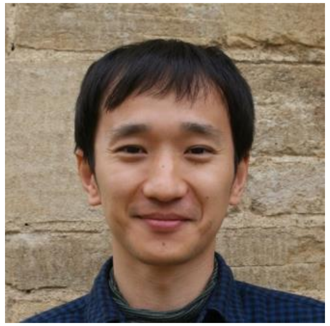
Corner singularities

Nick Trefethen, University of Oxford

Abi Gopal

André Weideman

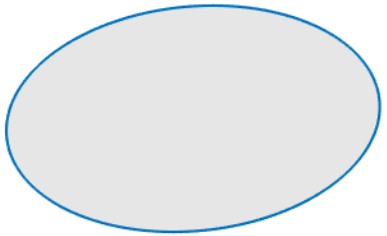
Pablo Brubeck



Yuji Nakatsukasa

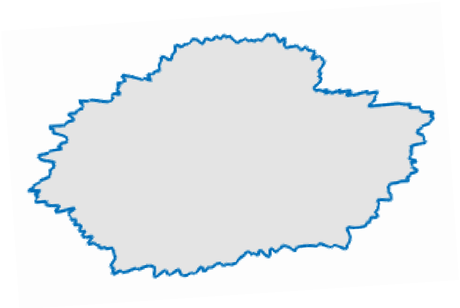
Kirill Serkh

Some problems are smooth.
Computations converge exponentially.



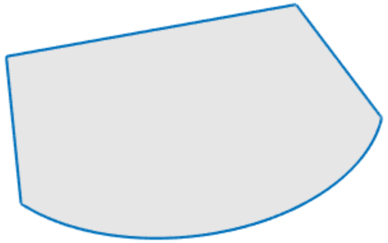
“18th century mathematics”

Some problems are not smooth.
Computations converge algebraically.



“20th century mathematics”

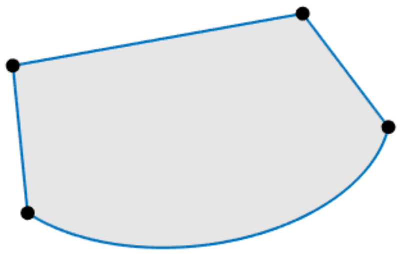
In practice, it’s usually a mix.
What are our options?



Analytic apart from isolated singularities.
In 2D, this means corner singularities.

~~multiscale~~ → twoscale

How to cope with corner singularities?



(1) Eliminate them analytically.

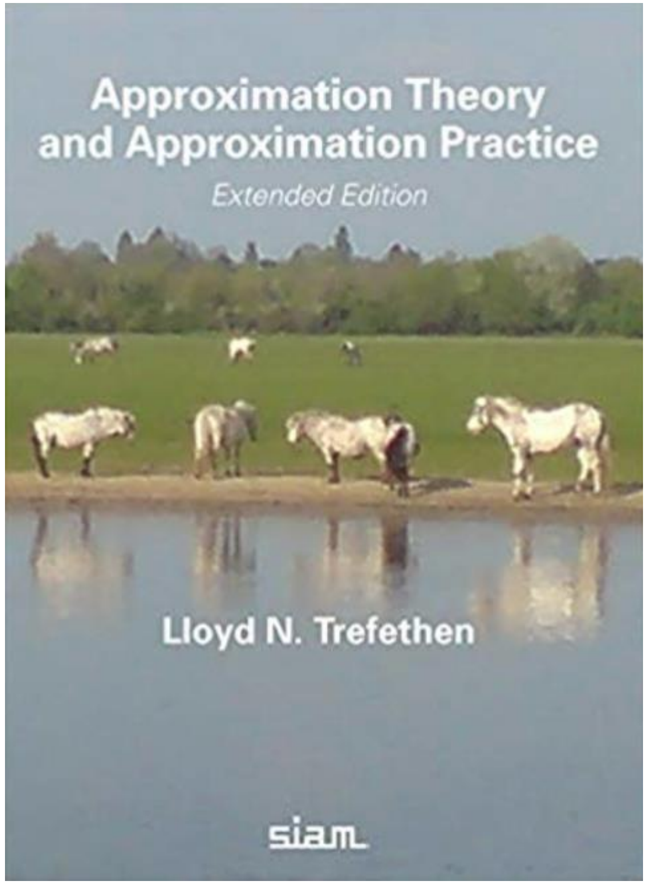
Allows exponential convergence at the cost of case-by-case analysis.
Fragile if the problem changes.

- Gauss-Jacobi quadrature — Works for integrand x^α, but what about $x^\alpha \log x$?
- Schwarz-Christoffel mapping — Works for polygons, but what if a side is curved?

(2) Resolve them with fast-converging approximations.

No analysis needed. Nearly as fast?
Robust if the problem changes.

