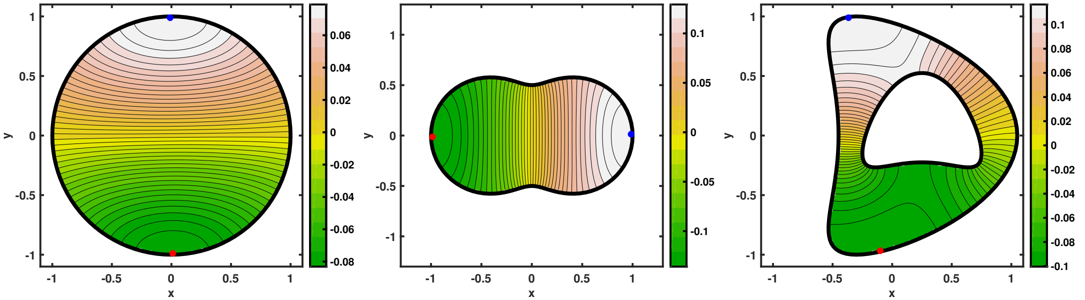

THE HOT SPOTS CONJECTURE CAN BE FALSE

Some numerical examples using boundary integral equations

UL Virtual Colloquium | March 25, 2021 | Andreas Kleefeld | Jülich Supercomputing Centre

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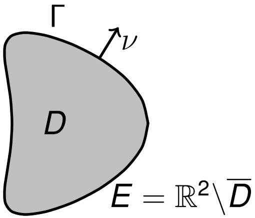
INTRODUCTION

Problem setup

Consider

- flat piece of metal
- which is insulated
- heat within piece diffuses over time
- (almost arbitrary) initial heat distribution is given



Mathematically

- $D \subset \mathbb{R}^2$ (bounded planar domain)
- homogeneous Neumann boundary condition (HNBC) $\partial_\nu u = 0$ on Lipschitz boundary Γ
- heat equation $\partial_t u = \Delta u$
- $u(x, 0) = f(x)$, $x \in D$

INTRODUCTION

Problem setup

- What happens if t is large?
- Consider smallest non-trivial eigenvalue of negative Laplacian in D with HNBC.
- $\Delta u + \kappa^2 u = 0$ in D with $\partial_\nu u = 0$ on Γ ($\lambda = \kappa^2$)
- Eigenvalues are discrete

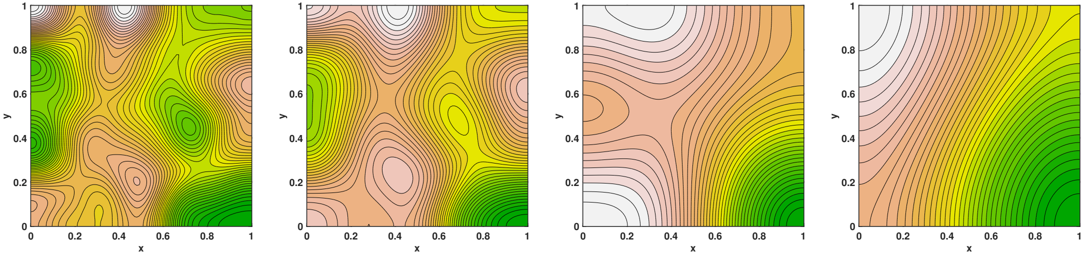
$$0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \ldots .$$

- If $\lambda_1 < \lambda_2$ and $\langle u(\cdot\,,0), u_1\rangle \neq 0$, then

$$u(x,t) = C + \mathrm{e}^{-\lambda_1 t}\,\langle u(\cdot\,,0), u_1\rangle\, u_1(x) + \text{lower terms}\,.$$

INTRODUCTION

Numerical solution of heat equation $\partial_t u = \tau \Delta u$, $\tau = 1/10$



(a) Solution at $t_1 = 1/200$ (b) Solution at $t_2 = 1/10$ (c) Solution at $t_3 = 1/2$ (d) Solution at $t_4 = 2$

Figure: Initial condition with standard normal random numbers and HNBC using ETD ($h = 1/100$ and $k = 1/100$).

E.O. Asante-Asamani, A. Kleefeld, & B.A. Wade, *A second-order exponential time differencing scheme for non-linear reaction-diffusion systems with dimensional splitting*, Journal of Computational Physics **415**, 109490 (2020).

