How integral equations help you solve PDEs

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Overview: what is numerical analysis?

Theory, Experiment, Computation: third branch of science

- E.g. in computer, real numbers $\mathbb{R}$ approximated by a finite set F

    'floating point' binary numbers: *e.g.* $0.11010111001 \times 2^{-1101}$

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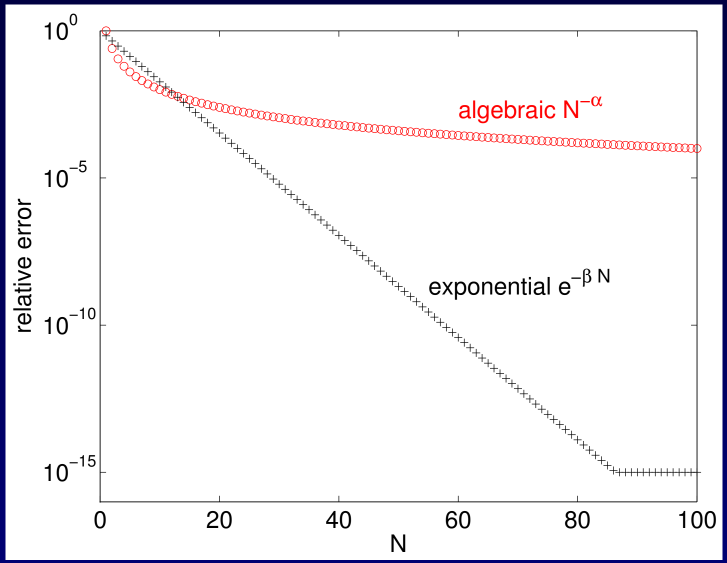

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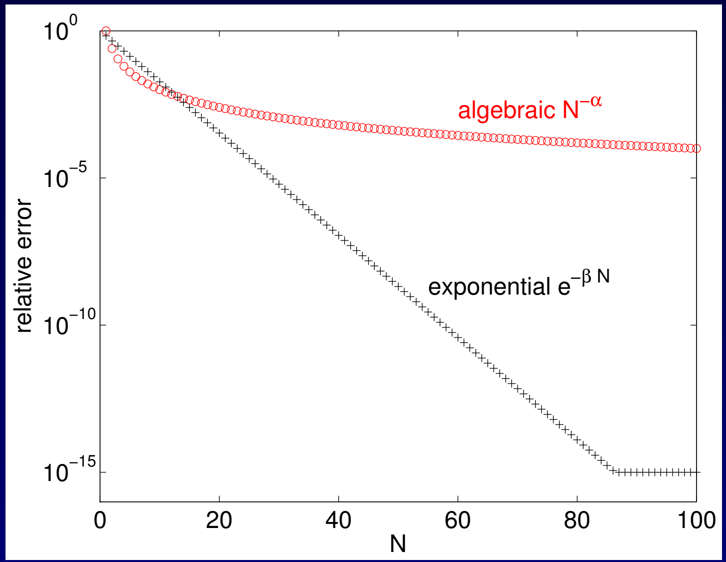

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- Engineering & technology relies on good computational algorithms:
  insensitive to rounding error, rapid convergence, robust, runs fast

Analysis: *proving* useful upper bounds on the error

What is an integral equation?

1D case: $\tau = \tau(x)$ function defined on interval $a \leq x \leq b$

Integral operator K takes function τ to $(K\tau)(x) := \int_a^b k(x,y)\tau(y)dy$

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- Apps: image deconvolution, radiosity (CG), solving PDEs, signals

Numerical solution: discretization to N-by-N linear system $A\boldsymbol{\tau} = \boldsymbol{b}$

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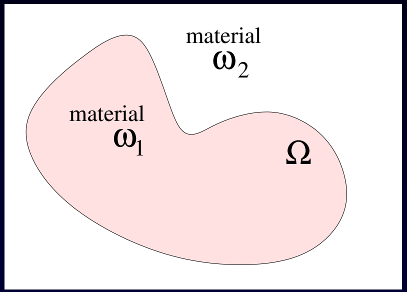
There are also Volterra equations where $(K\tau)(x) := \int_a^x k(x,y)\tau(y)dy$

- Apps: age-structured population models, IVPs. Well-behaved!

Piecewise-constant coefficient PDEs

Ω bounded domain in $\mathbb{R}^d$, $d = 2$ or 3 in most apps



Interior BVP: $\Delta u = 0$ in Ω, $\quad u = f$ on bdry $\partial\Omega$

Laplace operator $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$, const coeff

apps: electrostatics (electron lenses), magnetostatics (eg MRI), heat/diffusion

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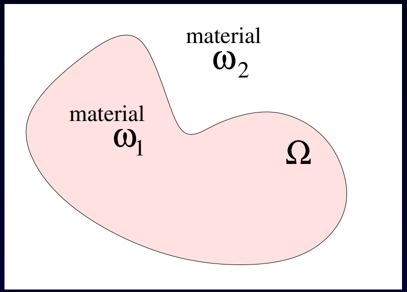

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Piecewise-constant case, composite of 2 or more materials, eg:

$(\Delta + \omega_1^2)u = 0$ in Ω Helmholtz eqn

$(\Delta + \omega_2^2)u = 0$ outside ...also matching/jumps on interfaces

- waves hitting optical devices (glass / air)
- diffuse optical imaging (muscle tissue / fat / tumor)
  modified Helmholtz $(\Delta - \omega^2)u = 0$
- protein configuration energy (molecule interior / water, Laplace)
- elastic modulus of composites (4th-order linear PDE)

Waves at constant frequency, in $\mathbb{R}^2$

waves at constant frequency (wavenumber) ω described by ...

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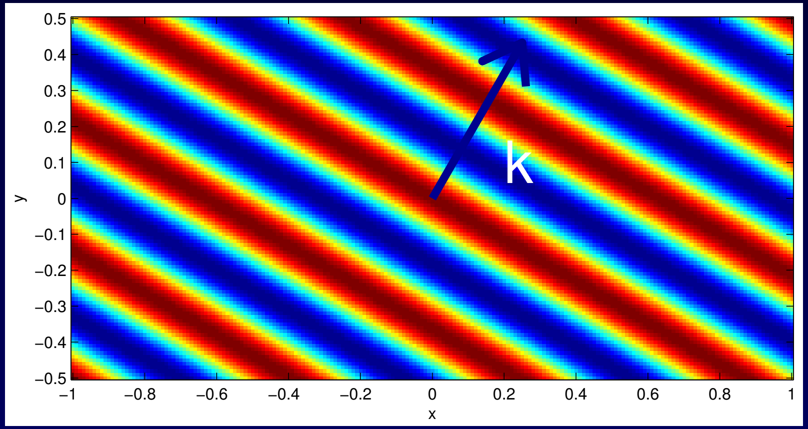
- E.g. plane wave solution

