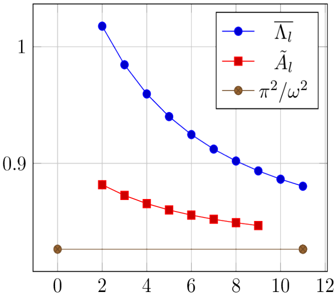
Goal:

- ▷ Approximate Λ

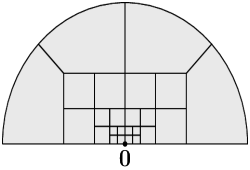
Problems:

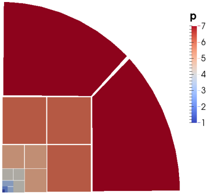
- ▷ RAYLEIGH-quotient minimization $\Rightarrow$ **upper bounds** $\overline{\Lambda}_\ell$, $\ell = 1, 2, \ldots$
- ▷ We need **lower bounds** $\underline{\Lambda} \leq \Lambda$ to ensure existence
  - **but** current two-sided bounds results rely on compactness arguments
- ▷ Λ is not attained in general, *i.e.* minimization sequences may escape $H^1(\Omega)$
  - approximation (from above) may becomes arbitrary difficult task





▷ **Decomposition** and analysis in **Babuška-Guo spaces** $\mathcal{B}^l_\beta$ motivate for *hp*-AFEM space U_{hp} with geom. grading $0 < \sigma < 1$ and linear polynomial slope $\mu > 0$.[6]





▷ Advantage: If u belongs to $\mathcal{B}^2_\beta(\Omega) \Rightarrow$ exponential convergence, *i.e.*

$$\exists b = C(\sigma, \beta, \mu)(1-\beta) > 0, \quad \text{s.t.} \quad \inf_{v \in U_{hp}} ||u - v||_{H^1(\Omega)} \leq C e^{-b \dim(U_{hp})^{1/3}}$$

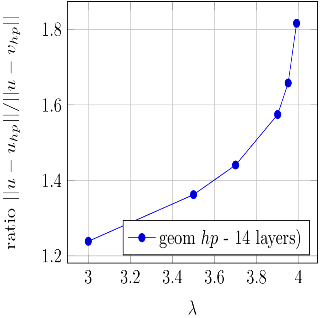
▷ **Problem:** As $\lambda \to \Lambda$, then $\beta \to 1$ and therefore $b \to 0$.

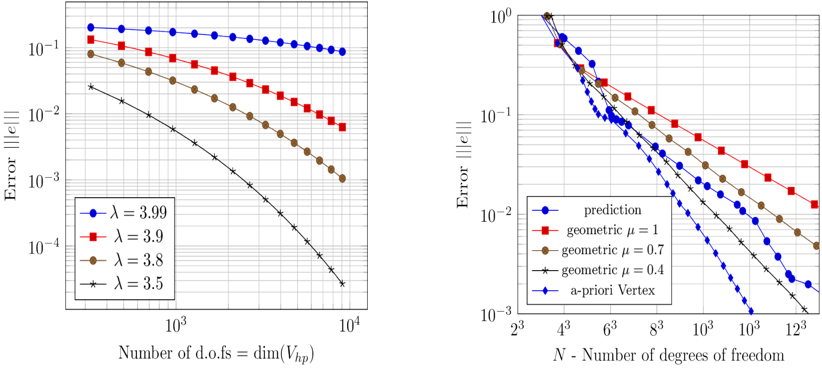
[6] *e.g.* Schwab, C., *p- and hp-finite element methods: Theory and applications in solid and fluid mechanics*, Oxford University Press, Oxford, UK, 1998

▷ **Difficulty:** Cea-Lemma yields

$$||u - u_{hp}||_{H^1(\Omega)} \leq C(\Lambda, \lambda) \inf_{v_{hp} \in U_{hp}} ||u - v_{hp}||_{H^1(\Omega)}$$

and $C(\Lambda, \lambda) \to \infty$ as $\lambda \to \Lambda$ due to coercivity constant.