INTRODUCTION

Hot spots conjecture (HSC)

- Hottest and coldest spot will appear on Γ when waiting for a long time.
- HSC by Jeffrey Rauch (1974): For each eigenfunction $u_1(x)$ corresponding to λ_1 which is not identically zero, we have

$$\inf_{x\in\Gamma} u_1(x) < u_1(y) < \sup_{x\in\Gamma} u_1(x) \qquad \forall\, y \in D\,.$$

J. Rauch *Lecture #1. Five problems: An introduction to the qualitative theory of partial differential equations*, in Partial differential equations and related topics (ed. J.A. Goldstein) **446**, 355–369, Lecture Notes in Mathematics, Springer (1974).

INTRODUCTION

Hot spots conjecture (HSC)

- Conjecture is true for parallelepipeds, balls, rectangles, cylinders, obtuse triangles, some convex and non-convex domains with symmetry, wedges, lip domains, convex domains with two axis of symmetry, convex $C^{1,\alpha}$ domains $(0 < \alpha < 1)$ with one axis of symmetry, a certain class of planar convex domains, sub-equilateral isosceles triangles, certain class of acute triangles, Euclidean triangles.

- HSC is open for arbitrary convex domains.
- As well as for arbitrary non-convex domains.
- No numerical results are available to show failure of HSC.

- Can we find easy to construct domains where HSC fails?

INTRODUCTION

Ingredients

- Method to find smallest non-trivial Neumann eigenvalue and corresponding eigenfunction for arbitrary domains.

  $\Rightarrow$ Boundary integral equations and its discretization.

- Non-linear eigenvalue solver.

  $\Rightarrow$ Complex analysis and integral equations.

- Optimization routines (standard).

NUMERICAL SOLUTION

Boundary integral equation

- Green's representation theorem

$$u(x) = \int_\Gamma \partial_{\nu(y)} u(y) \cdot \Phi_\kappa(x,y) - u(y) \cdot \partial_{\nu(y)} \Phi_\kappa(x,y)\,\mathrm{d}s(y)\,, \quad x \in D$$

with $\Phi_\kappa(x,y) = \mathrm{i}H_0^{(1)}(k\|x-y\|)/4$, $x \neq y$.

- Using $\partial_\nu u = 0$ on Γ, yields

$$u(x) = -\mathrm{DL}_\kappa u(x)\,, \quad x \in D \tag{1}$$

with acoustic double layer potential and density ψ

$$\mathrm{DL}_\kappa \psi(x) = \int_\Gamma \psi(y) \cdot \partial_{\nu(y)} \Phi_\kappa(x,y)\,\mathrm{d}s(y)\,, \quad x \in D\,.$$

NUMERICAL SOLUTION

Boundary integral equation

- Letting $x \in D$ approach Γ and using jump relation of DL_κ, gives

$$u(x) = -\left\{\mathrm{D}_\kappa u(x) - (1 - \Omega(x))\, u(x)\right\}, \quad x \in \Gamma$$

with double layer operator

$$\mathrm{D}_\kappa \psi(x) = \int_\Gamma \psi(y) \cdot \partial_{\nu(y)} \Phi_\kappa(x, y)\, \mathrm{d}s(y), \quad x \in \Gamma.$$

- $\Omega(x) = -\mathrm{D}_0\, 1\, (x)$ interior solid angle (½ a.e. for Lipschitz domains).

NUMERICAL SOLUTION

Boundary integral equation

- Can be written as

$$\Omega \cdot u + \mathrm{D}_\kappa u = 0 \quad \text{on } \Gamma\,.$$

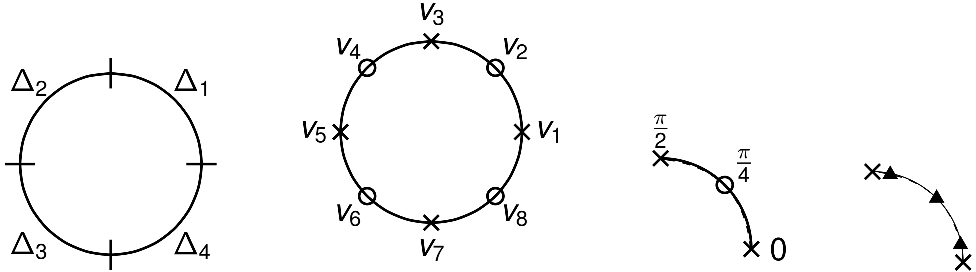
- Abstractly as non-linear eigenvalue problem $\mathrm{M}(\kappa)u = 0$ with