- Generalized Gauss quadrature — Bremer, Gimbutas, Rokhlin, Serkh, ….
- Lightning and log-lightning approximations — This talk.



25. Two Famous Problems

Famous problem #1: Newman 1964

Rational approximation of $|x|$ on $[-1,1]$: root-exponential convergence.
→ lightning approximation. Gopal & T., *SINUM* 2019.

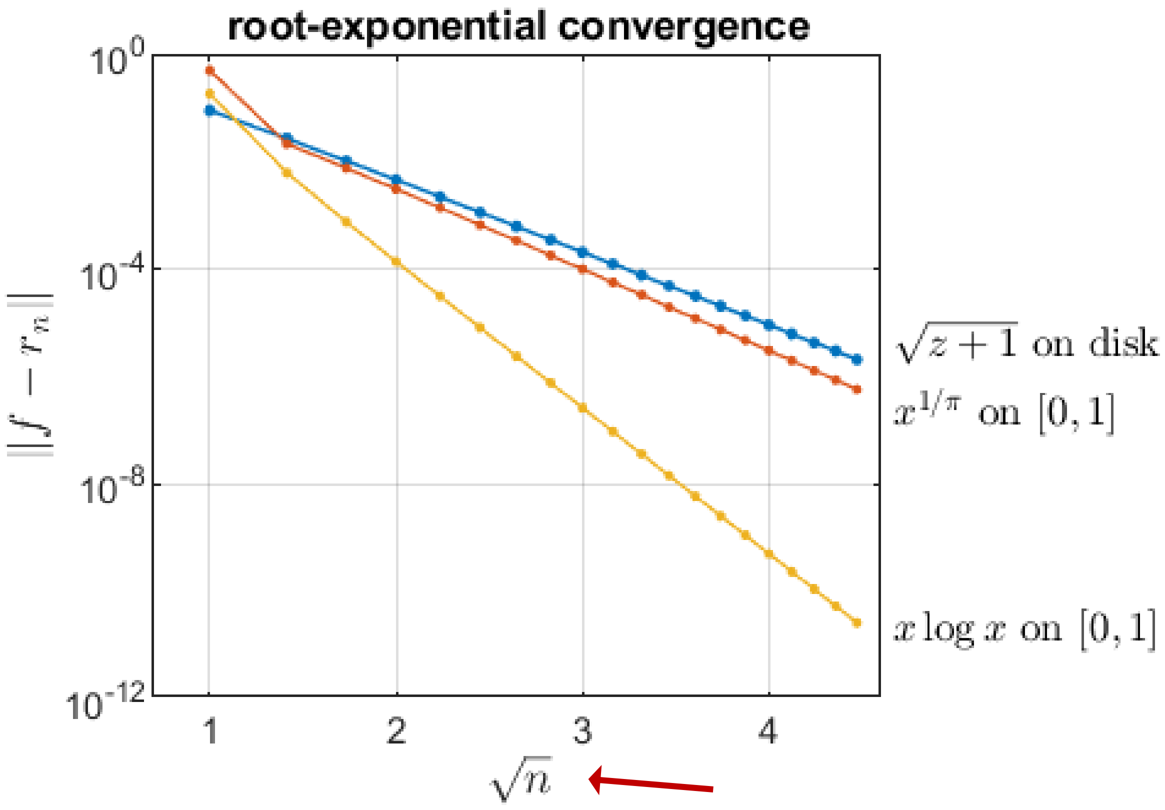
Famous problem #2: Cody, Meinardus & Varga 1969

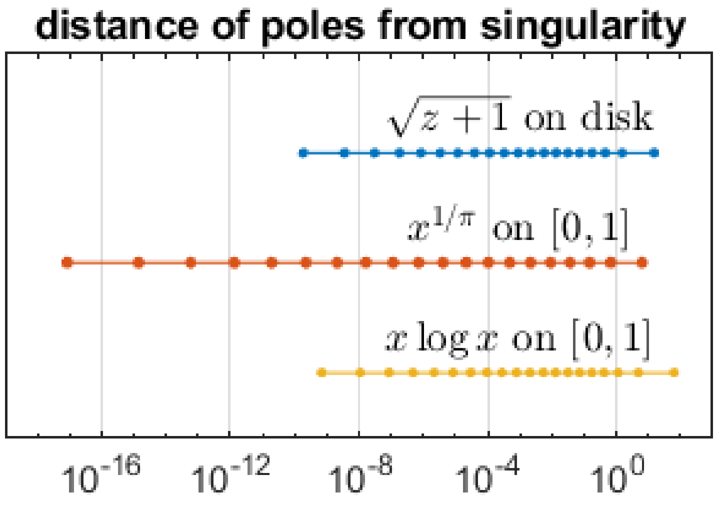
Rational approximation of e^x on $(-\infty, 0]$: exponential convergence.
→ log-lightning approximation. Nakatsukasa & T., in preparation.