- **left:** $\lambda \to \Lambda = 4$ dependence with $\mu = 1, \sigma = 0.5$,
- **right:** μ dependence with $\lambda = 3.9, \sigma = 0.5$ and other adaptive strategies

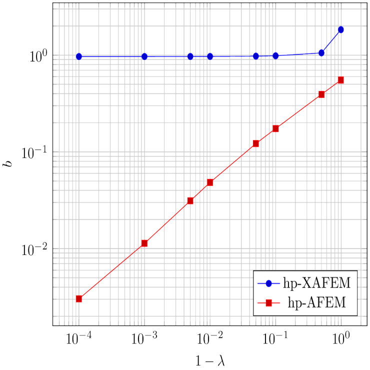
- Recall $u = u_{\text{sing}} + u_{\text{reg}}$ and $u_{\text{sing}} := \chi \sum_{i=1}^{I} u_i r^{\alpha_i} s(i;\theta)$ and set

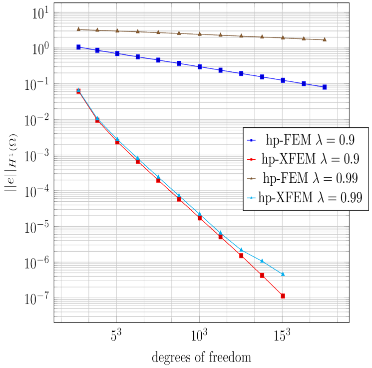
$$X_{hp} := \left\{ u_{xhp} \in H^1_{\Gamma_0}(\Omega) \,|\, u_{xhp} = u_{hp} + \chi \sum_{i=1}^{I} a_i \phi_i^{\text{XFEM}},\, u_{hp} \in U_{hp} \right\} \subset H^1_{\Gamma_D}(\Omega).$$

- Mesh must resolve the cutoff χ, and choose size of $\operatorname{supp}\chi$ with care
- Enrichment yields systemmatrix of the form

$$\mathbb{A} = \left[\begin{array}{c|c} A & b \\ \hline b^T & s \end{array} \right]$$

- **Advantages:** best approximation result now scales with $\inf_{v \in U_{hp}} ||u_{\text{reg}} - v_{hp}||_{H^1(\Omega)}$
- **Feature:** for particular situations necessarily $I > 1$ to ensure $u_{\text{reg}} \in H^2$, in particular different from POISSON problem.





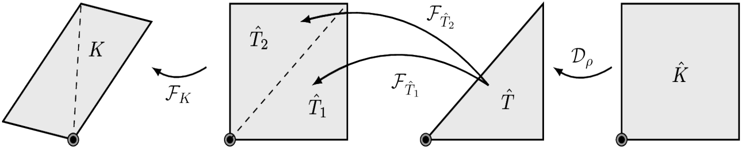
- **left:** $\Lambda = 1$, exponential convergence rate dependends on $\lambda \to \Lambda$ and method
- **right:** Demonstration of increased convergence speed for different values of $\lambda = 0.9, 0.99 < \Lambda = 1$, with $\mu = 1, \sigma = 0.5$

- When (locally) assembling $\mathbb{A}$, need of accurate integration of $\int_K \frac{q(\mathbf{x})}{r^\alpha}\,\mathrm{d}\mathbf{x}$, $\mathbf{0} \in \overline{K}, \alpha < 2$

Definition (Generalized DUFFY transform[7])

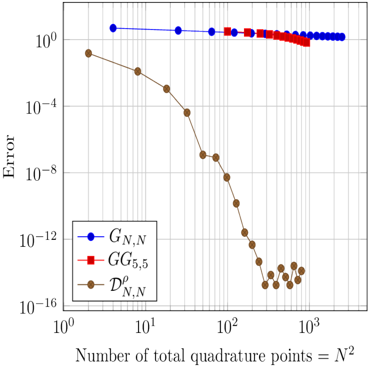
Let $\rho > 0$, then the generalized Duffy transform $\mathcal{D}_\rho$ is defined as