$$\mathrm{M}(\kappa) = \Omega \cdot \mathrm{I} + \mathrm{K}(\kappa)\,.$$

- $\mathrm{K}(\kappa)$ is compact operator from $\mathcal{H}^{-1/2}(\Gamma)$ to $\mathcal{H}^{1/2}(\Gamma)$.
- $\mathrm{M}(\kappa)$ Fredholm of index zero for $\kappa \in \mathbb{C} \backslash \mathbb{R}_{\leq 0}$.
- Therefore, theory of eigenvalue problems for holomorphic Fredholm operator-valued functions applies.

NUMERICAL SOLUTION

Boundary integral equation and its approximation



1. Subdivide boundary in n_f pieces.
2. Define discretization points.
3. Approximate boundary pieces.
4. Discretize unknown function on each piece.
5. Require residual to be zero at $n_c = 3 \cdot n_f$ 'collocation points'.
6. Leads to non-linear eigenvalue problem $\mathbf{M}(\kappa)\vec{u} = \vec{0}$ with $\mathbf{M}(\kappa) \in \mathbb{C}^{n_c \times n_c}$.

NUMERICAL SOLUTION

Boundary integral equation and its approximation

- Consider

$$\lambda\,\psi(x) + \int_\Gamma \psi(y)\partial_{\nu(y)}\Phi_\kappa(x,y)\,\mathrm{d}s(y) = h(x)\,,\quad x\in\Gamma\,.$$

- Parameter $\lambda \neq 0$ and h are given.
- Then

$$\lambda\,\psi(x) + \sum_{j=1}^{n_f}\int_{\Delta_j} \psi(y)\partial_{\nu(y)}\Phi_\kappa(x,y)\,\mathrm{d}s(y) = h(x)\,,\quad x\in\Gamma\,.$$

NUMERICAL SOLUTION

Boundary integral equation and its approximation

- For each j there exists a bijective map $m_j : \sigma = [0,1] \mapsto \Delta_j$.
- Then,

$$\lambda\,\psi(x) + \sum_{j=1}^{n_f} \int_\sigma \psi(m_j(s))\partial_{\nu(m_j(s))}\Phi_\kappa(x, m_j(s))J(s)\,\mathrm{d}s(s) = h(x)\,, \quad x \in \Gamma\,.$$

- Jacobian given by $J(s) = \|\partial_s m_j(s)\|$.

NUMERICAL SOLUTION

Boundary integral equation and its approximation

- We approximate each $m_j(s)$ by a quadratic interpolation polynomial

$$m_j(s) \approx \widetilde{m}_j(s) = \sum_{i=1}^{3} v_{(i+2(j-1)+1) \bmod (2n_f)} L_i(s)\,.$$

- Lagrange basis functions for the quadratic interpolation polynomials are

$$L_1(s) = t\cdot(1-2s)\,, \quad L_2(s) = 4s\cdot t\,, \quad \text{and} \quad L_3(s) = s\cdot(2s-1)$$

with $t = 1 - s$.

NUMERICAL SOLUTION

Boundary integral equation and its approximation

- 'Collocation nodes' $\widetilde{v}_{j,k}$ are given by $\widetilde{v}_{j,k} = \widetilde{m}_j(q_k)$ for $j = 1, \ldots, n_f$ and for $k = 1, 2, 3$ where $q_1 = \alpha$, $q_2 = ½$, and $q_3 = 1 - \alpha$ with $0 < \alpha < ½$ a given and fixed constant.
- Ensures that collocation nodes are always lying within a piece of the boundary and at those points the interior solid angle is ½.
- Specific choice of α can improve the overall convergence rate.

NUMERICAL SOLUTION

Boundary integral equation and its approximation

- Unknown function $\psi(\widetilde{m}_j(s))$ is now approximated on the j-th piece by a quadratic interpolation polynomial of the form

$$\sum_{k=1}^{3} \psi(\widetilde{m}_j(q_k))\widetilde{L}_k(s) = \sum_{k=1}^{3} \psi(\widetilde{v}_{j,k})\widetilde{L}_k(s)\,.$$

- Here, $\widetilde{L}_k(s)$ are the Lagrange basis functions

$$\widetilde{L}_1(s) = \frac{t-\alpha}{1-2\alpha}\frac{1-2s}{1-2\alpha}\,,\quad \widetilde{L}_2(s) = 4\frac{s-\alpha}{1-2\alpha}\frac{t-\alpha}{1-2\alpha}\,,\quad \widetilde{L}_3(s) = \frac{s-\alpha}{1-2\alpha}\frac{2s-1}{1-2\alpha}$$

with $t = 1 - s$ and $0 < \alpha < ½$.

