AAA-LS rational approximation and solution of Laplace problems

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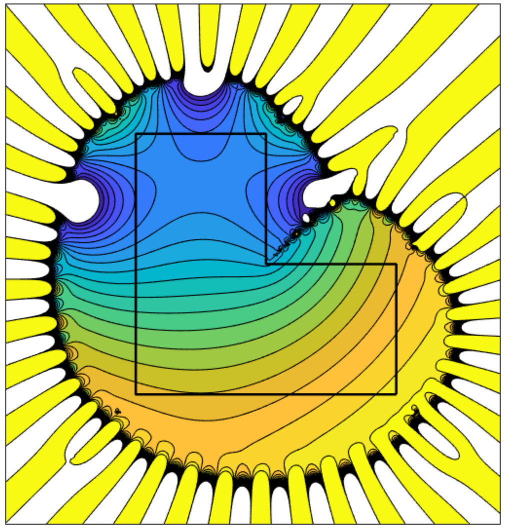

Paper to appear in the proceedings, available at my website

Collaborators on rational functions

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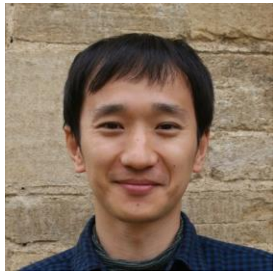

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Three representations for rational approximation on a domain Ω

Quotient of polynomials

$$r(z) = p(z)/q(z)$$

Advantage: mathematically simple
Disadvantage: numerical failure when poles are clustered

Partial fractions

$$r(z) = \sum \frac{a_k}{z - z_k}$$

Advantages: computationally simple
easy to work with the real part (harmonic)
easy to exclude poles from Ω
Disadvantage: where do we put the poles?
→ lightning PDE solvers (2019)

(2)

Barycentric
(= quotient of partial fractions)

$$r(z) = \sum \frac{a_k}{z-z_k} \Big/ \sum \frac{b_k}{z-z_k}$$

Advantages: outstanding numerics if $\{z_k\}$ are well chosen
decoupling of support pts z_k and coeffs a_k, b_k
Disadvantage: no way to exclude poles from Ω
→ AAA rational approximation (2018)

(1)

AAA-LS

(3)

1. Free poles and AAA approximation

AAA (Chebfun, running in MATLAB)

```
Z = rand(2000,1) + 1i*rand(2000,1);
plot(Z,'.k','markersize',4), axis([-1 2 -1.5 1.5]),
axis square
F = sqrt(Z.*(1-Z));
tic, [r,pol] = aaa(F,Z); toc
hold on, plot(pol,'.r','markersize',10)

norm(F-r(Z),inf)

phaseplot(r)
```

AAA algorithm (= "adaptive Antoulas-Anderson")

THE AAA ALGORITHM FOR RATIONAL APPROXIMATION

YUJI NAKATSUKASA*, OLIVIER SÈTE†, AND LLOYD N. TREFETHEN‡

For Jean-Paul Berrut, the pioneer of numerical algorithms based on rational barycentric representations, on his 65th birthday.

SISC 2018

$$r(z) = \frac{n(z)}{d(z)} = \sum_{k=1}^{m} \frac{a_k}{z - z_k} \bigg/ \sum_{k=1}^{m} \frac{b_k}{z - z_k}$$

- Fix $a_k = f_k b_k$, so that we are in "interpolatory mode": $r(z_k) = f_k$.
- Taking $m = 1,2, \dots,$ choose support points z_m one after another.
- Next support point: sample point ζ_i where error $|f_i - r(\zeta_i)|$ is largest.
- Barycentric weights $\{b_k\}$ at each step:
  chosen to minimize linearized least-squares error $||fd - n||$.

AAA is remarkably effective, quickly producing approximations within factor ~ 10 of optimal.
The support points cluster near singularities, giving stability even in extreme cases.

No such fast, flexible methods have existed before.

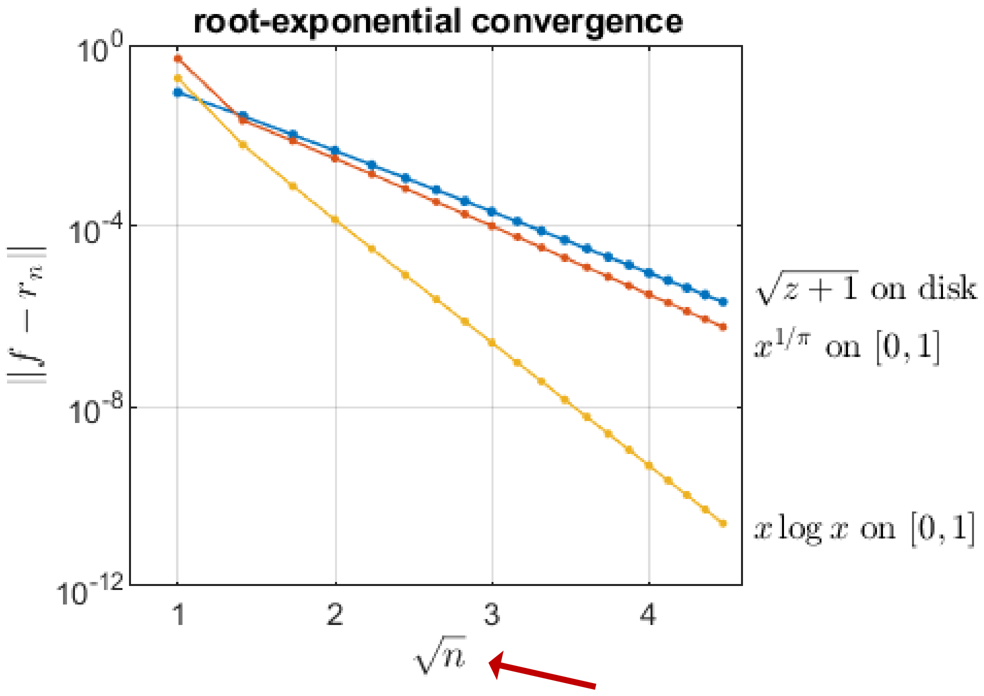
Root-exponential convergence at branch point singularities