1. Lightning approximation

Newman effect: $O(\exp(-C\sqrt{n}\,))$ convergence for rational approximation of branch point boundary singularities, made possible by exponential clustering of poles and zeros.

Proofs: Hermite contour integral formula… potential theory. (Gopal & T., *SINUM* 2019, building on Walsh, Gonchar, Rakhmanov, Stahl, Saff, Totik, Aptekarev, Suetin,…)

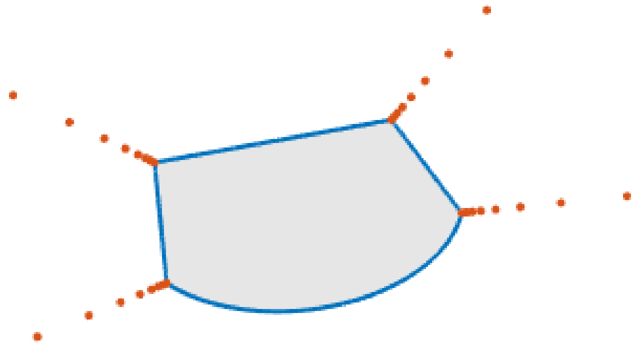




K. Serkh had the idea (September 2018).

We know that good approximations have exponentially clustered poles.

How about prescribing such poles and then getting coefficients
for approximations by linear least-squares fitting?

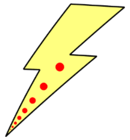


Base application: Laplace problem $\Delta u = 0$ on a domain with corners.

(Corner singularities:
Wasow 1957, Lehman 1959)

$u \approx \mathrm{Re}(r)$, r = rational function.

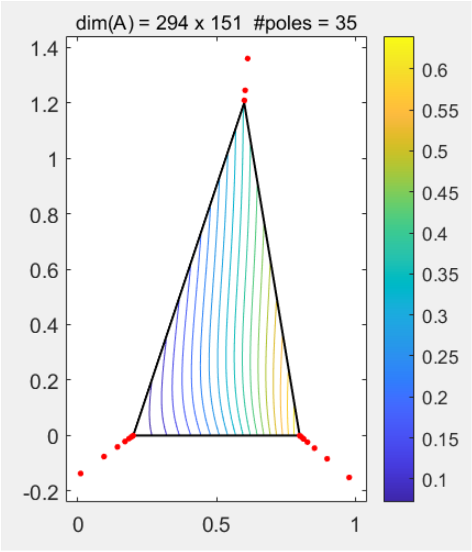
Lightning Laplace solver



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

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

"Newman + Runge“,
a partial fractions representation



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

An error bound comes from the maximum principle.
The harmonic conjugate also comes for free.

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, …)

Demonstration

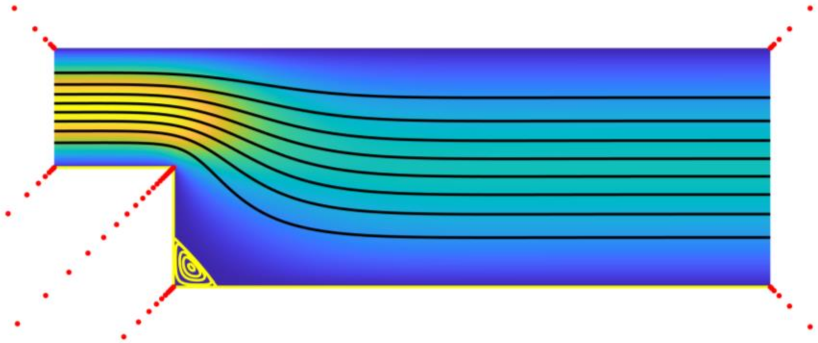
Lightning Stokes solver

(Brubeck & T., work in progress)

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.



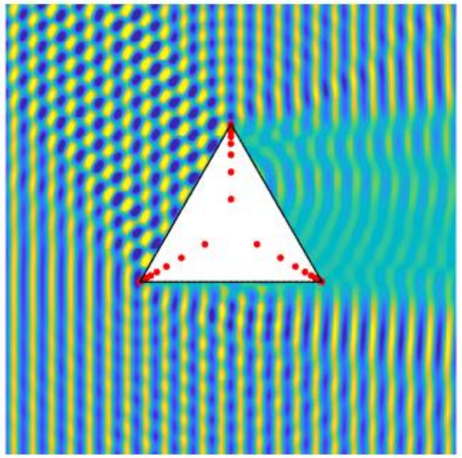
Lightning Helmholtz solver

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

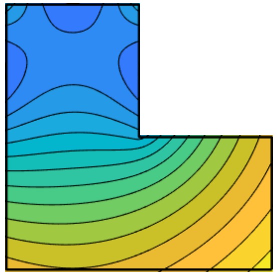
Helmholtz eq. $\Delta u + k^2 u = 0.$

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

Root-exponential convergence to 10 digits.