NUMERICAL SOLUTION

Boundary integral equation and its approximation

- We obtain

$$\lambda\,\psi(x) + \sum_{j=1}^{n_f}\sum_{k=1}^{3}\int_\sigma \partial_{\nu(\widetilde{m}_j(s))}\Phi_\kappa(x,\widetilde{m}_j(s))\|\partial_s\widetilde{m}_j(s)\|\widetilde{L}_k(s)\,\mathrm{d}s(s)\psi(\widetilde{v}_{j,k}) - h(x) = r(x)$$

  with $r(x)$ the residue which is due to the various approximations.
- We set $r(\widetilde{v}_{i,\ell}) = 0$. Boundary element collocation method

NUMERICAL SOLUTION

Boundary integral equation and its approximation

- In our case $\lambda = ½$.
- We obtain the linear system of size $3n_f \times 3n_f$

$$\frac{1}{2}\psi(\widetilde{v}_{i,\ell}) + \sum_{j=1}^{n_f}\sum_{k=1}^{3} a_{i,\ell,j,k}\psi(\widetilde{v}_{j,k}) = h(\widetilde{v}_{j,k})$$

with the resulting integrals

$$a_{i,\ell,j,k} = \int_{\sigma} \partial_{\nu(\widetilde{m}_j(s))}\Phi_{\kappa}(\widetilde{v}_{i,\ell}, \widetilde{m}_j(s))\|\partial_s \widetilde{m}_j(s)\|\widetilde{L}_k(s)\,\mathrm{d}s(s)\,.$$

- Approximate them by adaptive Gauss-Kronrod quadrature.
- Can be written abstractly as $\mathbf{M}(\kappa)\vec{\psi} = \vec{h}$.

NUMERICAL SOLUTION

Boundary integral equation and its approximation

- In our case

$$\mathbf{M}(\kappa)\vec{u} = \vec{0}\,.$$

After we obtain κ and $\vec{u}$ on the boundary, we insert this into (1) to compute the potential inside the domain at any point we want.

- Discretization done as explained previously yields

$$u(x) = -\mathrm{DL}_\kappa[u](x) \approx -\sum_{j=1}^{n_f}\sum_{k=1}^{3} \hat{a}_{j,k}\, u(\widetilde{v}_{j,k})$$

with

$$\hat{a}_{j,k} = \int_\sigma \partial_{\nu(\widetilde{m}_j(s))}\Phi_\kappa(x,\widetilde{m}_j(s))\|\partial_s \widetilde{m}_j(s)\|\widetilde{L}_k(s)\,\mathrm{d}s(s)$$

for an arbitrary point $x \in D$.

NUMERICAL SOLUTION

Solving the non-linear eigenvalue problem

- Consider non-linear eigenvalue problem

$$\mathbf{M}(\kappa)\vec{u} = \vec{0}\,, \quad \vec{u} \in \mathbb{C}^{n_c}\,, \quad \vec{u} \neq 0\,, \quad \kappa \in \mathbb{D} \subset \mathbb{C}\,, \quad \gamma = \partial\mathbb{D}\,.$$

- Large scale problem $n(\gamma) \ll n_c$ ($n(\gamma)$ is number of eigenvalues including multiplicities inside γ).
- Problem can be reduced to linear eigenvalue problem of dimension $n(\gamma)$ (Keldysh's theorem).
- One has to use complex-valued contour integrals.

W.-J. Beyn, *An integral method for solving nonlinear eigenvalue problems*, Linear Algebra and its Applications **436**, 3839–3863 (2012).

NUMERICAL SOLUTION

Solving the non-linear eigenvalue problem

- Specify 2π-periodic contour γ of class C^1 within the complex plane.
- Need a contour that is enclosing a part of the real line where the smallest non-zero eigenvalue is expected.
- Usually use a circle with radius R and center $(\mu, 0)$.
- In this case, we have $\varphi(t) = \mu + R\cos(t) + \mathrm{i}R\sin(t)$ which satisfies $\varphi \in C^\infty$.