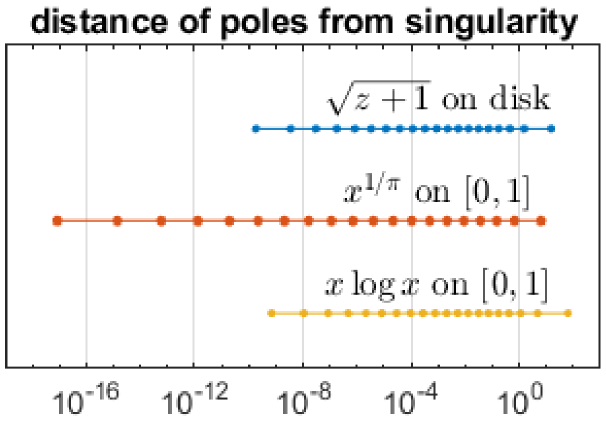
Donald Newman 1964:

$O(\exp(-C\sqrt{n}\,))$ convergence for degree n rational best approximation of $|x|$ on $[-1,1]$ made possible by exponential clustering of poles and zeros near the singularity.

Same result holds for general branch point singularities on boundaries of domains. (Gopal & T., *SINUM* 2019)

Proof: Hermite contour integral formula… potential theory. (Walsh, Gonchar, Rakhmanov, Stahl, Saff, Totik, Aptekarev, Suetin,…)





These data are for best approximations.
AAA would be similar but noisier.

2. Fixed poles and lightning PDE solvers

The idea

Inspired by Newman, we'd like to use AAA to solve Laplace and related PDE problems.
But we don't know how to do AAA for harmonic as opposed to analytic functions.

Kirill Serkh (U. of Toronto) made a suggestion in Sepember 2018.
We know poles should cluster near singularities.
Why not *fix* the poles that way, giving an easy linear approximation problem?

Much of my last three years have been spent developing this idea.

Abi Gopal
Pablo Brubeck
Yuji Nakatsukasa
André Weideman
Stefano Costa
Peter Baddoo

Lightning Laplace solver

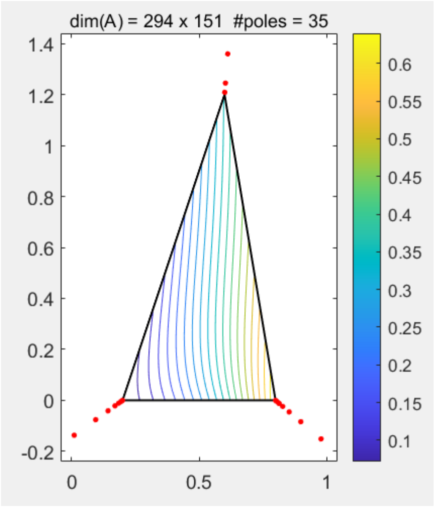
Gopal & T., *SINUM* 2019 and *PNAS* 2019
Software: `people.maths.ox.ac.uk/trefethen/`

Given: Laplace problem $\Delta u = 0$ on a 2D domain with corners.
Corner singularities are inevitable. (Wasow 1957, Lehman 1959)

Approximate $u \approx \mathrm{Re}(r)$ by matching boundary data by linear least-squares,
where r has fixed poles exponentially clustered at the corners.

$$r(z) = \sum_{j=1}^{n_1} \frac{a_j}{z - z_j} + p_{n_2}(z)$$

"Newman + Runge",
a partial fractions representation
plus a polynomial term



`laplace([.2 .8 .6+1.2i])`

An error bound comes from the maximum principle.
The harmonic conjugate also comes for free: Hilbert transform or
Dirichlet-to-Neumann map.

This is a variant of the Method of Fundamental Solutions, but with exponential clustering and complex poles instead of logarithmic point charges.
(Kupradze, Bogomolny, Katsurada, Karageoghis, Fairweather, Barnett & Betcke, …)

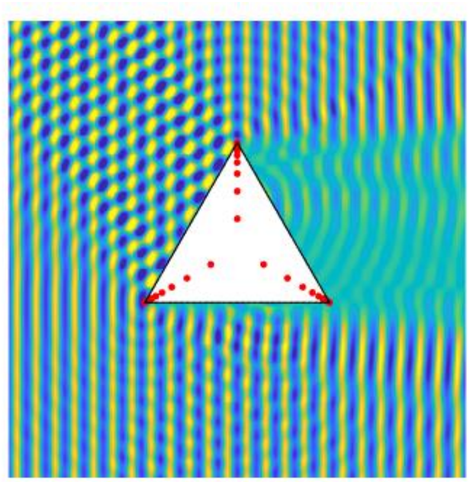
Lightning Helmholtz solver

(Gopal & T., *PNAS*, 2019)

Helmholtz eq. $\Delta u + k^2 u = 0.$

Instead of sums of simple poles $(z - z_j)^{-1}$, use sums of complex Hankel functions $H_1(k|z - z_j|)\,\exp(\pm i \arg(z - z_j)).$

Root-exponential convergence to 10 digits.