$$u(x, y) = e^{i(k_x x + k_y y)} = e^{i\boldsymbol{k}\cdot\boldsymbol{x}}$$

with $|\boldsymbol{k}| = \omega$



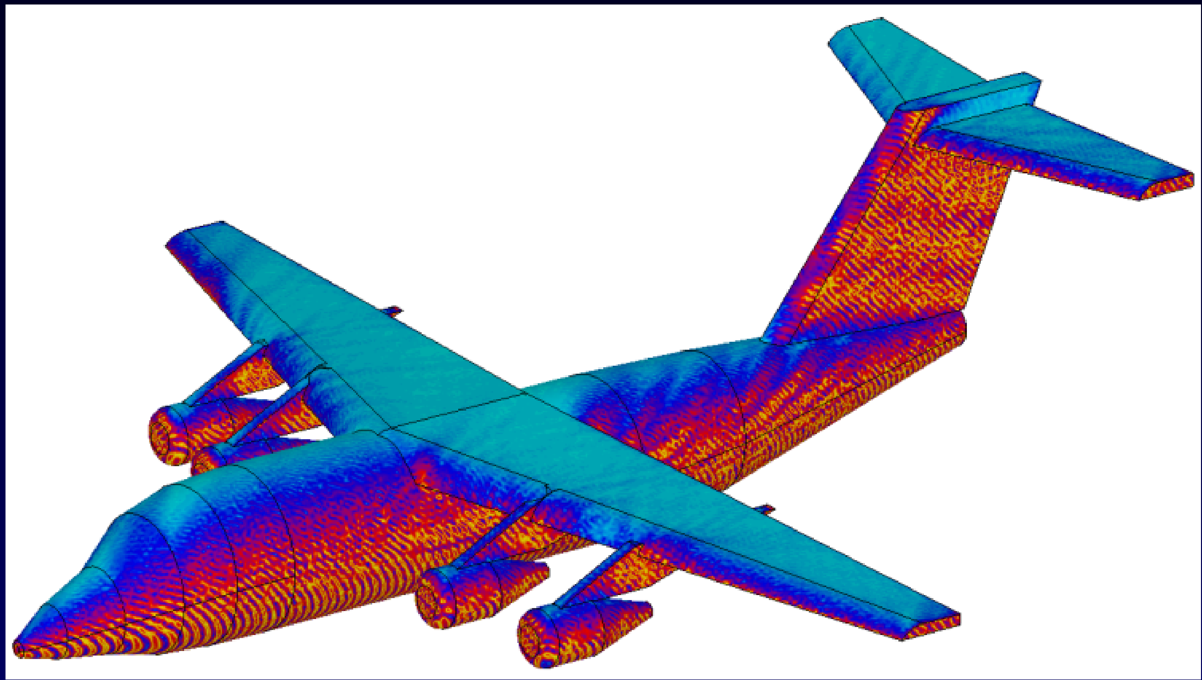
traveling waves from distant source

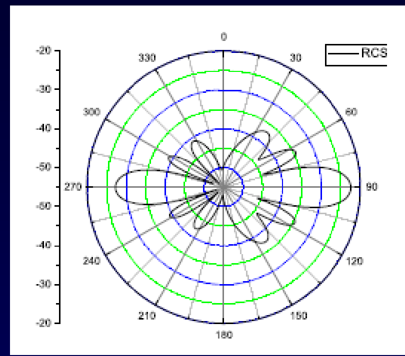
What happens when these waves hit an obstacle? Applications:

- electromagnetics: radar, cellphones, communications
- optics: microscopic devices e.g. internet backbone switches
- acoustics: ultrasound imaging, architectural, musical

Challenges of wave scattering

$\omega \approx$ size of body in wavelengths. $\omega \gg 10^2$ can't be solved via FEM





- backscattered intensity: radar cross section

N unknowns scales as *volume* in wavelengths $O(\omega^3)$ for FEM
N scales only as *surface area* $O(\omega^2)$ for boundary integral eqns (BIE)

- FEM for Helmholtz also has 'pollution error' (BIE doesn't):
  for FEM, number of elements per wavelength must grow to keep accurate

Applications of periodic scattering problems

Diffraction gratings, filters, antennae, meta-materials, solar energy…

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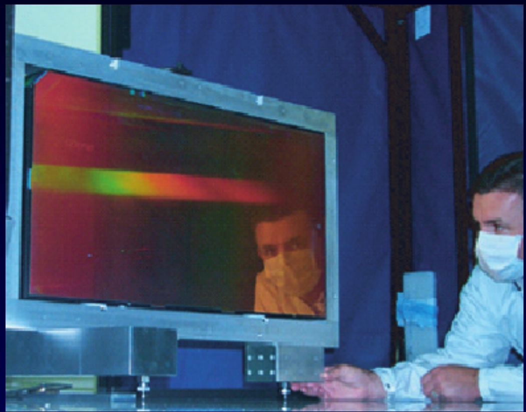
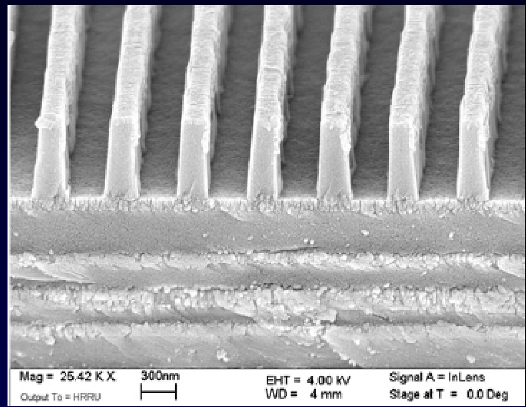


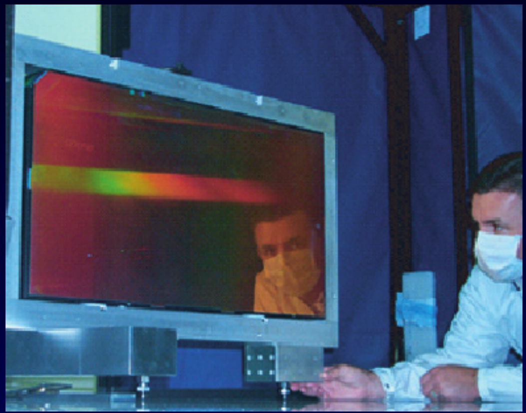


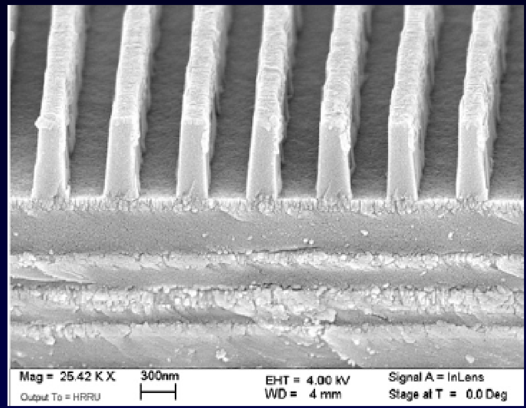
multi-layer dielectric diffraction grating, NIF lasers (LLNL)

2×10^6 periods! (Barty '04)

Applications of periodic scattering problems

Diffraction gratings, filters, antennae, meta-materials, solar energy…





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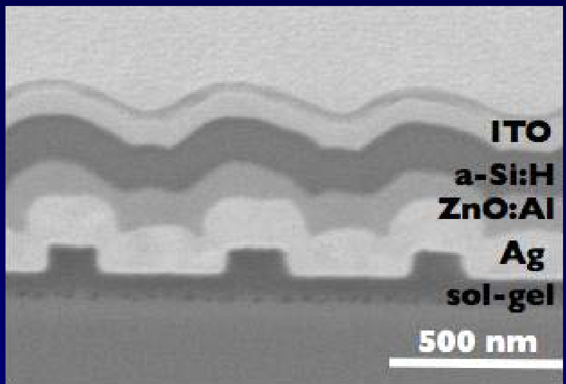
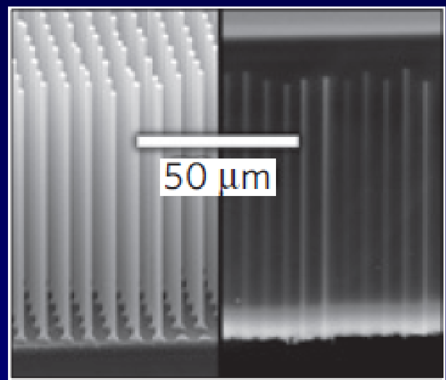


plasmonic solar cell (Atwater ’10)



Si microwires absorber (Kelzenberg ’10)

↕ high aspect ratio

- Design optimization
- Simulation at $>10^3$ inc. angles, frequencies
- Related: photonic crystals which *trap* light inside periodic structures