NUMERICAL SOLUTION

Solving the non-linear eigenvalue problem

- Approximate

$$A_0 = \frac{1}{2\pi\mathrm{i}} \int_\gamma \mathbf{M}^{-1}(\kappa)\,\mathrm{d}s(\kappa) \approx \frac{1}{\mathrm{i}N}\sum_{j=0}^{N-1} \mathbf{M}^{-1}(\varphi(t_j))\varphi'(t_j) = A_{0,N}\,,$$

$$A_1 = \frac{1}{2\pi\mathrm{i}} \int_\gamma \kappa\mathbf{M}^{-1}(\kappa)\,\mathrm{d}s(\kappa) \approx \frac{1}{\mathrm{i}N}\sum_{j=0}^{N-1} \varphi(t_j)\mathbf{M}^{-1}(\varphi(t_j))\varphi'(t_j) = A_{1,N}\,.$$

- Parameter N is given and equidistant nodes are $t_j = 2\pi j/N$, $j = 0,\dots,N$.
- Note that choice $N = 24$ is sufficient due to exponential convergence rate.

NUMERICAL SOLUTION

Solving the non-linear eigenvalue problem

- Compute an SVD of $A_{0,N} = V\Sigma W^{\mathrm{H}}$ with $V \in \mathbb{C}^{n_c\times n_c}$, $\Sigma \in \mathbb{C}^{n_c\times n_c}$, and $W \in \mathbb{C}^{n_c\times n_c}$.
- Perform a rank test for the matrix $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \dots, \sigma_{n_c})$ for a given tolerance $\epsilon = \mathrm{tol}_{\mathrm{rank}}$ (usually $\epsilon = 10^{-4}$).
- That is, find $n(\gamma)$ such that $\sigma_1 \geq \dots \geq \sigma_{n(\gamma)} > \epsilon > \sigma_{n(\gamma)+1} \geq \dots \geq \sigma_{n_c}$.
- Define $V_0 = (V_{ij})_{1\leq i\leq n_c, 1\leq j\leq n(\gamma)}$, $\Sigma_0 = (\Sigma_{ij})_{1\leq i\leq n(\gamma), 1\leq j\leq n(\gamma)}$, and $W_0 = (W_{ij})_{1\leq i\leq n_c, 1\leq j\leq n(\gamma)})$ and compute the $n(\gamma)$ eigenvalues κ_i and eigenvectors $\vec{s}_i$ of the matrix

$$B = V_0^{\mathrm{H}} A_{1,N} W_0 \Sigma_0^{-1} \in \mathbb{C}^{n(\gamma)\times n(\gamma)}\,.$$

- The i-th non-linear eigenvector $\vec{u}_i$ is given by $V_0\vec{s}_i$.

NUMERICAL RESULTS

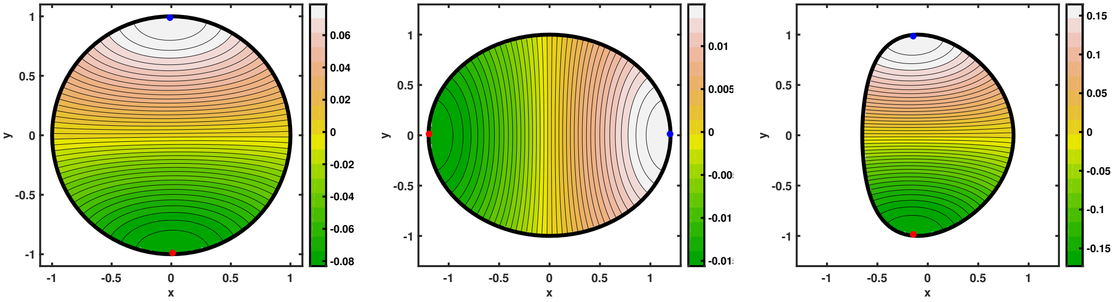
Estimated order of convergence (EOC)