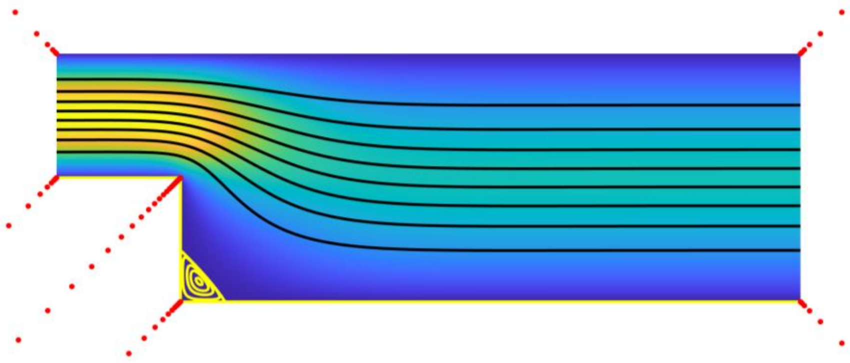
Lightning Stokes solver

(Brubeck & T., *SISC*, submitted)

Biharmonic eq. $\Delta^2 u = 0.$

Reduce to Laplace problems via Goursat representation $u = \mathrm{Re}(\,\overline{z} f + g).$

Root-exponential convergence to 10 digits.



Lightning Stokes solver — triangular lid-driven cavity

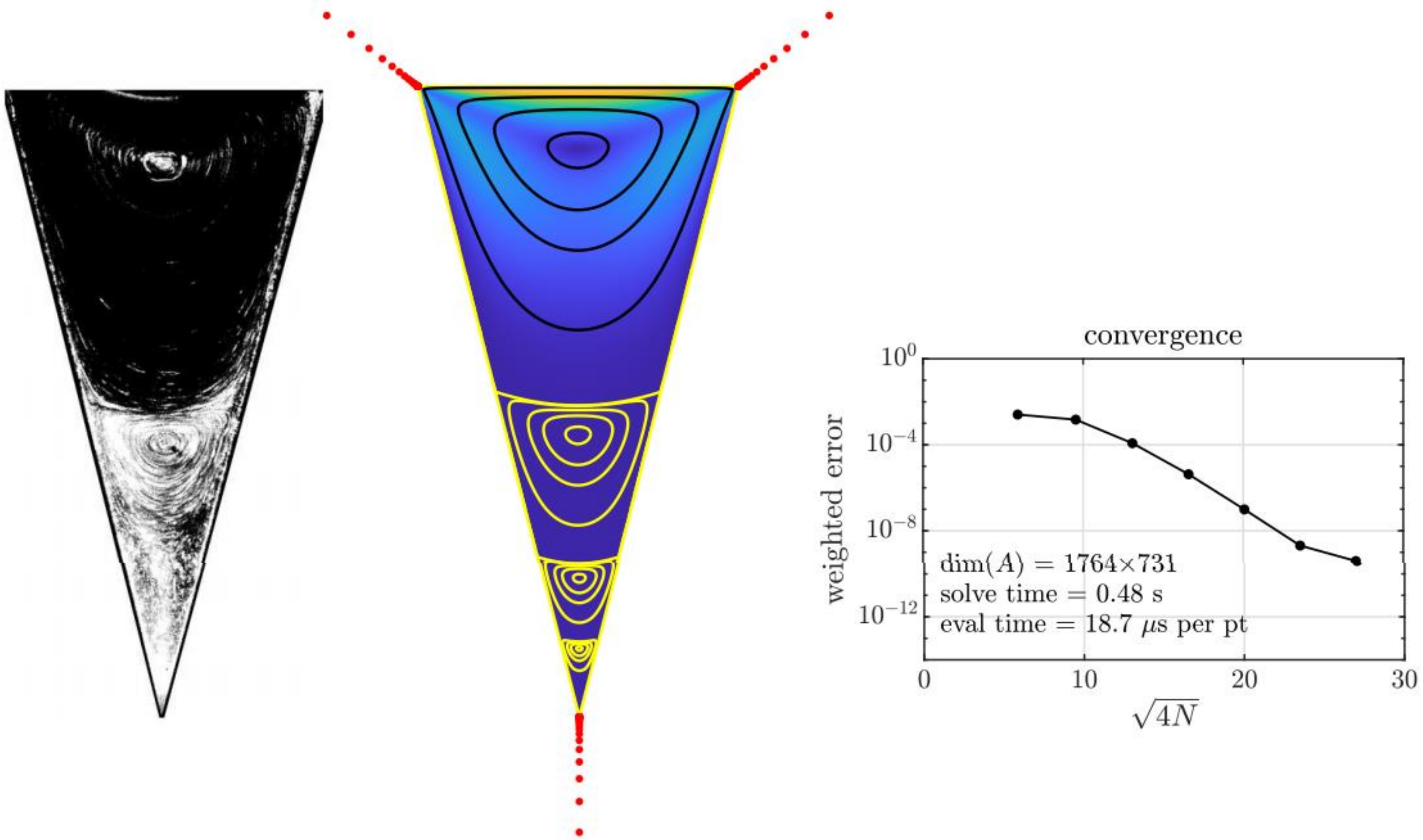


FIG. 5.4. *Stokes flow in a triangular lid-driven cavity of vertex angle* $2\alpha = 28.5°$. *There are* 49 *poles at each corner, of which* 7 *at the lower corner and* 5 *at each upper corner lie outside the plotting axes. The computed result matches Taneda's experiment from* 1979 [35].

```
laplace('L');
laplace('L', 'tol', 1e-10);
laplace('iso');
laplace(12);

helm(20)
helm(-40)

stokes
```

3. New algorithm: AAA-LS

= Adaptive Antoulas-Anderson—Least-Squares

Laplace problem: given Ω and real bndry data h, find u s.t. $\Delta u = 0$ in Ω and $u = h$ on $\partial\Omega$.

AAA-LS finds a complex rational function r s.t. $||f - r|| < \varepsilon$ on $\partial\Omega$, discards poles in $\overline{\Omega}$, then computes a least-squares fit to $\mathrm{u} \approx h$ by real parts of the remaining poles.

AAA-LS LAPLACE SOLVER

(1) Run AAA to get rational approx $r \approx h$ with poles both in and outside Ω.
(2) Discard poles in $\overline{\Omega}$.
(3) Solve $Ax \approx b$ to construct a new fit involving just the poles outside $\overline{\Omega}$.

barycentric
↓
partial fractions

Core code, given column vectors **Z**, **H** of sample pts and data, row vector **pol** of poles.