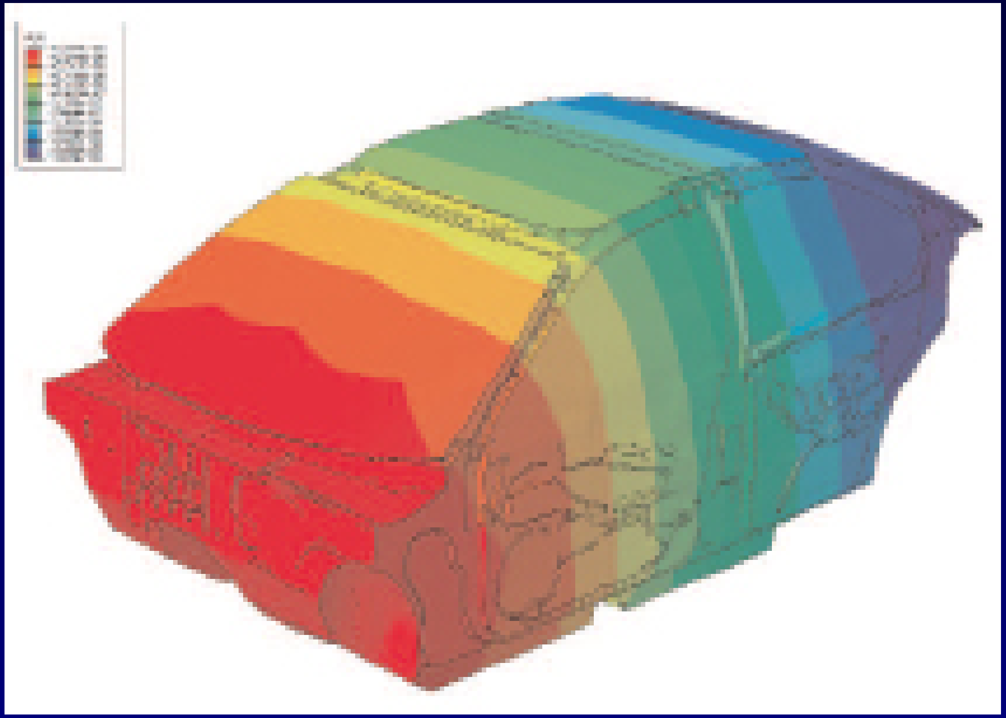
Eigenmodes and applications

$$-\Delta u = \omega^2 u \quad \text{in } \Omega, \qquad u = 0 \text{ on boundary}$$

homogeneous problem ($u = 0$ is always a solution).

For what discrete frequencies $\omega_0 < \omega_1 \leq \omega_2 \cdots$ is non-trivial u possible?

- resonances of cavities (optical, microwave, acoustic, quantum)



automobile interior
acoustic resonance

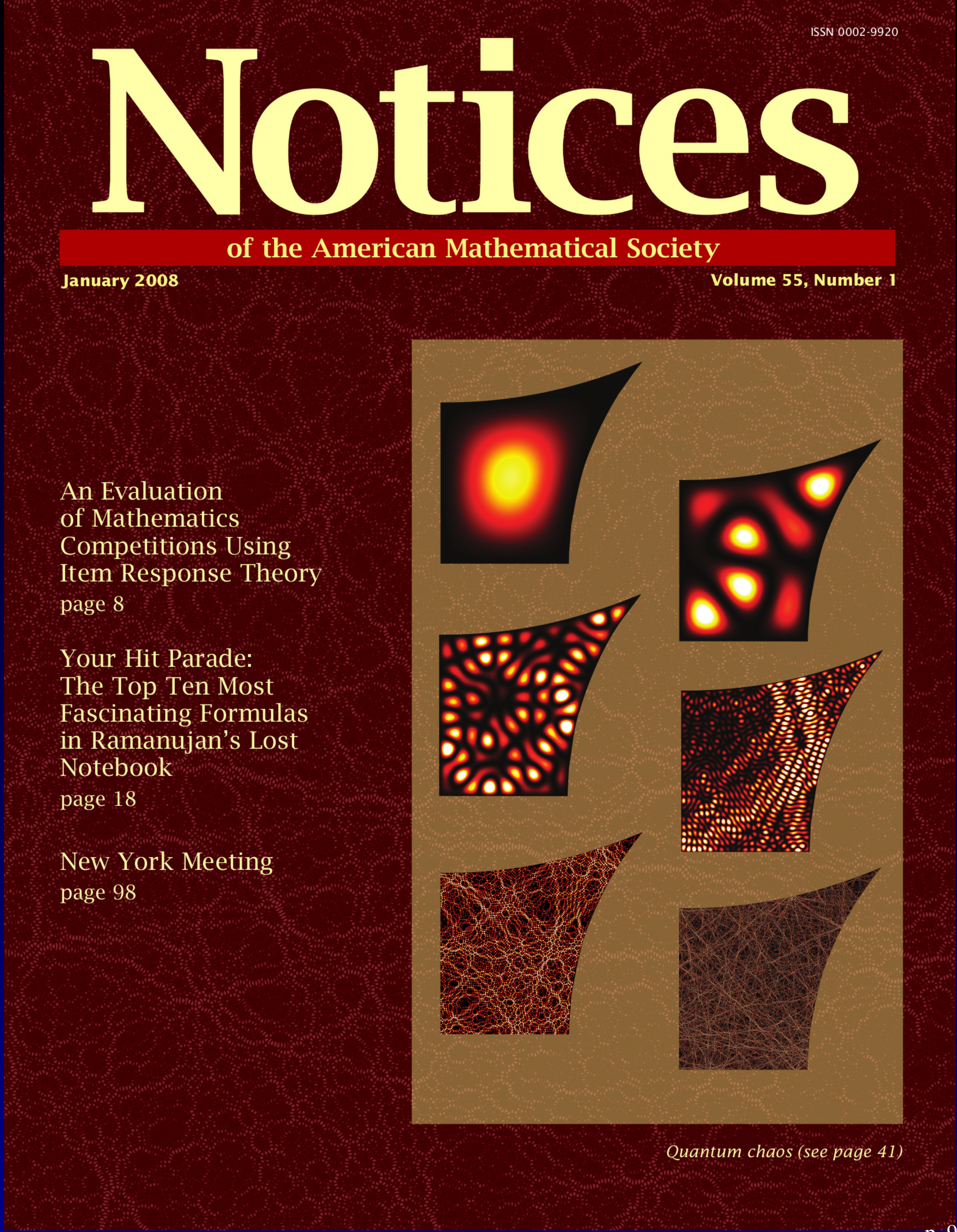
- mathematical interest: spectrum of drums, quantum chaos

Numerical study

- High-freq. asymptotic study of Ω with chaotic ray dynamics (B ’06)