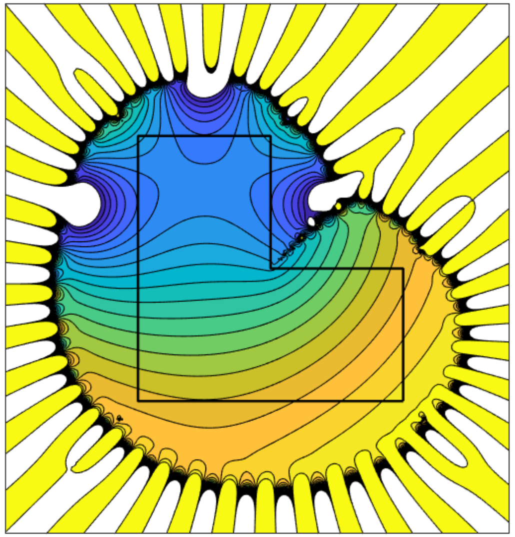


Lightning solvers vs. integral equations



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,...)



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 as an explicit formula.

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

2. Log-lightning approximation

A new idea came along two months ago.

Change from rational to reciprocal-log approximation.

Convergence rate may speed up to exponential !

Singularity at 0: $$g(z) = c_0 + \sum_{k=1}^{n} \frac{c_k}{\log(z) - s_k}$$

Singularities at $z_1 \ldots, z_m$: $$g(z) = \sum_{j=1}^{m} \sum_{k=1}^{n_j} \frac{c_{jk}}{\log(z - z_j) - s_{jk}} + p_0(z)$$

Why should this work?

Suppose we want to approximate z^a on $[0,1]$.

Change variables: $s = \log(z)$, $z = e^s$.

You get approximation of e^{as} on $(-\infty, 0]$. → Famous problem #2 !
Exponential convergence.

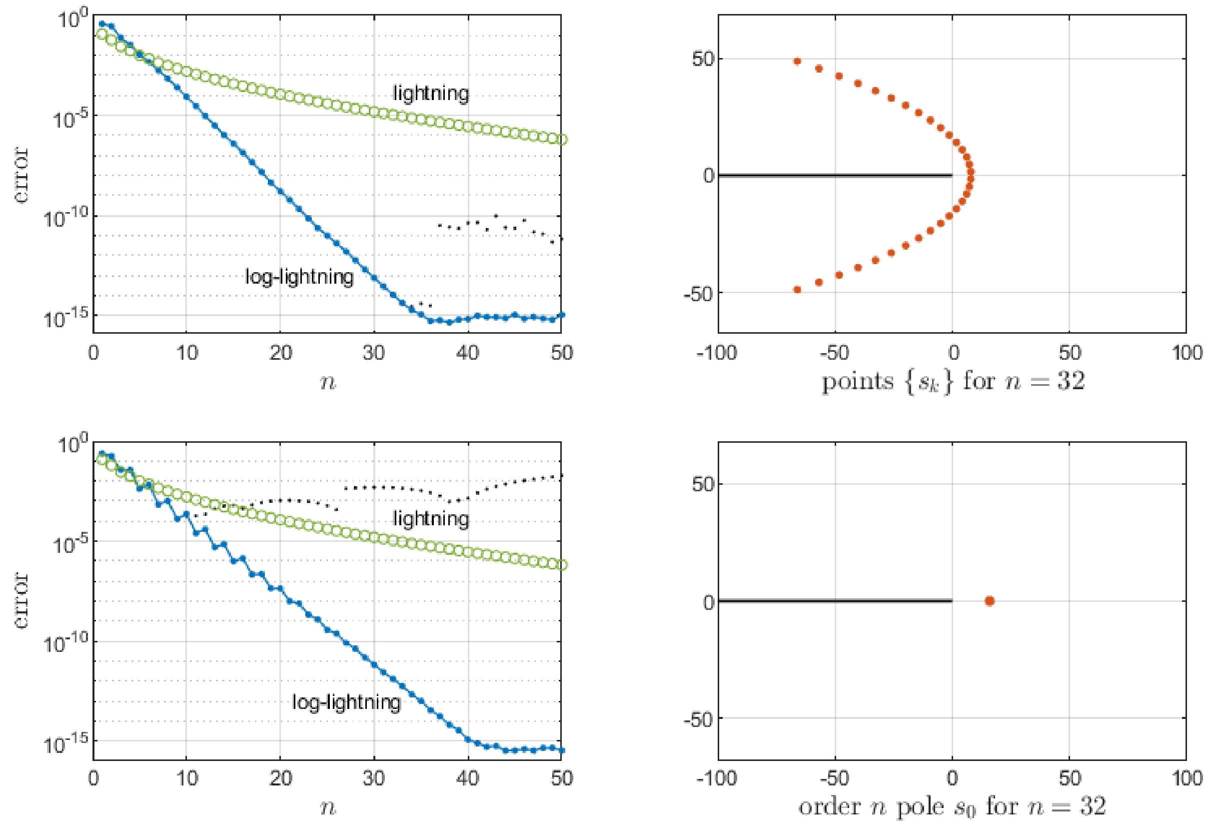
$$e^{as} \approx \sum_{k=1}^{n} \frac{c_k}{s - s_k} \quad \Longleftrightarrow \quad z^a \approx \sum_{k=1}^{n} \frac{c_k}{\log(z) - s_k}$$