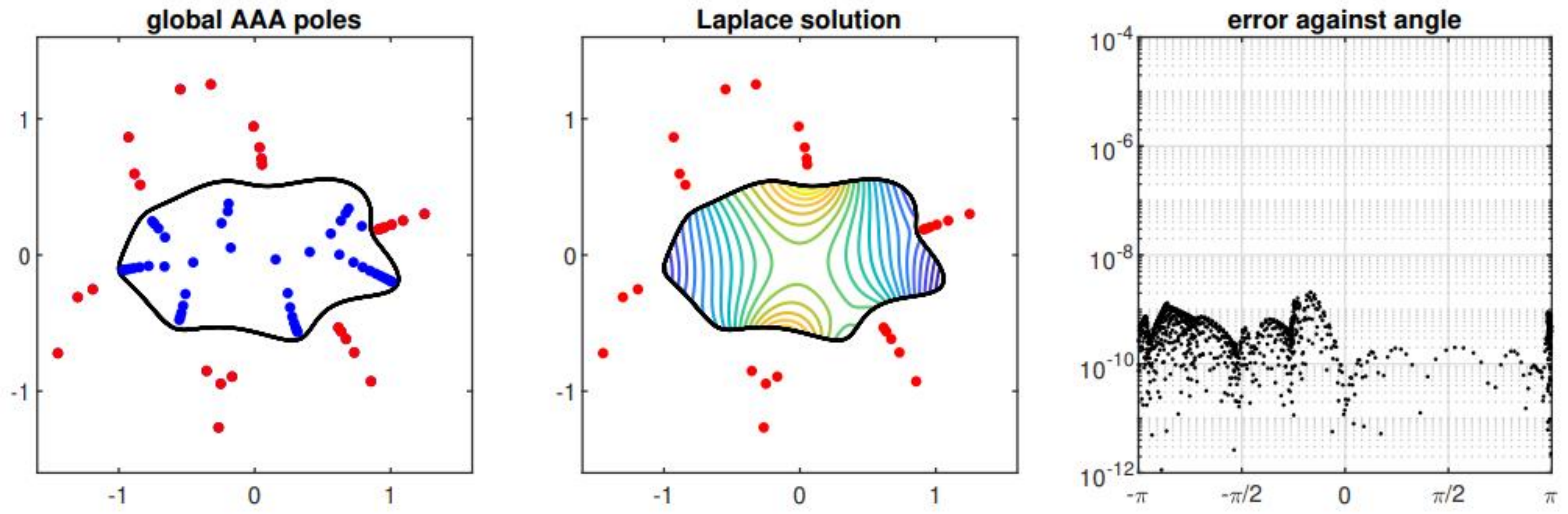
```
d = min(abs(Z-pol),[],1);                % for column normalization
P = Z.^(0:n); Q = d./(Z-pol);            % polynomial & rational columns
A = [real(P) real(Q) -imag(P) -imag(Q)]; % fitting matrix
c = reshape(A\H),[],2)*[1;1i];           % least-squares solve
```

better stability: use Vandermonde with Arnoldi orthogonalization for polynomial term

FASTER "LOCAL AAA-LS" VARIANT

(1') Use separate AAA fits near different corners or other singularities.