  shown: mode numbers $j = 1, 10, 10^2, 10^3, 10^4, 10^5$

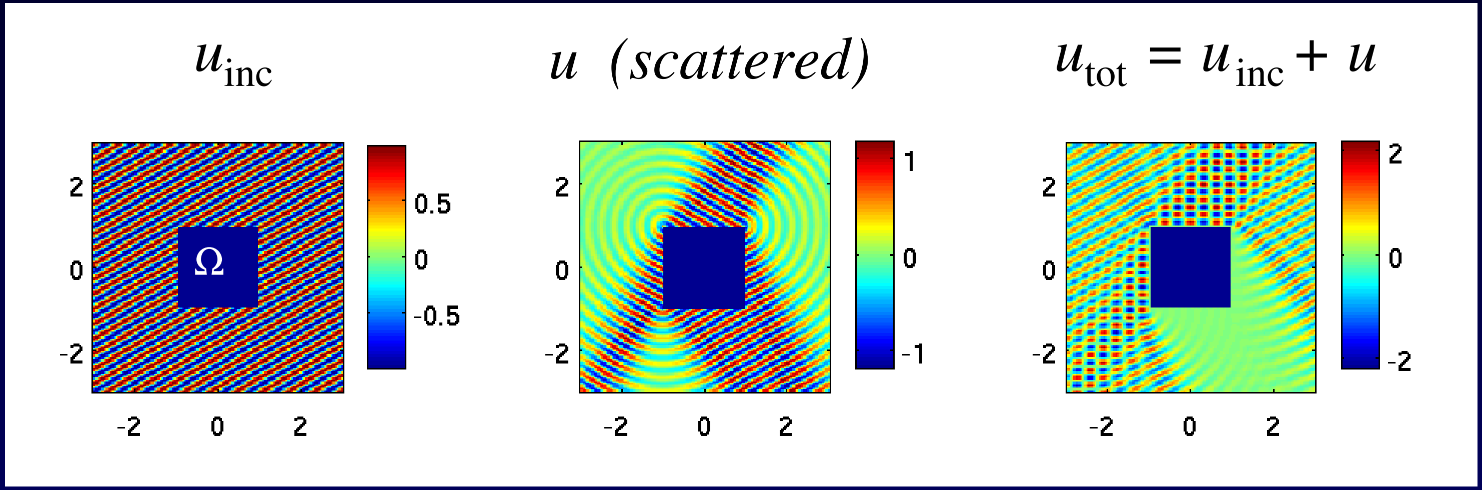
- 30000 modes
- new methods: impossible with FEM



Setup: scattering of waves

$u_{\text{inc}}(x) = e^{i\boldsymbol{k}\cdot\boldsymbol{x}}$ hitting obstacle $\Omega \subset \mathbb{R}^2$?

Decompose total field into sum of incident and scattered...



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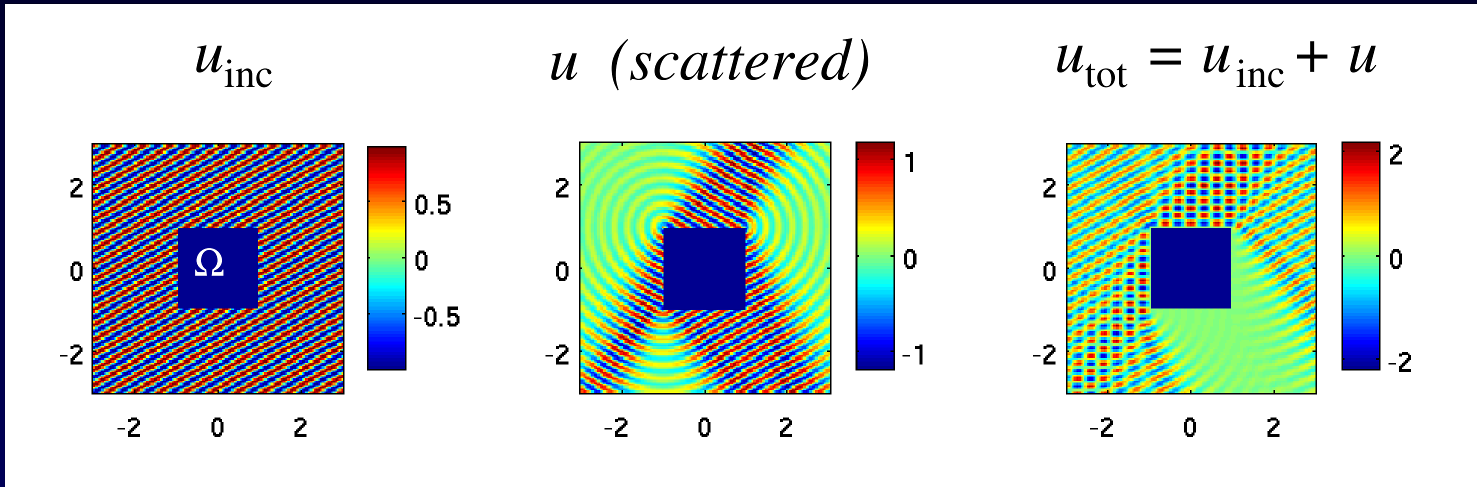

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Exterior boundary-value problem (BVP) for u:

$$\begin{aligned} (\Delta + \omega^2)u &= 0 && \text{in } \mathbb{R}^2 \setminus \overline{\Omega} \\ u &= -u_{\text{inc}} && \text{on } \partial\Omega \\ u & \text{ ‘radiative’ (outgoing towards } \infty) \end{aligned}$$

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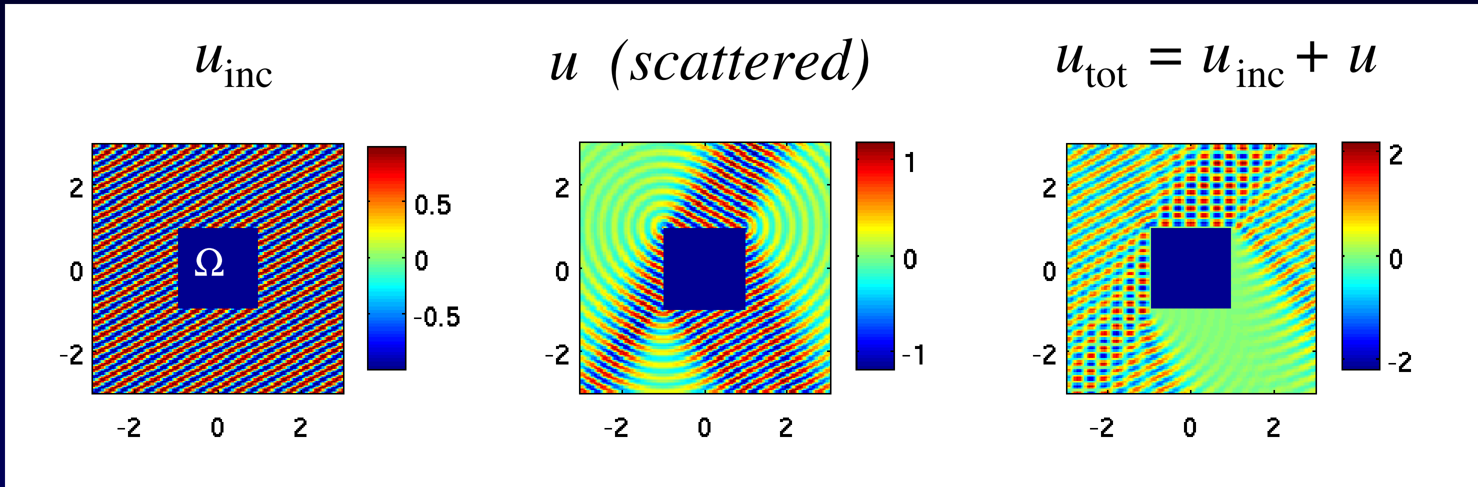

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Note: $\Omega =$ square, is quite hard due to singularities at *corners* (Barnett-Betcke)

Tool: potential theory

‘charge’ (source of waves) distributed along curve Γ w/ density func.

