Diffraction gratings and photonic crystals: numerical analysis of waves

Grad Open House, Apr 2, 2011

Alex Barnett

Mathematics Department, Dartmouth College

Current research areas

- Numerical analysis: efficient computational methods for PDEs
  wave scattering, periodic problems, eigenvalue problems
  inventing new methods, coding them up, analyzing them
  (NSF Grant DMS-0811005)

- Mathematical physics: ‘quantum chaos’
  high-frequency waves trapped in an ergodic dynamical system

- Other applied mathematics:
  mathematical ecology, animal movement models
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Study it at grad school = versatile + interdisciplinary + employable

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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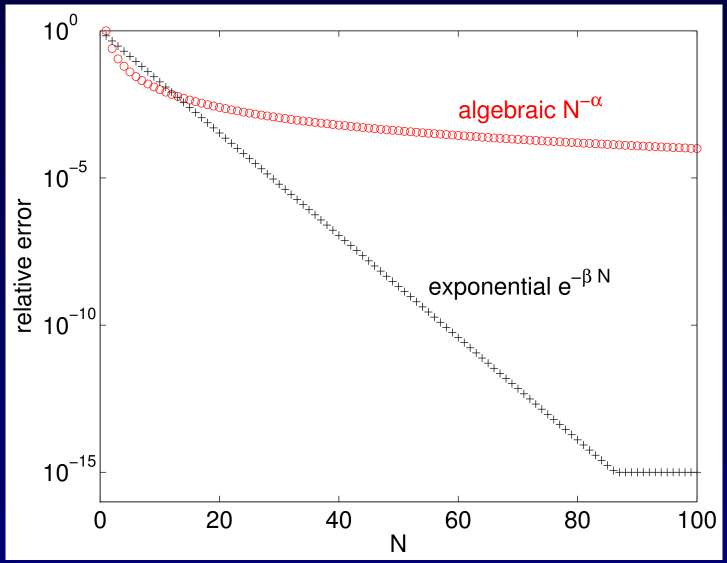

e.g. solving PDEs: how does error scale with N = effort ?

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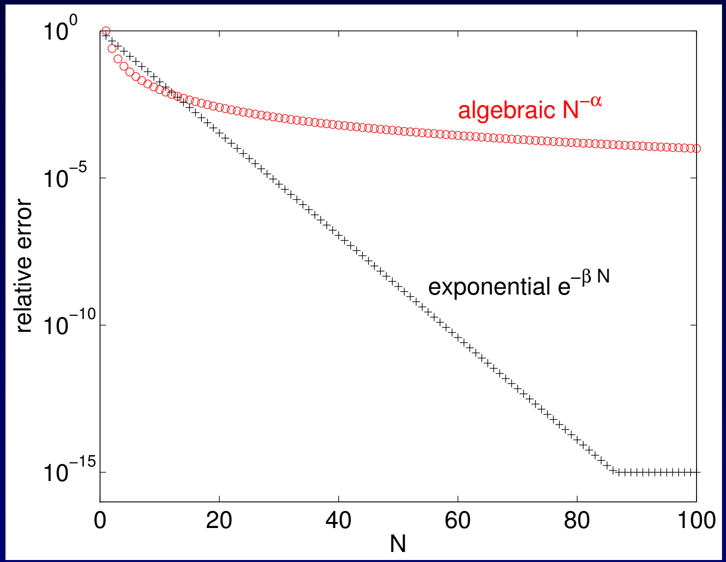

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- Engineering & technology relies on good computational algorithms: insensitive to rounding error, rapid convergence, robust, runs fast

Analysis: *proving* useful upper bounds on the error

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

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

waves at constant frequency ω described by function $u : \mathbb{R}^2 \to \mathbb{C}$