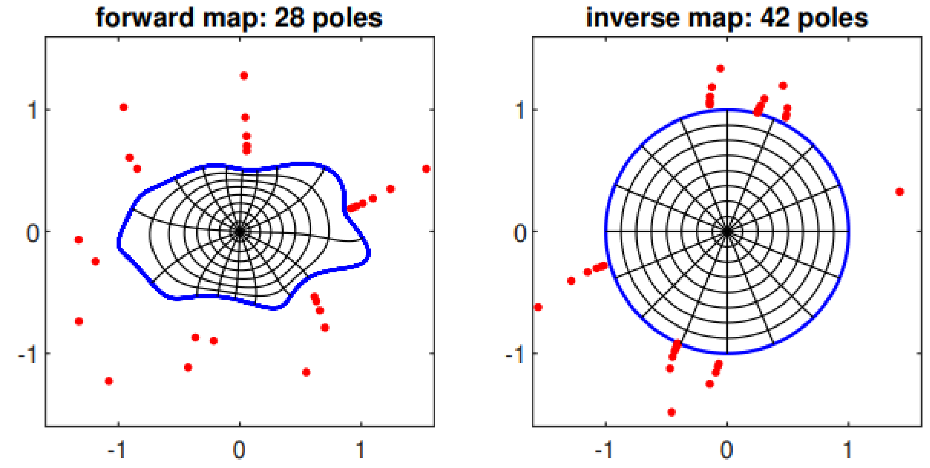
AAA-LS example: smooth domain



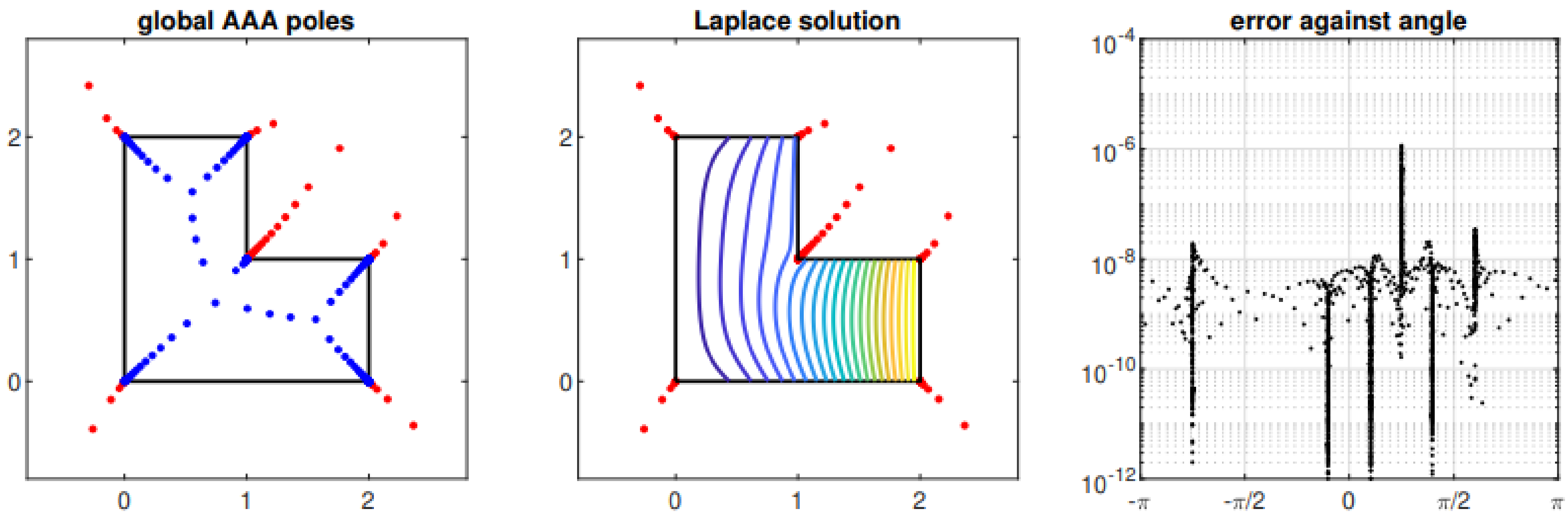
global variant

46 poles inside, discarded.
30 poles outside, retained.
9-digit accuracy in 0.7 secs.

From a Laplace solver it's an
easy step to conformal mapping.

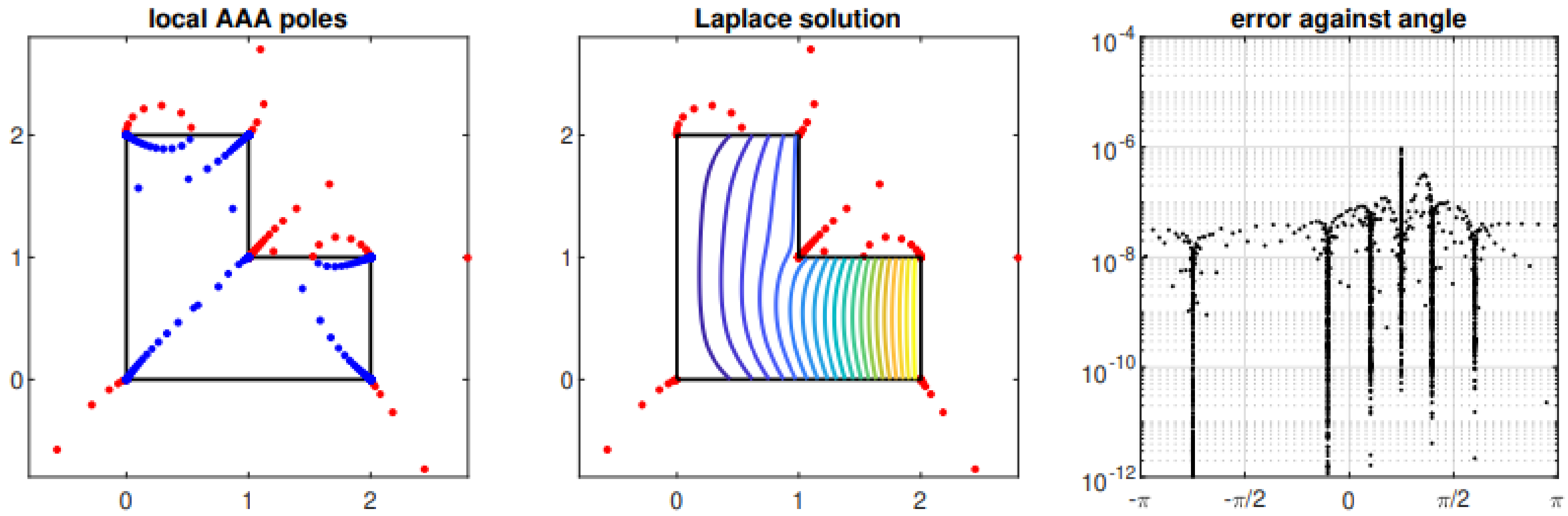


AAA-LS example: L-shaped domain



global variant

12 secs. (global AAA, 294 poles)