RATIONAL APROXIMATION ON $(-\infty, 0]$

RECIPROCAL-LOG APROXIMATION ON $[0,1]$

Log-lightning approximation of $\sqrt{x}$ on $[0,1]$

$$g(z) = c_0 + \sum_{k=1}^{n} \frac{c_k}{\log(z) - s_k}$$



← singularities $\{s_k\}$ on a Hankel contour

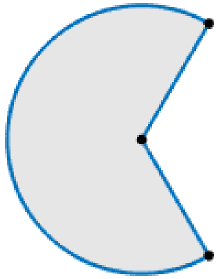
← confluent singularities $\{s_k\}$

Numerical stability: Vandermonde + Arnoldi = Stieltjes orthogonalization.
Black dots show results if you don't stabilize.

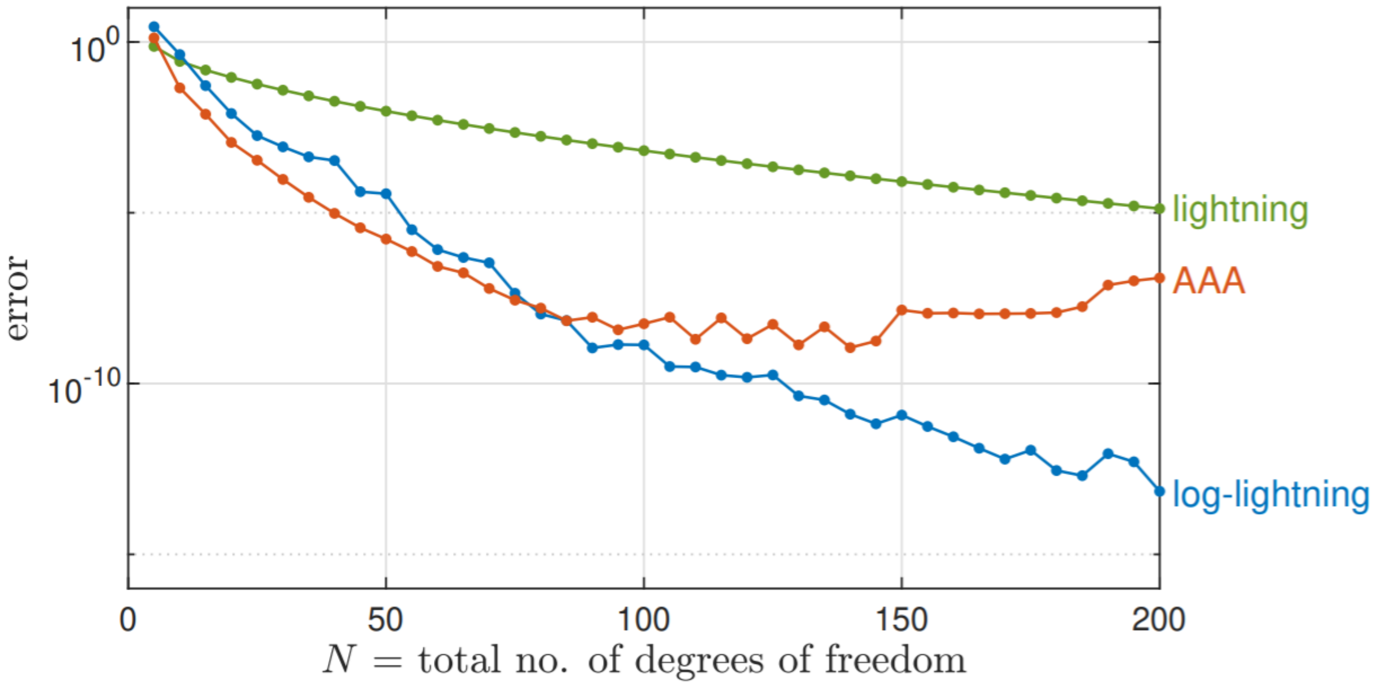
Brubeck, Nakatsukasa & T, *SIREV*, to appear.