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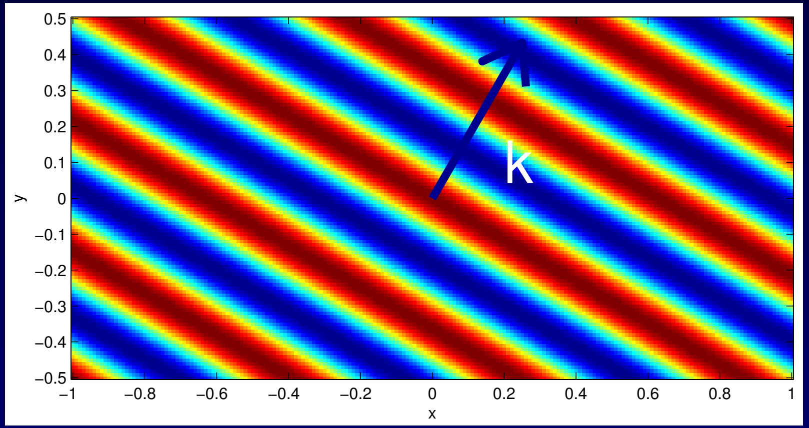
- E.g. plane wave solution

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

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

traveling waves from distant source



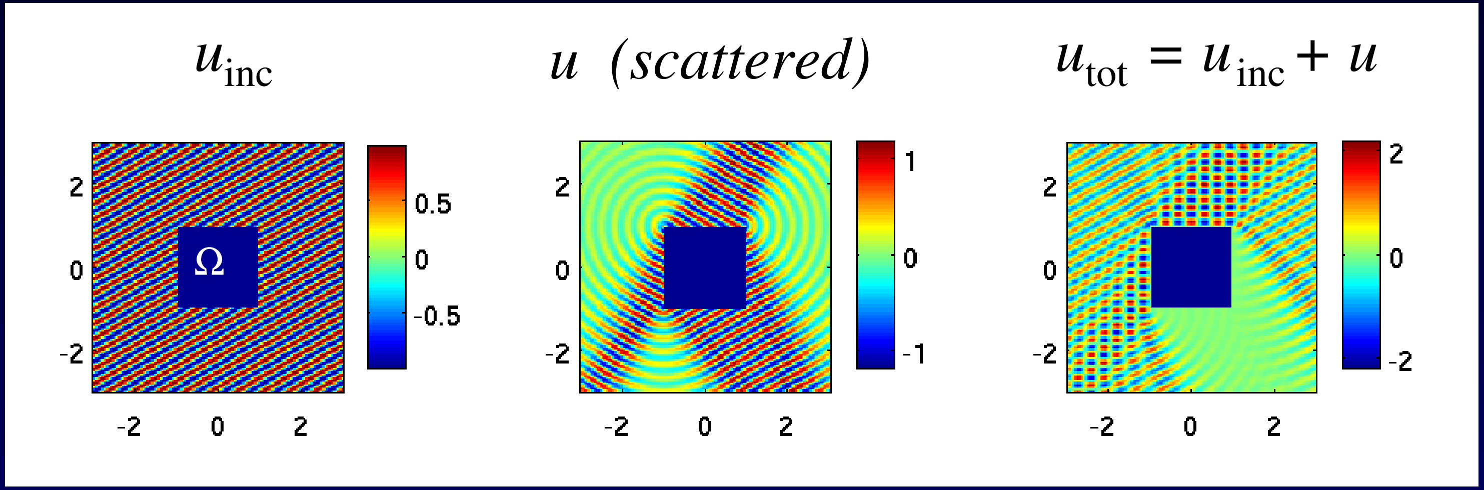
What happens when these waves hit an obstacle? Applications:

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

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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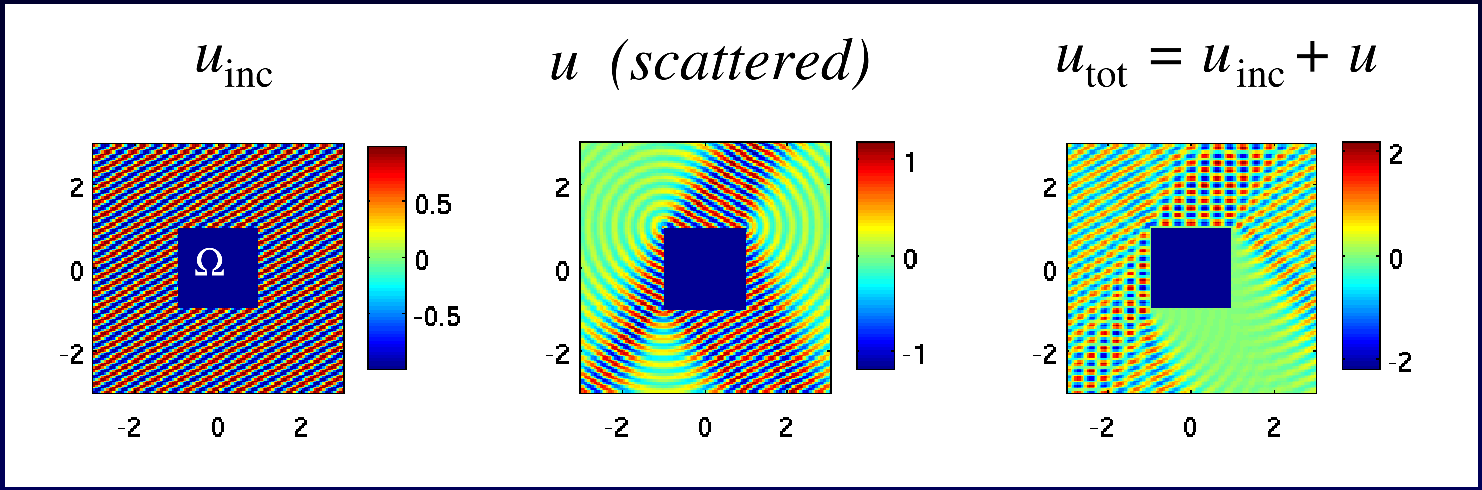

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PDE Boundary-value problem (BVP) for u:

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

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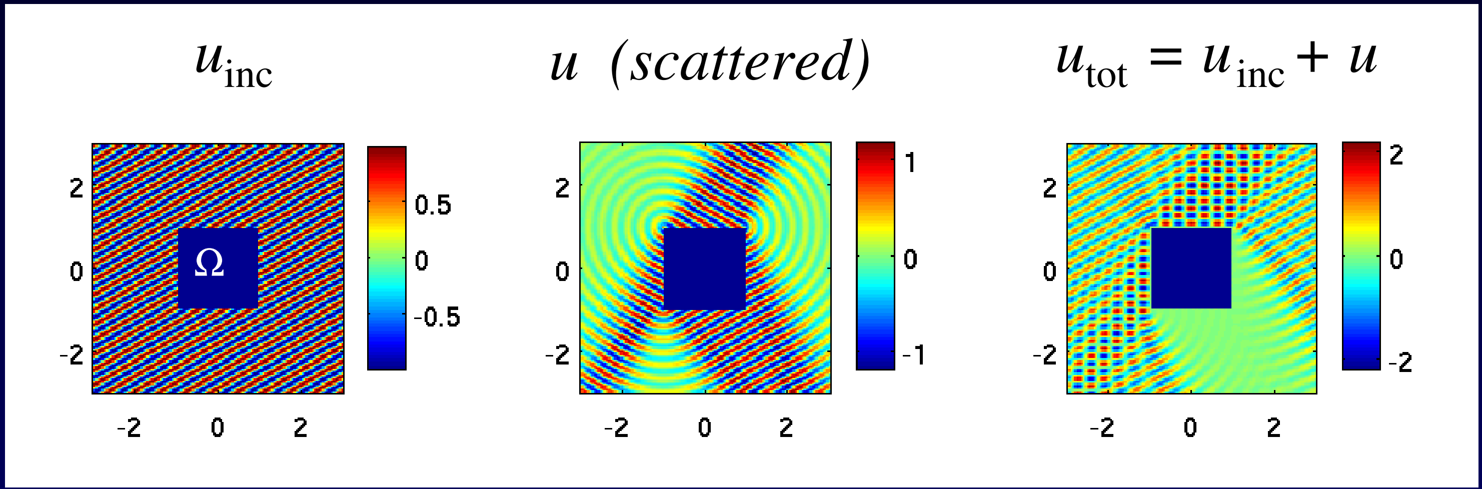

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Note: Ω = square, is quite hard due to singularities at *corners*: research area!