Single-, double-layer potentials, $\mathbf{x}, \mathbf{y} \in \mathbb{R}^2$

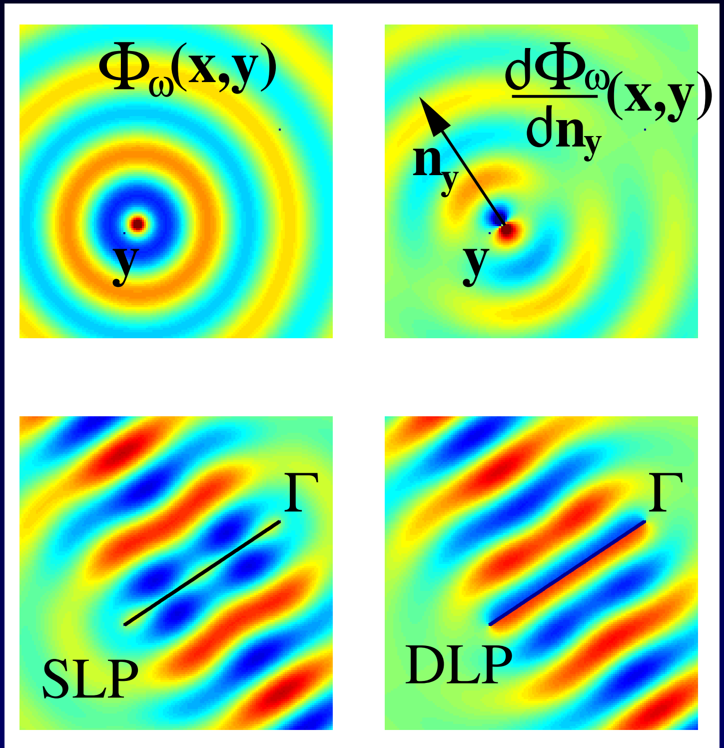
$$v(\mathbf{x}) = \int_\Gamma \Phi_\omega(\mathbf{x}, \mathbf{y})\sigma(\mathbf{y})ds_\mathbf{y} := (\mathcal{S}\sigma)(\mathbf{x})$$

$$u(\mathbf{x}) = \int_\Gamma \frac{\partial \Phi_\omega}{\partial n_\mathbf{y}}(\mathbf{x}, \mathbf{y})\tau(\mathbf{y})ds_\mathbf{y} := (\mathcal{D}\tau)(\mathbf{x})$$

$$\Phi_\omega(\mathbf{x}, \mathbf{y}) := \Phi_\omega(\mathbf{x} - \mathbf{y}) = \frac{i}{4} H_0^{(1)}(\omega|\mathbf{x} - \mathbf{y}|)$$

kernel is *fundamental solution* to PDE:

$(\Delta + \omega^2)\Phi_\omega = 0$, except at origin



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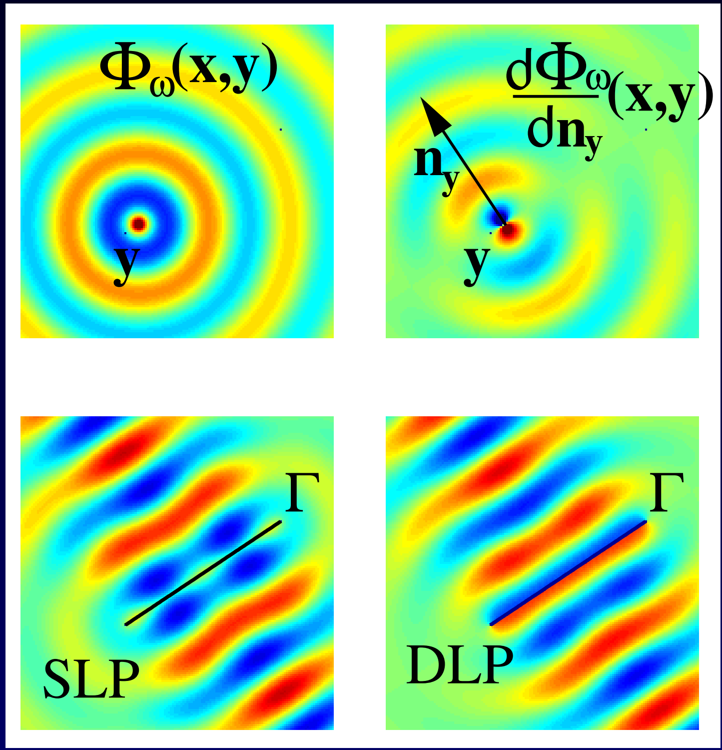

Jump relation: field limit as $\mathbf{x} \to \Gamma$ can depend on which side ($\pm$):

$$u^\pm = D\tau \pm \tfrac{1}{2}\tau$$

D is Fredholm integral operator, mapping continuous functions τ on Γ to continuous functions on Γ

Solve BVP via boundary integral equations

Say represent scattered field by $u = \mathcal{D}\tau$ double-layer on $\partial\Omega$ ($=\Gamma$)

Jump relation (u^+) gives: $(D + \frac{1}{2})\tau = -u_{\text{inc}}|_{\partial\Omega}$

2nd-kind Fredholm int. eqn. Parametrize $\partial\Omega$ via $\mathbf{y}(t)$, $0 \le t \le 2\pi$:

$$(D\tau)(s) = \int_0^{2\pi} \frac{\partial \Phi_\omega}{\partial n_{\mathbf{y}(t)}}(\mathbf{y}(s), \mathbf{y}(t))\, \tau(t)\, |\mathbf{y}'(t)| dt\ , \qquad 0 \le s \le 2\pi$$

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Numerical solution:

- insert a quadrature rule $\displaystyle\int_0^{2\pi} f(t)dt \;\approx\; \sum_{j=1}^{N} w_j f(t_j)$

Get N-by-N linear system, Nyström method,

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How well does this discretized solution approx true solution?

- Thm (Anselone): Nyström converges just like quad. rule for integrand

Periodic numerical quadrature

The simplest rule to approximate $\int_0^{2\pi} f(t)dt$ is sometimes the best: sum N equally spaced samples of f !

$\boxed{\text{MATLAB demo}}$

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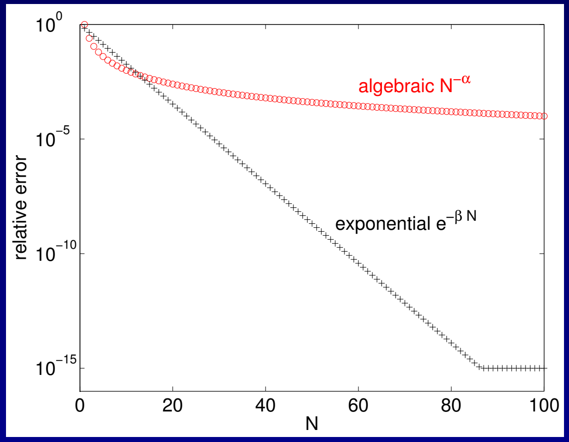
Theorem (Davis '59): Let f be 2π-periodic, and *real analytic*, meaning $f(z)$ is bounded and analytic in some strip $|\,\mathrm{Im}\, z| \le a$ of half-width $a > 0$. Then there is a const $C > 0$ (indep. of N) such that the error is

$$\left| \frac{2\pi}{N} \sum_{j=1}^{N} f\left(\frac{2\pi}{N} j\right) - \int_0^{2\pi} f(t)dt \right| \le Ce^{-aN}$$

- If kernel k analytic (eg $\partial\Omega$ analytic, $\omega = 0$) exponential convergence in N:

  very desirable: can get accuracies of 10^{-14}

  w/ small $N < 10^2$, little effort. (3D analogous)



But $\omega > 0$ needs $f(t) + \ln(4\sin^2 \frac{t}{2})g(t)$

Proof

Residue Thm: $\quad 2\pi i \sum$ residues $=$ closed contour integral in $\mathbb{C}$