Approximation on a planar region with 3 singularities

$$g(z) = \sum_{j=1}^{m} \sum_{k=1}^{n_j} \frac{c_{jk}}{\log(z - z_j) - s_{jk}} + p_0(z)$$

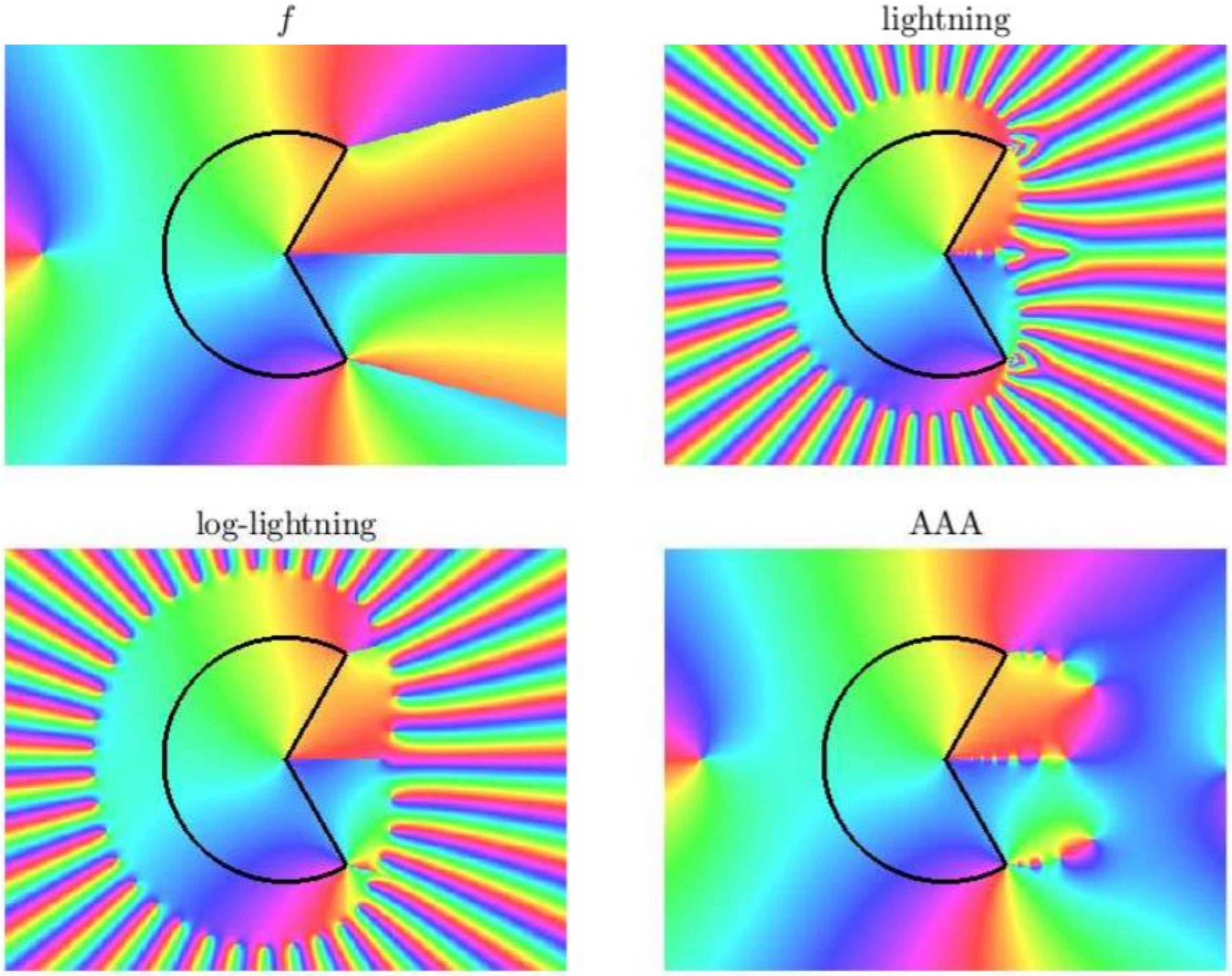


$$f(z) = z \log(-\tfrac{1}{2}z) \cdot (1 - z/\omega)^{1/2} \cdot (1 - z/\bar{\omega})^{3/2}$$



(confluent singularities $\{s_k\}$)

Phase portraits for three approximations, $N = 100$



Theorems

$$g(z) = \sum_{j=1}^{m} \sum_{k=1}^{n_j} \frac{c_{jk}}{\log(z - z_j) - s_{jk}} + p_0(z)$$

Approximation $f \approx g$ on a simply-connected compact set E in the complex plane.

With Hermite integral formula + potential theory we can show:

$\|f - g\|_{\mathrm{E}} = O(\exp(-Cn))$ if f is analytic in the whole plane except for branch points.

The proof uses points $\{e^{s_k}\}$ growing exponentially with n, which may be confluent.

$\|f - g\|_{\mathrm{E}} = O(\exp(-Cn/\log n))$ if f is analytic in a nbhd of E except for branch points.