n_f	n_c	abs. error $E^{(1)}_{n_f}$	$\mathrm{EOC}^{(1)}$	abs. error $E^{(2)}_{n_f}$	$\mathrm{EOC}^{(2)}$	abs. error $E^{(3)}_{n_f}$	$\mathrm{EOC}^{(3)}$
5	15	5.8503_{-3}		1.2817_{-2}		1.6335_{-2}	
10	30	4.7818_{-4}	3.6129	1.1543_{-3}	3.4729	1.3081_{-3}	3.6424
20	60	4.5775_{-5}	3.3849	1.2187_{-4}	3.2437	1.3133_{-4}	3.3162
40	120	5.0168_{-6}	3.1897	1.4173_{-5}	3.1041	1.5147_{-5}	3.1161
80	240	5.9173_{-7}	3.0838	1.7199_{-6}	3.0428	1.8416_{-6}	3.0401
160	480	7.2096_{-8}	3.0369	2.1229_{-7}	3.0182	2.2788_{-7}	3.0146
320	960	8.9069_{-9}	3.0169	2.6386_{-8}	3.0082	2.8373_{-8}	3.0057
640	1920	1.1072_{-9}	3.0080	3.2895_{-9}	3.0038	3.5406_{-9}	3.0024
1280	3840	1.3803_{-10}	3.0039	4.1066_{-10}	3.0018	4.4225_{-10}	3.0011

Table: Absolute error and EOC of first three non-trivial interior Neumann eigenvalue for a unit circle.

NUMERICAL RESULTS

Convex domains

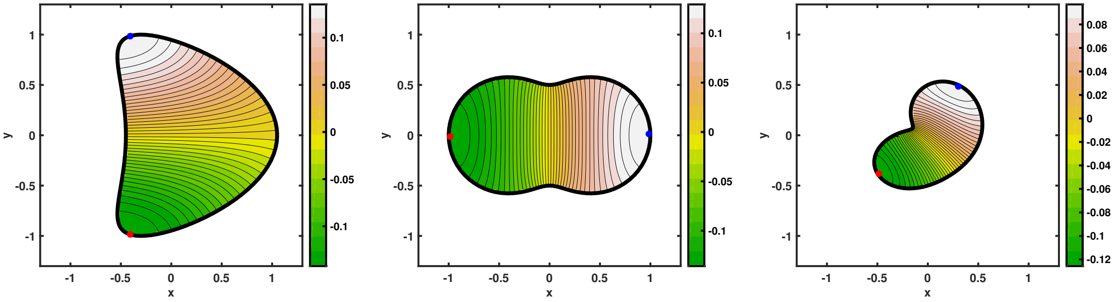


(a) Circle (b) Ellipse (c) Deformed ellipse

Figure: u_1 for a circle, an ellipse, and a deformed ellipse.

NUMERICAL RESULTS

Non-convex domains



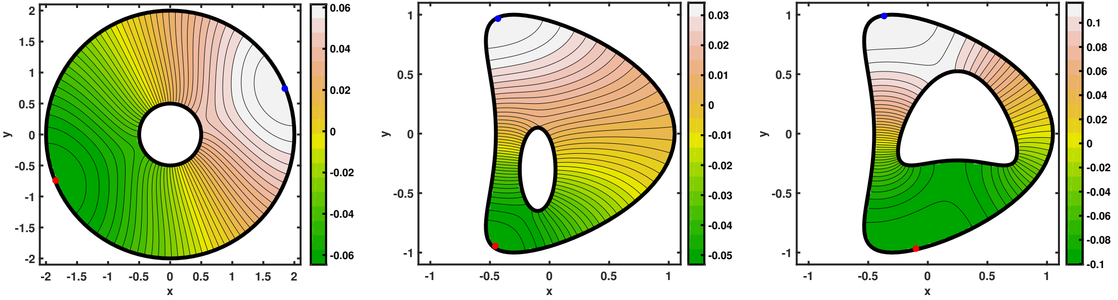
(a) Deformed ellipse (b) Peanut (c) Apple

Figure: u_1 for deformed ellipse, peanut, and apple.

NUMERICAL RESULTS

Domains with one hole

- What about objects with one hole?
- HSC is true for an annuli (exact solution available) and other domains (my numerical results)



(a) Annulus (b) Domain with hole (c) Domain with hole

Figure: u_1 for an annulus and two other domains with a hole.

NUMERICAL RESULTS

Domains with one hole

- Krzysztof Burdzy & Wendelin Werner (1999) showed that there is a domain with one hole such that HSC fails.
- “...domains with bizarre shape...”
- A recent domain with one hole given by Burdzy (2005) is a theoretical one, too (epsilon domain, very thin).
- Proof includes stochastic arguments.