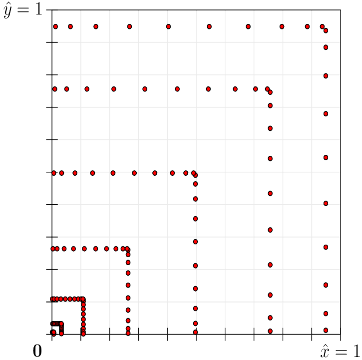
$$\mathcal{D}_\rho \colon \hat{K} \to \hat{T}, \quad \hat{\mathbf{x}} = (\hat{x}, \hat{y}) \mapsto \mathcal{D}_\rho(\hat{x}, \hat{y}) = (\hat{x}^\rho, \hat{x}^\rho \hat{y}).$$



- **Advantage:** $\int_K \frac{q(\mathbf{x})}{r^\alpha}\,\mathrm{d}\mathbf{x} = \sum_{i=1}^{2} \int_{\hat{K}} F_i(\hat{x}^\rho, \hat{y})\hat{x}^{2\rho-1-\alpha\rho}\,\mathrm{d}\hat{\mathbf{x}}$, with smooth function $F_i, i = 1, 2$.
- Duffy-Gauß-Jacobi/Legendre integration after own choice of ρ yields fast approximation

[7] Mousavi, S.E. and Sukumar, N., *Generalized Duffy transformation for integrating vertex singularities*, Computational Mechanics, 45(2-3), 2010





- **left:** Comparison for $\alpha = 1.8$ on $K = \hat{K}$, with geometric Gauss quadrature
- **right:** typical structure of Duffy points

- Current state of explicit and implicit residual error estimators not suitable for full range of $\lambda \in (-\infty, \Lambda)$
  - $u/|\mathbf{x}|^2 \notin L^2(\Omega)$, $a_\lambda|_K(.,.)$ is not positive on interior functions if $\lambda > 0$
  - Need of Interpolation operator $I \colon U \to U_{hp}$, s.t.

$$\left|\left|\frac{v - I_v}{|.|}\right|\right|_{L^2(K)} \leq C h_K^{\alpha} ||v||_{H^1(\omega_K)},$$

- For $\lambda < 0$ implicit estimators yield results, but standard proofs will not work
- Hierachical estimator[8] successfull applied for low-order approximation and $\lambda < 0$
- others, *e.g.* gradient recovery, mixed formulations based on *hypercircle* method not yet analysed

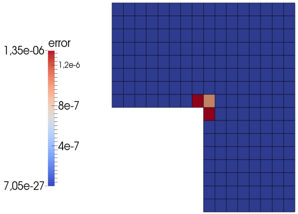
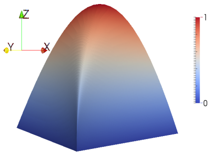


Figure : implicit estimator, with $\lambda < 0$

[8] Li, H. and Ovall, J. S., *A posteriori error estimation of hierarchical type for the Schrödinger operator with inverse square potential*, Numerische Mathematik, 128(4), 2014

- We analysed equation involving a inverse square potential

$$-\Delta - \frac{\lambda}{|\mathbf{x}|^2}$$



- Well-posedness and Non-Existence with the help of HARDY constants extended on non-zero trace spaces $H^1_{\Gamma_D}(\Omega)$
- We illustrated features of this type of equation, *i.e.* strong singularities, best approximation issues (related to coercivity)
- We were able to accurate approximate via extended *hp*-AFEM.
- Accurate assembling based on Duffy transform.

Open problems:

- Singular behaviour for non-conical behaviour of Ω. $\rightarrow$ Clear since 06.07.2016
- Finding rigorous a-posteriori analysis, in particular for $\lambda > 0$.
- Extend regularity analysis to the multi-polar case and adapt the numerical tools.

Thank you for your attention

Main references:

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