The proof uses bounded points $\{e^{s_k}\}$, which lie on $O(n)$ sheets of the Riemann surface of f.

3. The amazing Cauchy integral

First we prove convergence for f with a single branch point.

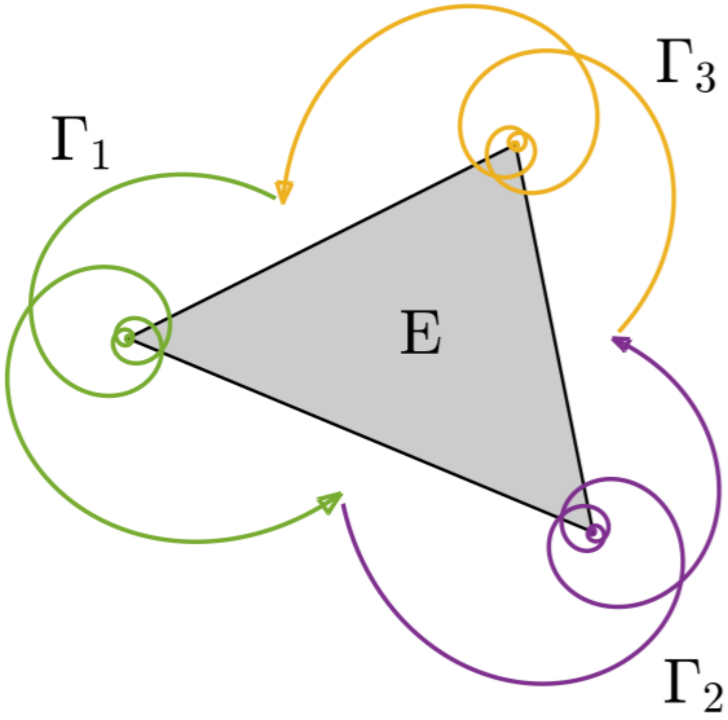
What if f has m branch points?

We break it into m pieces f_k via Cauchy integrals over arcs, a subject full of puzzles and paradoxes.

$$f(z) = \frac{1}{2\pi i}\oint_{\Gamma} \frac{f(t)}{t-z}\,dt$$

$$f = f_1 + \cdots + f_m$$

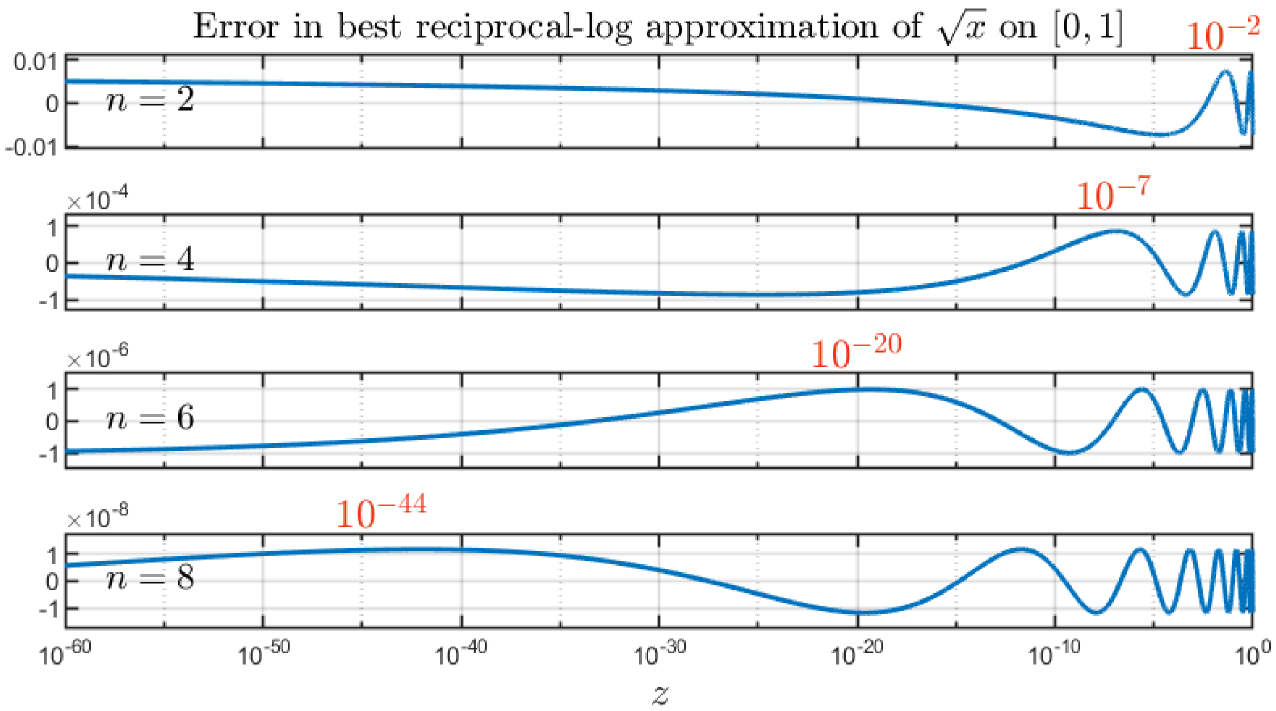
$$f_k(z) = \frac{1}{2\pi i}\int_{\Gamma_k} \frac{f(t)}{t-z}\,dt$$



The arcs Γ_k must be
logarithmic spirals on the Riemann surface of f.