Tools: potential theory

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

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

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

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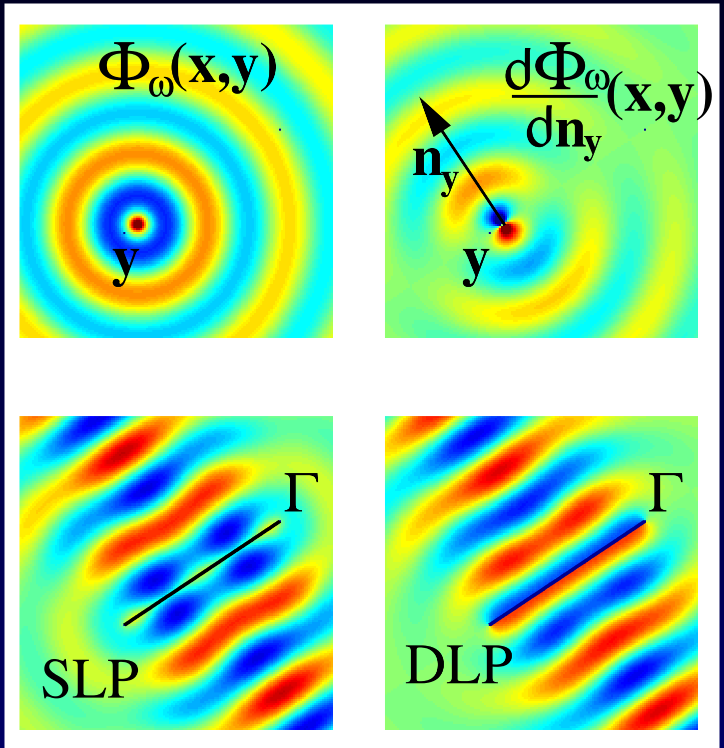
$$\Phi_\omega(\mathbf{x}, \mathbf{y}) := \Phi_\omega(\mathbf{x} - \mathbf{y}) = \frac{i}{4}H_0^{(1)}(\omega|\mathbf{x} - \mathbf{y}|)$$

kernel is *fundamental solution* to PDE:

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



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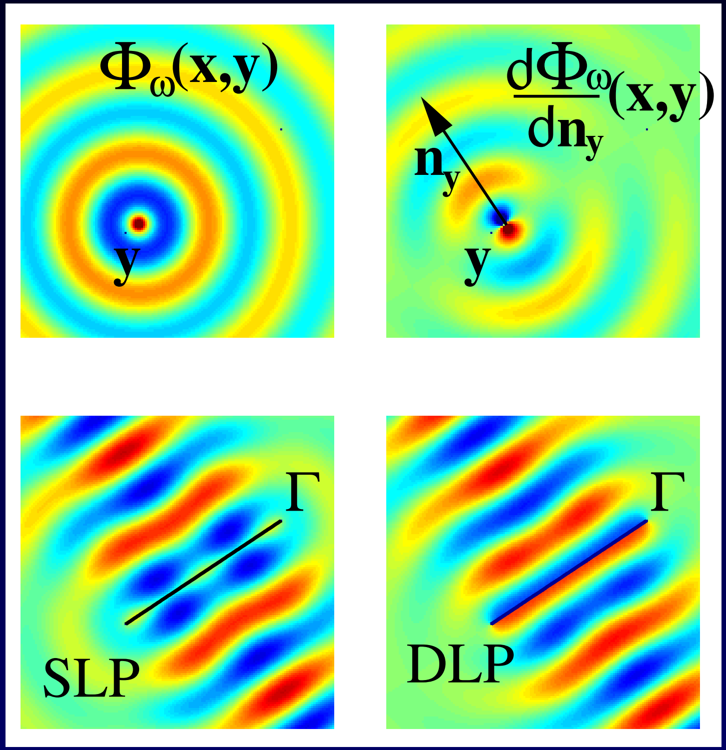

Jump relation: field limit as $\mathbf{x} \to \Gamma$ can depend on which side ($\pm$):

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

D is a *linear integral operator* mapping continuous functions $\tau \in C(\Gamma)$ to continuous functions $C(\Gamma)$

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

Is a *Fredholm integral equation*, operator D acts like

$$(D\tau)(s) = \int_0^{2\pi} k(s,t)\tau(t)dt$$

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Numerical solution must restrict to finite set of N unknowns:

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

This gives an N-by-N linear system,

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How well does this discretized solution approx true solution?

- need analysis of quadrature: let me show you a cute proof. . .