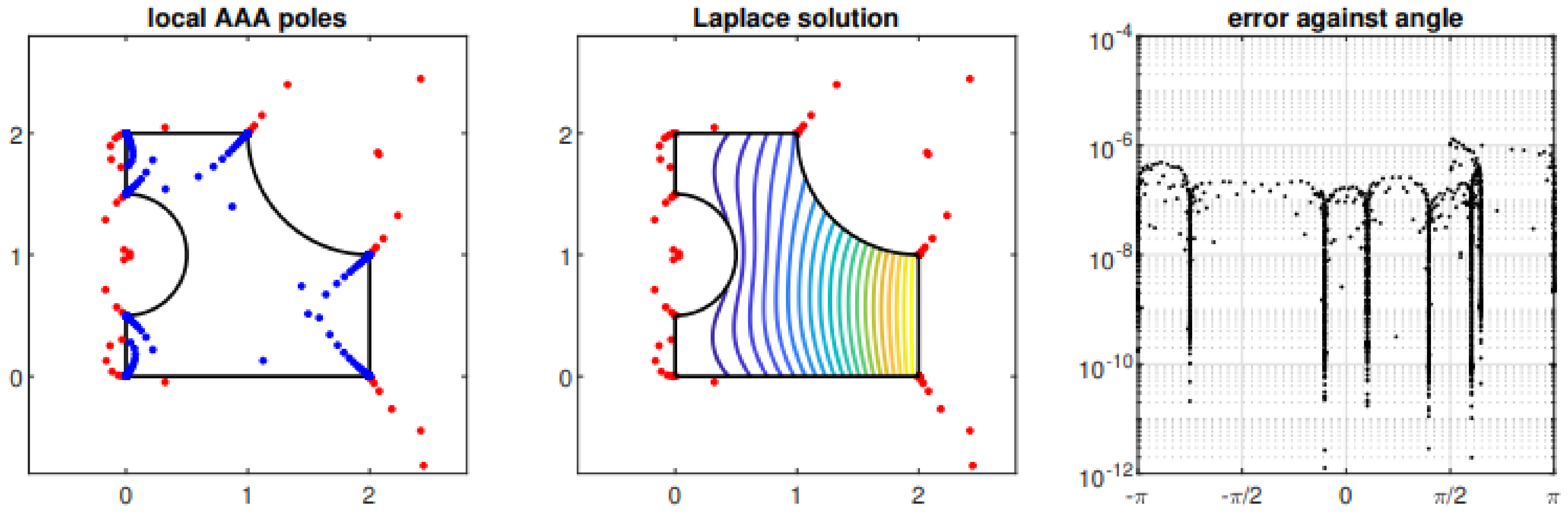


local variant

0.7 secs. (6 local AAA fits)

NA Digest test value
$u(.99 + .99i) \approx 1.0267919261$
accurate to 10 digits.

AAA-LS example: domain with curved sides

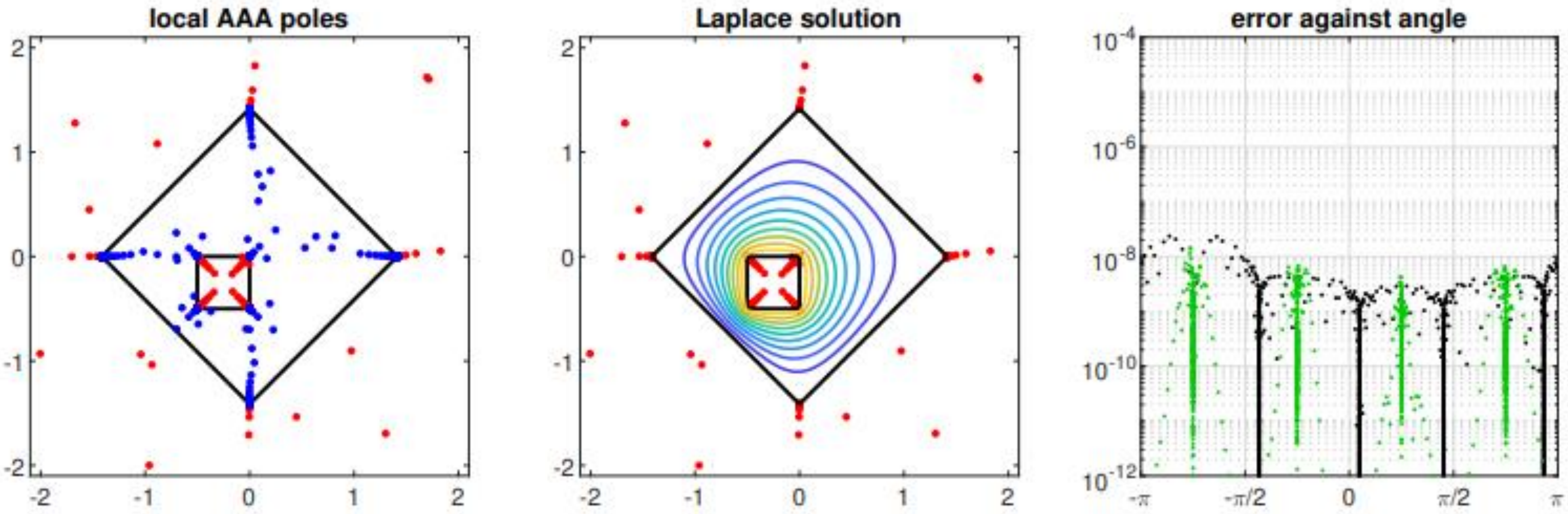


local variant

102 poles outside.
6-digit accuracy in 0.5 secs.

No new issues arise with this problem.
These methods converge root-exponentially so long as the boundary is piecewise analytic.

AAA-LS example: doubly connected domain



local variant

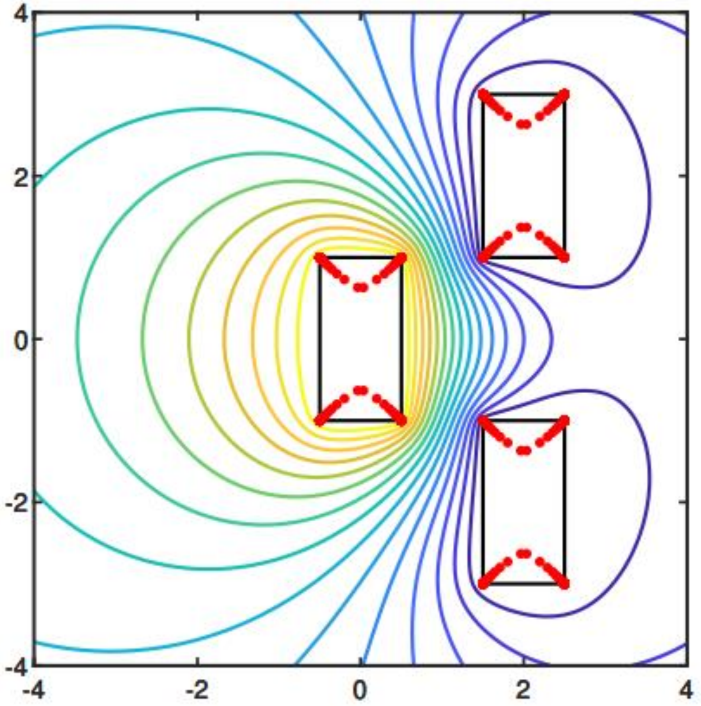
397 poles outside.
8-digit accuracy in 1.7 secs.