- Issue: No numerical results given (cannot be given for this domain).

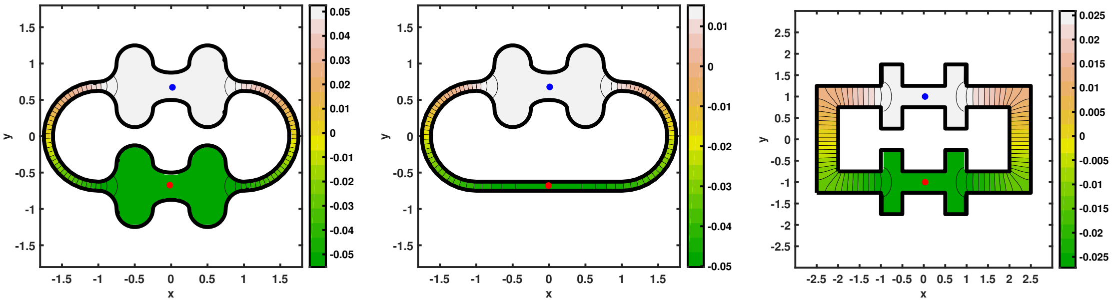
K. Burdzy, *The hot spots problem in planar domains with one hole*, Duke Mathematical Journal **129**, 481–502 (2005).

K. Burdzy & W. Werner, *A counterexample to the “hot spots” conjecture*, Annals of Mathematics **149**, 309–317 (1999).

NUMERICAL RESULTS

Domains with one hole

Some counter-examples



(a) ‘Teether’ domain (b) Variant of ‘teether’ (c) ‘Brick’ domain

Figure: u_1 for the teether, its variant, and the brick.

A. Kleefeld, *The hot spots conjecture can be false: Some numerical examples*, arXiv:2101.01210.

NUMERICAL RESULTS

Domains with one hole

- Use optimization routine (Nelder-Mead) to find max (min) location in D.
- Max (min) on Γ known, too.
- Define ratio of max (min) in D and max (min) on Γ as $\aleph_{max}$ ($\aleph_{min}$).

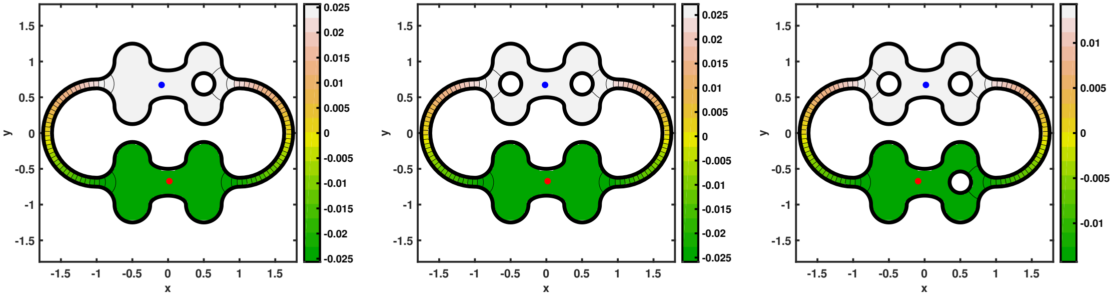
D	location max	location min	$\aleph_{max}$	$\aleph_{min}$
T	$(-3.805_{-8}, 6.877_{-1})^\top$	$(3.299_{-8}, -6.877_{-1})^\top$	$1 + 1.221_{-4}$	$1 + 1.221_{-4}$
V	$(-1.968_{-7}, 6.877_{-1})^\top$	——	$1 + 1.438_{-3}$	——

Table: Location of max and min inside domain along with ratios $\aleph_{max} > 1$ and/or $\aleph_{min} > 1$ for teether T and its variant V that fail HSC.

NUMERICAL RESULTS

Domains with more than one hole

Some counter-examples



(a) Domain with two holes (b) Domain with three holes (c) Domain with four holes

Figure: u_1 for teether with more than one hole.

SUMMARY AND OUTLOOK

- Introduced HSC.
- Showed how to find highly accurate first non-trivial Neumann eigenvalue and eigenfunction via boundary integral equations.
- Illustrated numerically that HSC can be false for domains with hole(s).

- Can you find easy to construct domains that fail HSC, too?
- Can you prove that HSC is true for simply-connected convex/non-convex domains?

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