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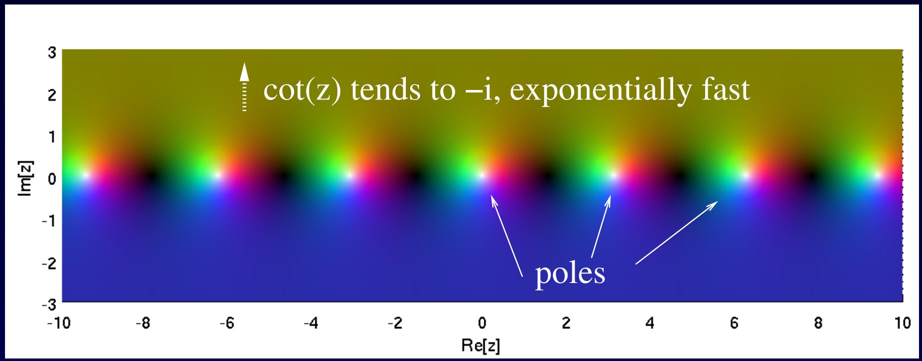
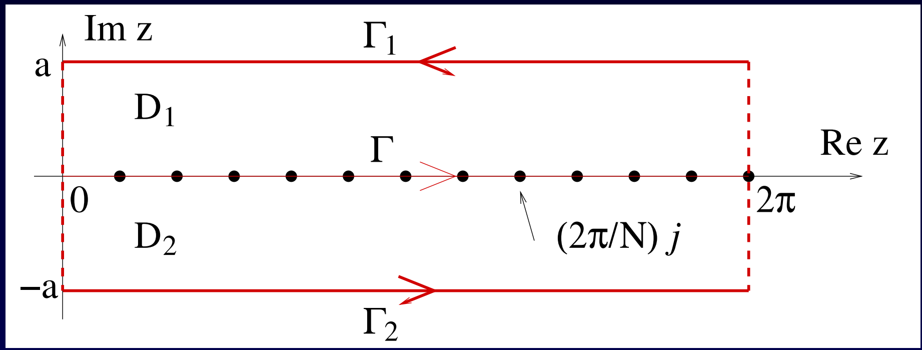
Beautiful cotangent function $\cot(z)$: poles at πj, $j \in \mathbb{Z}$, residues 1





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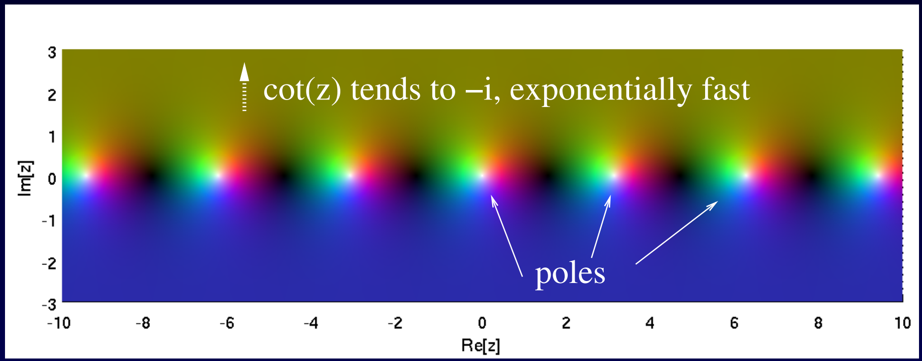

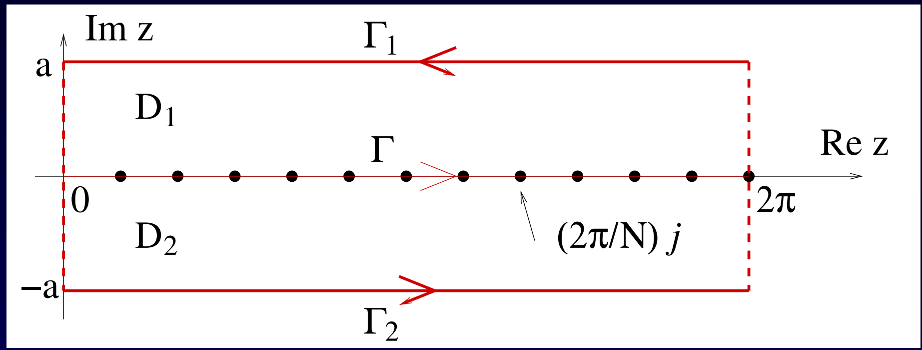

f analytic $\quad \frac{1}{2i} f(z) \cot(\frac{N}{2} z)$: $\quad$ poles at $\frac{2\pi}{N} j$, $\quad$ residues $\frac{1}{iN} f(\frac{2\pi}{N} j)$

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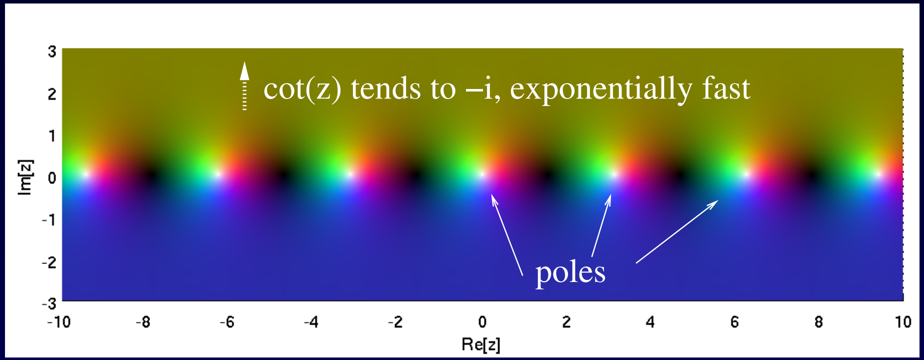
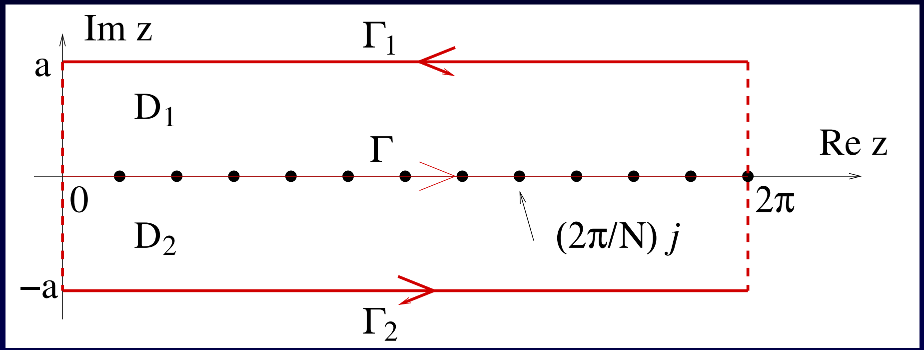
Beautiful cotangent function $\cot(z)$: $\quad$ poles at πj, $j \in \mathbb{Z}$, $\quad$ residues 1





f analytic $\quad \frac{1}{2i} f(z) \cot(\frac{N}{2} z)$: $\quad$ poles at $\frac{2\pi}{N} j$, $\quad$ residues $\frac{1}{iN} f(\frac{2\pi}{N} j)$

Res. Thm in strip:
$$\frac{2\pi}{N} \sum_{j=1}^{N} f\left(\frac{2\pi}{N} j\right) = \int_{\Gamma_1+\Gamma_2} \frac{1}{2i} f(z) \cot\left(\frac{N}{2} z\right) dz$$

Proof

Residue Thm: $2\pi i \sum$ residues $=$ closed contour integral in $\mathbb{C}$

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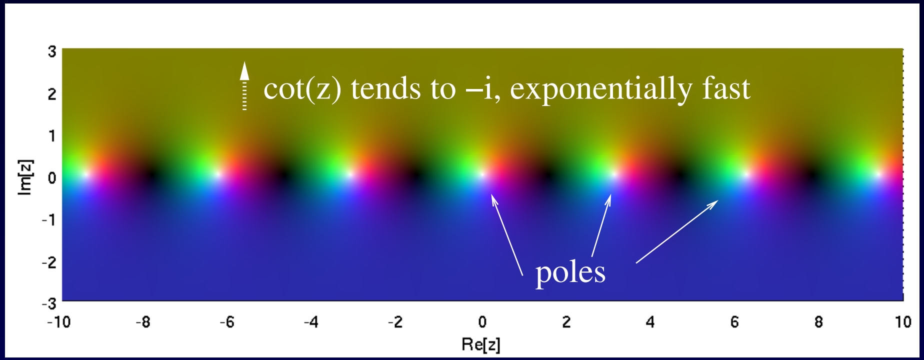