Black: outer boundary
Green: inner boundary

To treat the hole, we include polynomials in both $(z - z_c)^{-1}$ and z. (Runge 1865)

We also include a term $\log|z - z_c|$. (Walsh 1929. See Axler in *MAA Monthly* 1986, "Harmonic functions from a complex analysis viewpoint".)

AAA-LS example: exterior domain, triply connected

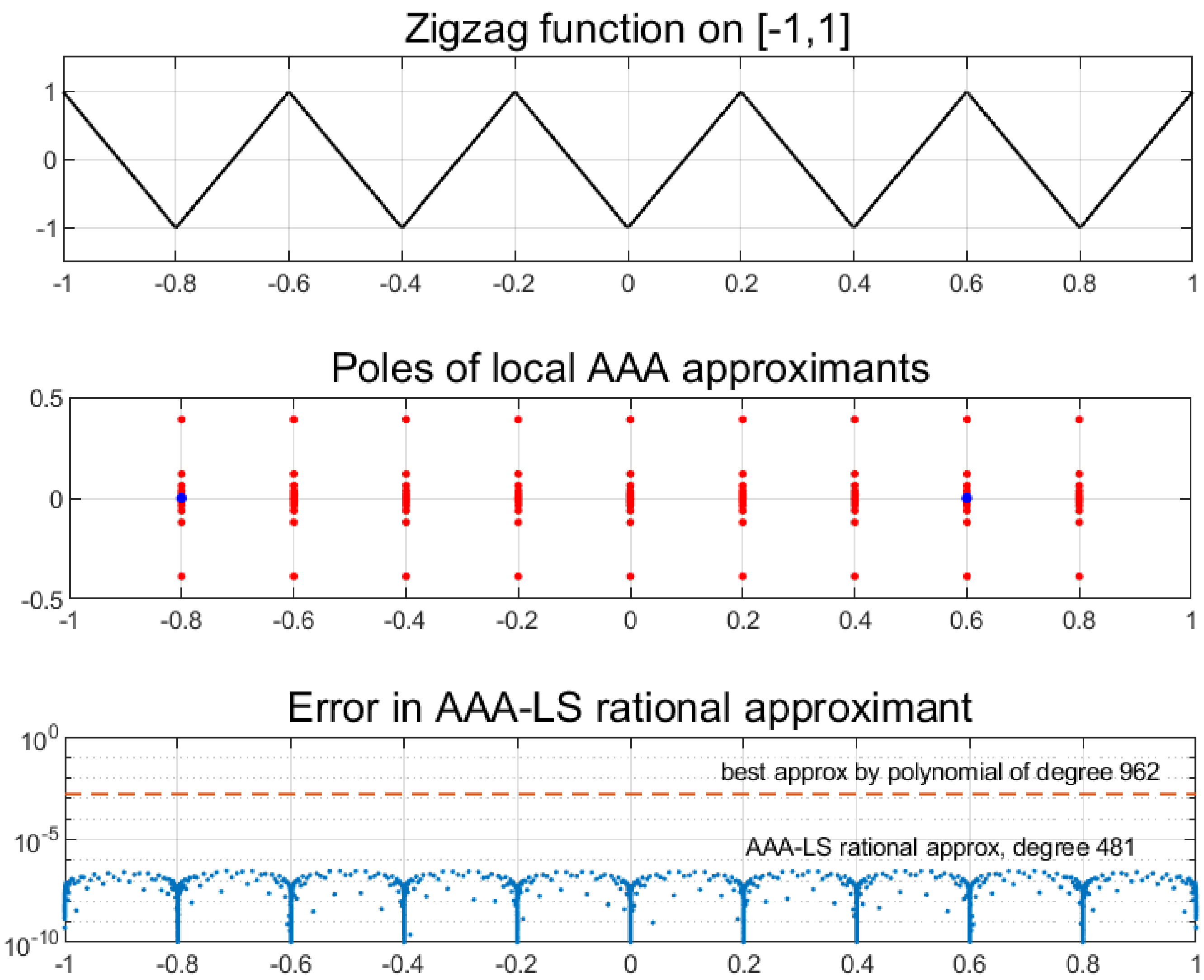


local variant

624 poles outside.
10-digit accuracy at $z = 1$ in 2 secs.

Now there are polynomials in three reciprocals $(z - z_j)^{-1}$, but no polynomial in z.
Also three log terms $\log|z - z_j|$.

AAA-LS example: real zigzag function



local variant

466 finite poles.
962 total degrees of freedom.
2 poles in $[-1,1]$ are discarded.
7-digit accuracy in 0.7 secs.