Periodic numerical quadrature

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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 $|\operatorname{Im} z| \le a$ of half-width $a > 0$. Then there is a const $C > 0$ (indep. of N) such that the error is

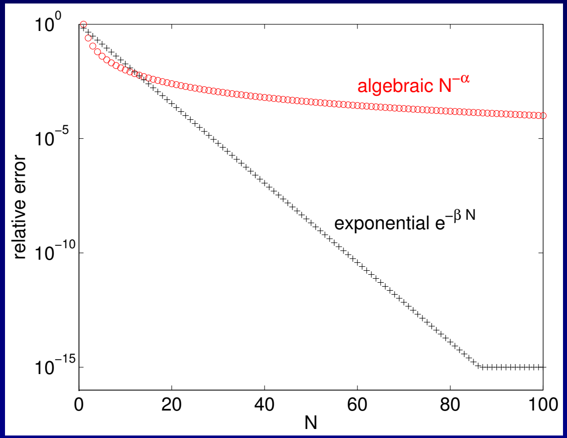
$$\left| \frac{2\pi}{N} \sum_{j=1}^{N} f\left(\frac{2\pi}{N} j\right) - \int_0^{2\pi} f(t)dt \right| \le Ce^{-aN}$$

- exponential convergence in N:

doubling N squares your accuracy

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

w/ little effort. Carries over to solving the PDE!



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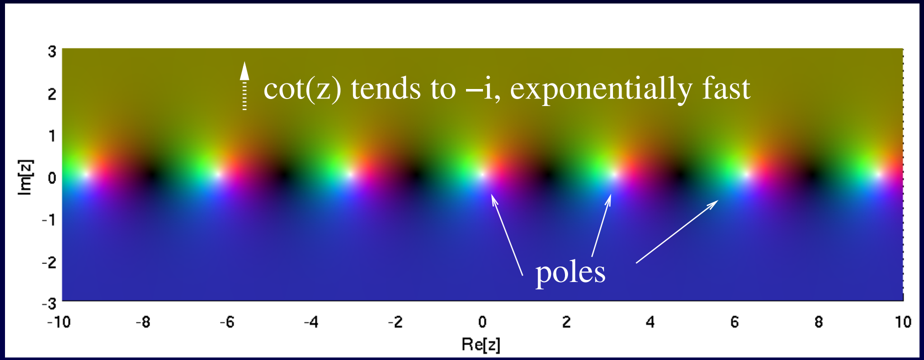

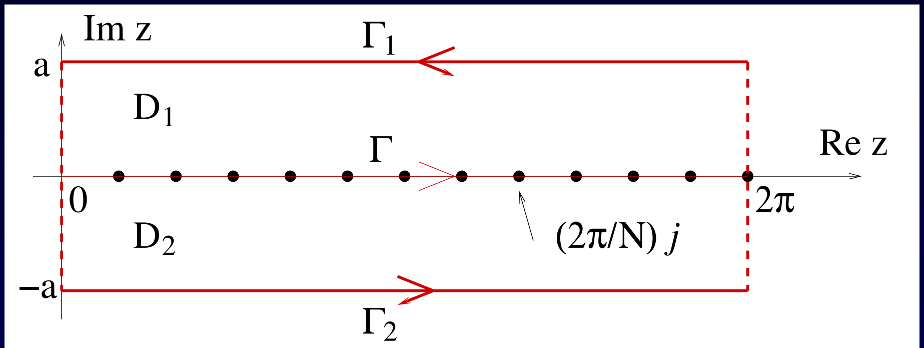

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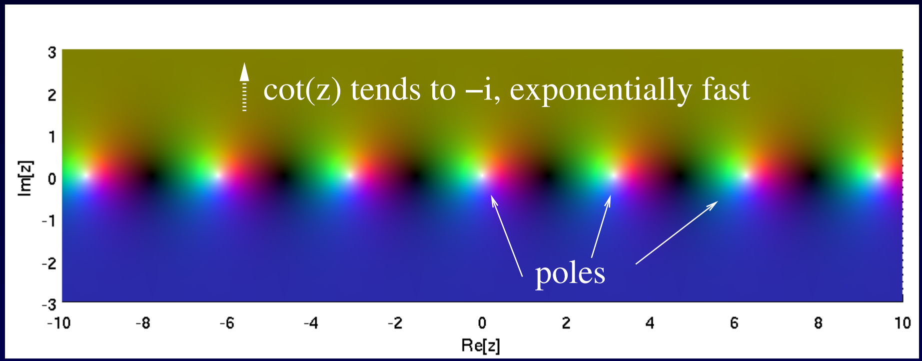