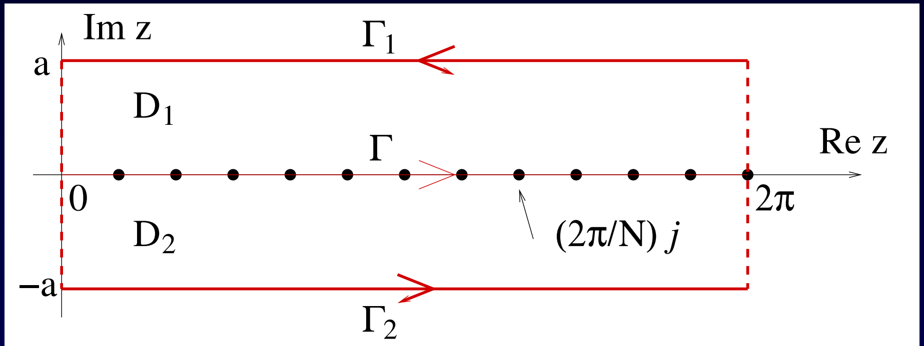

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integrand pure Im on $\mathbb{R}$, so

Re parts antisymmetric $\updownarrow$ add

Im parts symmetric $\updownarrow$ cancel

$$= \operatorname{Re} \int_{\Gamma_1} (-i) f(z) \cot\left(\frac{N}{2} z\right) dz$$

$$\frac{2\pi}{N}\sum_{j=1}^{N} f\left(\frac{2\pi}{N}j\right) \;=\; \mathrm{Re}\int_{\Gamma_1} (-i) f(z)\cot\left(\frac{N}{2}z\right) dz$$

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Cauchy integral formula in D_1 (since f analytic):

$$-\int_{\Gamma} f(z)dz \;=\; \int_{\Gamma_1} f(z)dz$$

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add Re part of this to previous eqn:

$$\frac{2\pi}{N}\sum_{j=1}^{N} f\left(\frac{2\pi}{N}j\right) - \int_{\Gamma} f(z)dz \;=\; \mathrm{Re}\int_{\Gamma_1} \left[1 - i\cot\left(\frac{N}{2}z\right)\right] f(z)dz$$

$$\frac{2\pi}{N}\sum_{j=1}^{N} f\left(\frac{2\pi}{N}j\right) \;=\; \mathrm{Re}\int_{\Gamma_1} (-i) f(z) \cot\left(\frac{N}{2}z\right) dz$$

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add Re part of this to previous eqn:

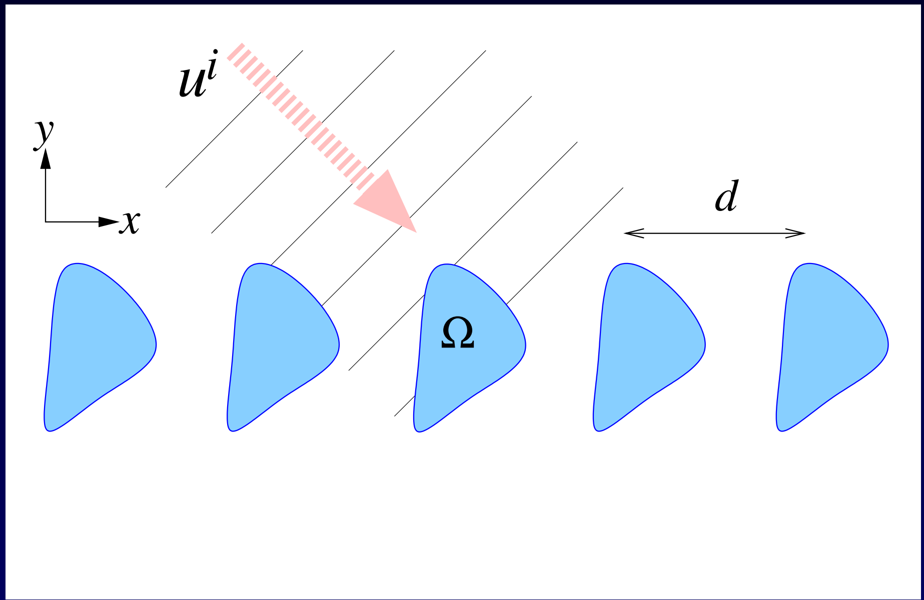
$$\frac{2\pi}{N}\sum_{j=1}^{N} f\left(\frac{2\pi}{N}j\right) \underset{\substack{\uparrow \\ \text{error of our quadrature}}}{-} \int_{\Gamma} f(z)dz \;=\; \mathrm{Re}\int_{\Gamma_1} \Big[1 - \underset{\substack{\uparrow \\ \text{exp. small} \le 2/(e^{aN}-1)}}{i\cot\left(\frac{N}{2}z\right)}\Big] \underset{\substack{\uparrow \\ \text{bnded in } D_1}}{f(z)}dz$$

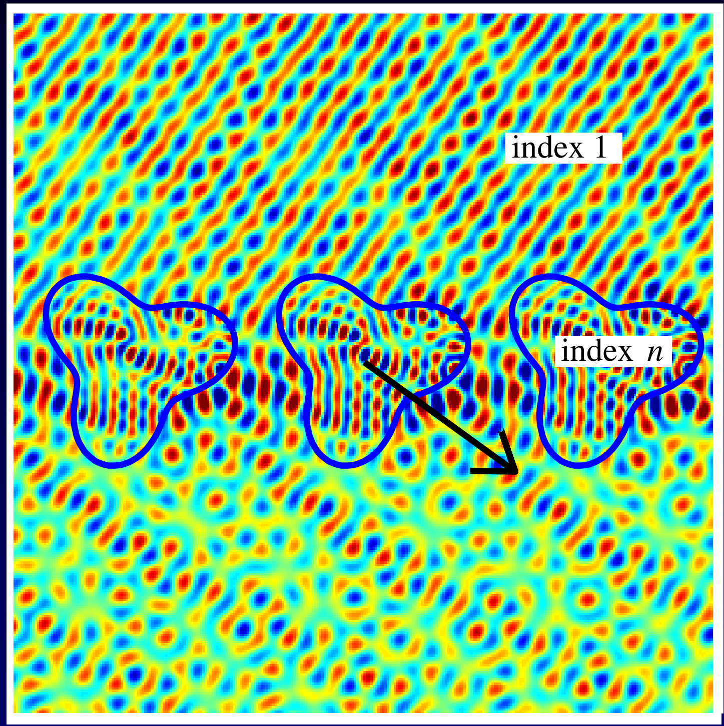
QED

- Research: good quadrature schemes for f's with *singularities*

Results: scattering from periodic grating

lattice of obstacles (hint: you don't want to discretize an ∞ long boundary!)





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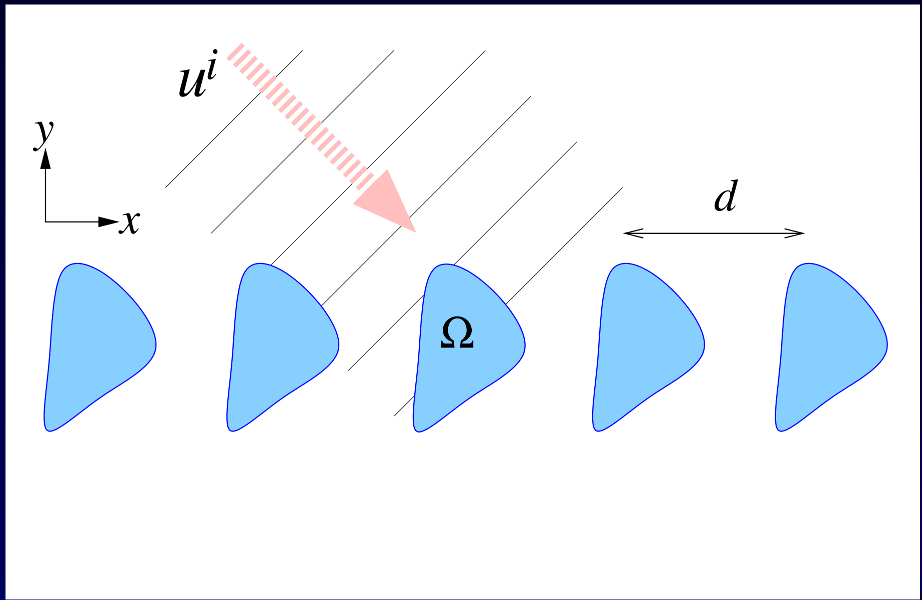