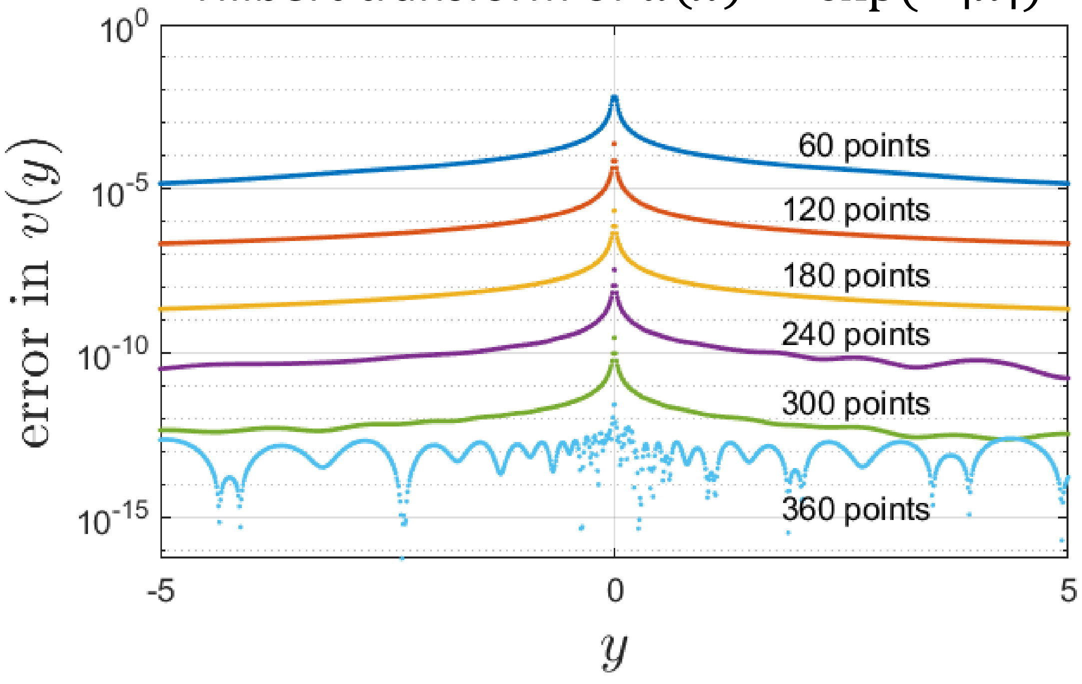
AAA-LS for computing the Hilbert transform on the real line

Hilbert transform ≈ principal value integral ≈ harmonic conjugate ≈ Dirichlet-to-Neumann map.
Comes for free from any rational approximation of a real function u.

Prototype code

```
function [v,f] = ht(u)
X = logspace(-10,10,300)'; X = [X; -X];
[~,pol] = aaa(u(X),X,'cleanup',0);
pol(imag(pol)>=0) = []; pol = pol.';
d = min(abs(X-pol),[],1);
A = d./(X-pol); A = [real(A) -imag(A)];
c = reshape(A\u(X),[],2)*[1;1i];
f = @(x) reshape((d./(x(:)-pol))*c,size(x));
v = @(x) imag(f(x));
```

Hilbert transform of $u(x) = \exp(-|x|)$



This plot was produced in 2 secs.

AAA-LS theory

Laplace problem: given Ω and real bndry data h, find u s.t. $\Delta u = 0$ in Ω and $u = h$ on $\partial\Omega$.

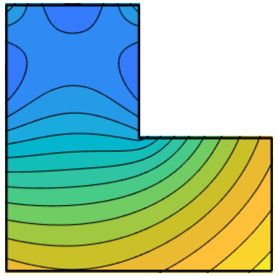
AAA-LS (the global variant) finds a complex rational function r s.t. $||f - r|| < \varepsilon$ on $\partial\Omega$, discards poles in $\overline{\Omega}$, and computes a least-squares fit to h by real parts of the remaining poles.

Theorem. *If Ω is a disk or half-plane, this method gives accuracy $< 2\varepsilon$.*

For a precise statement and proof, see the paper.

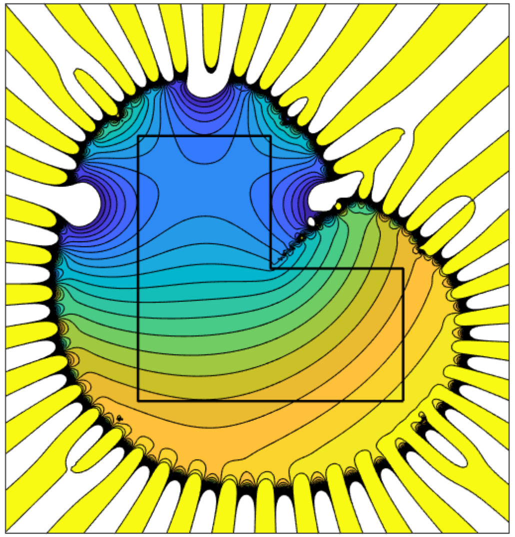
If Ω is not a disk or half-plane, examples show that the method can fail, but it appears such examples are nongeneric. Further investigation needed.

Integral equations vs. rational functions for solving PDEs



Integral equation methods compute a continuous charge distribution
on the boundary, uniquely determined.
The integrals are singular, treated by clever quadrature.
The solution is evaluated by further integrals.

(Barnett, Betcke, Bremer, Bruno, Bystricky, Chandler-Wilde, Gillman, Greengard, Helsing, Hewitt, Hiptmair, Hoskins, Klöckner, Martinsson, Ojala, O'Neil, Rachh, Rokhlin, Serkh, Tornberg, Ying, Zorin,…)



AAA/Lightning methods compute a discrete charge distribution
outside the boundary, nonunique (redundant bases).
This is done by linear least-squares with no special quadrature.
The solution is evaluated by an explicit formula.

Note the branch cut, which the computation captures by a string of poles.
The yellow stripes come from the polynomial "Runge" term (cf. Jentzsch's thm).

These rational approximations are prototypes of "thinking beyond the boundary." I believe we'll see more of that in the years ahead. With luck, maybe even in 3D.

In closing: what is a function?

"18th century view": singularities nowhere

Default assumption: analytic.
Use polynomials and aim for exponential convergence.

"20th century view": singularities everywhere

Default assumption: continuous.
Real analysis is built on this, with regularity as the central concern.
Likewise much of numerical analysis (finite elements, Sobolev spaces,…).
Use piecewise polynomials. Convergence rates will be limited by regularity.

"Applied mathematics view": singularities here and there

Default assumption: analytic except for isolated singularities.
Sometimes, we can "nail the singularities" and get exponential convergence.
More generally, use rational functions and aim for root-exponential convergence.
Not mentioned in this talk: "log-lightning" approximations with near-exponential convergence.

(Nakatsukasa & T., *SINUM*, submitted; Baddoo & T., in preparation)