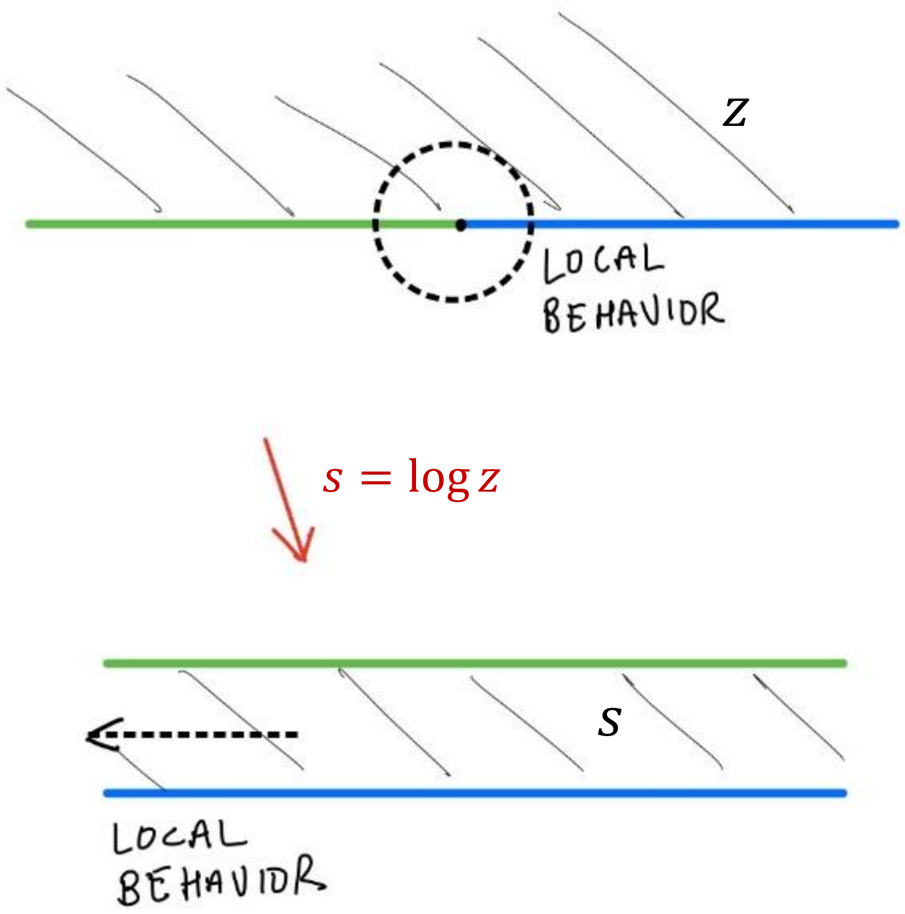
4. The amazing log change of variables

I’ve spent the COVID era analysing singularities.
This has led me to apply $s = \log z$ to everything in sight.
My favorite MATLAB command has become “semilogx”.



Reciprocal-log approximation was born of the log transformation and has some consequently extreme features.

Note e.g. how these extrema are *doubly*-exponentially small.



In the problem space, it may not be obvious that space scales are exponentially decoupled.

Taking the log makes it obvious (St. Venant’s principle).

To appear in *Numer. Math.*:

Exponential node clustering at singularities for rational approximation, quadrature, and PDEs

Lloyd N. Trefethen · Yuji Nakatsukasa · J. A. C. Weideman

Summary

- Reciprocal log approximation: a new problem in approximation theory.
- Exponential/near-exponential convergence, whereas rationals get just root-exponential.
- The approximations exploit analytic continuation onto a Riemann surface (but that's all implicit: calculations happen just on the approximation domain).
- In particular, slit domains are no problem.
- Related mathematics arises with DE (e.g. tanh-sinh) quadrature.
- Application to fast solution of Laplace eq. with corner singularities.
- But we haven't actually tried this yet! — so software is certainly not yet available.
- Beating lightning Laplace may be tough. Evaluating $1/z$ is 3-4 times faster than $\log(z)$.
- Other eqs. such as Helmholtz? We don't know yet.
- 3D? No opinion.

Thank you!