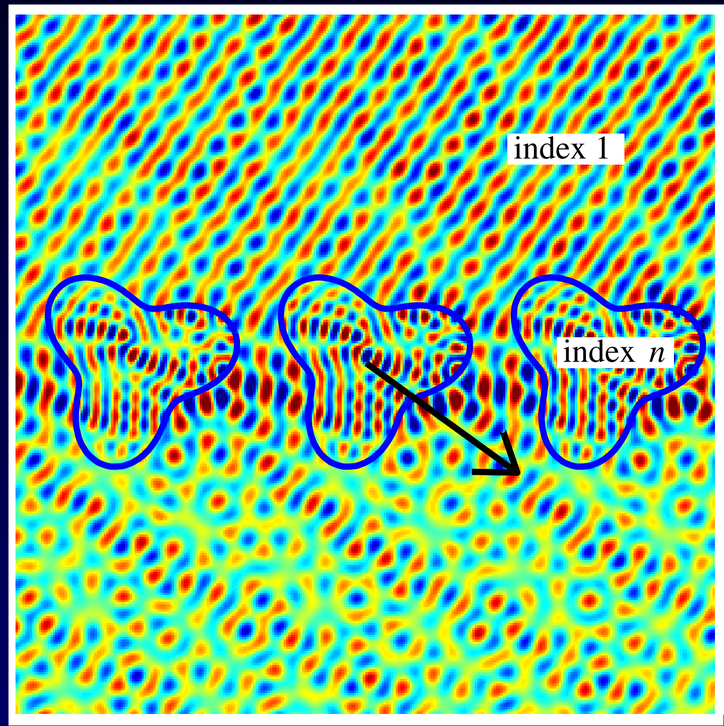

u_{inc} quasi-periodic, so u is too:

$$u(x+d,y) \;=\; \alpha u(x,y)$$ Bloch phase α

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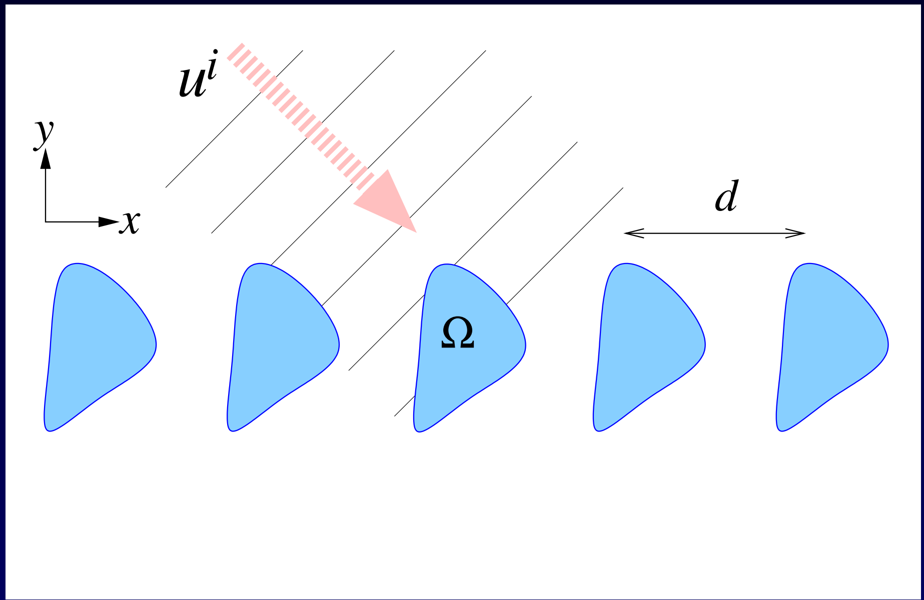

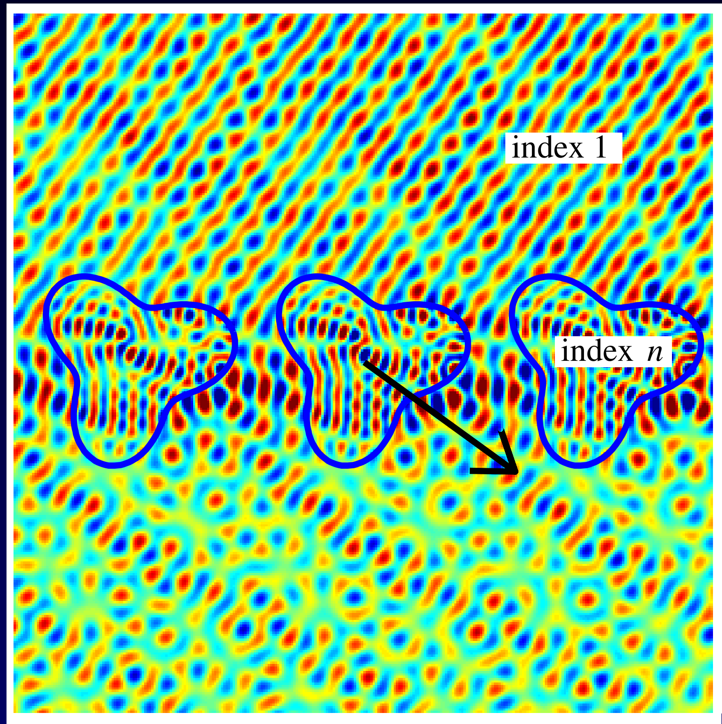

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Results to 12 digits accuracy with $N \sim 100$ (Barnett-Greengard) MOVIE 1

- Research: *robust* way to 'periodize' integral equations in 3D?

Advanced topics, issues

- fast multipole methods (FMM (Greengard-Rokhlin)): Nyström matrix A can be applied to vector $\boldsymbol{\tau}$ in $O(N \log N)$ time (naive is N^2)

Huge speedup! (like FFT) enables much larger problems, *if* can use iterative solve.

- 3D is hard to get accurate (BEM is done with low-order finite elements on boundary).

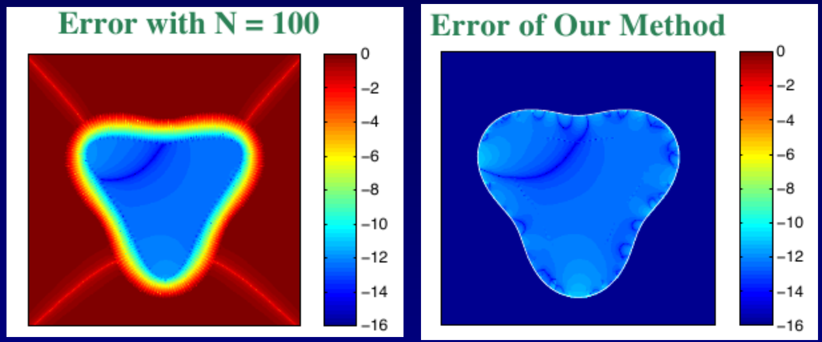
    high-order singular quadrature near diagonal for Nyström messy

- Handling *corners* to high accuracy: v. hard (Bremer, Helsing)

    can add 10^3 to N for each corner in 2D, more in 3D. How compress & use less?

- Accurate evaluation of u from layer potential up to the boundary:

Hanh Nguyen '14 poster
Thursday at Wetterhahn Symposium:



- Fundamental soln Φ, hence BIE, for graded-index media (Mahoney)