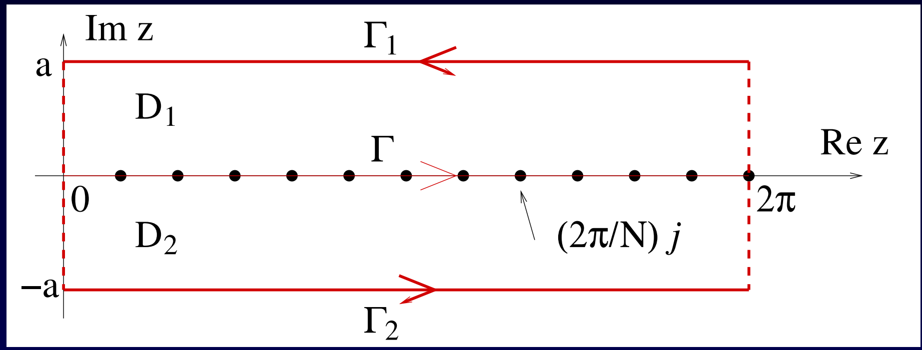

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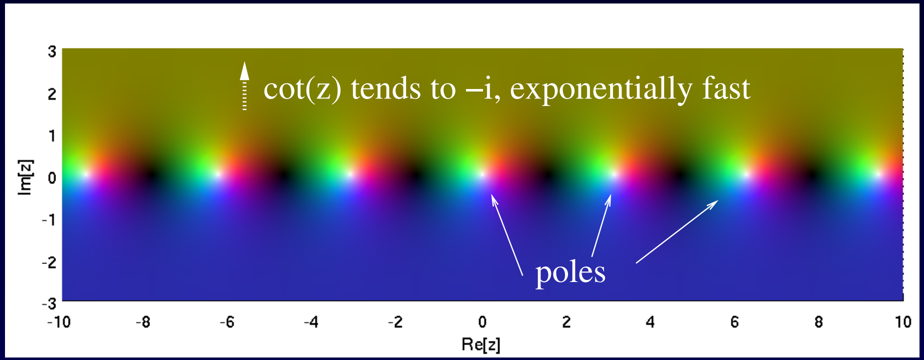

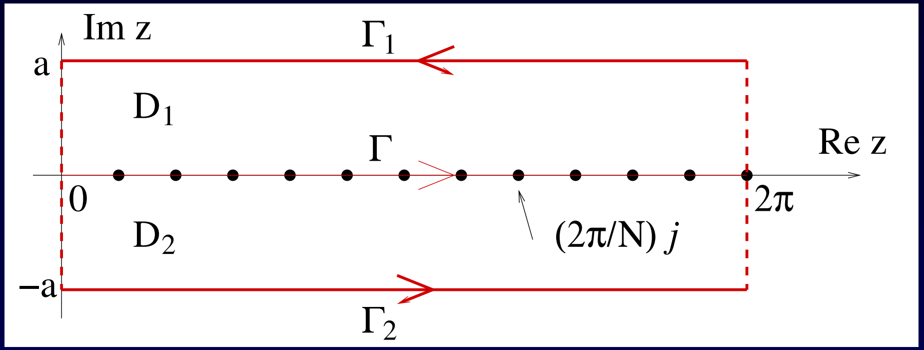

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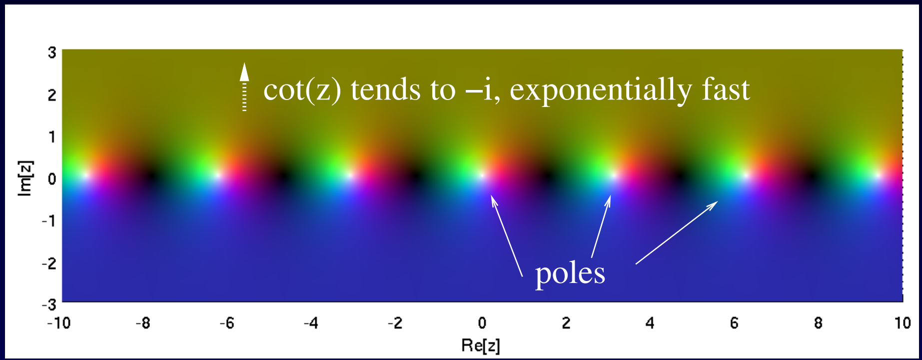

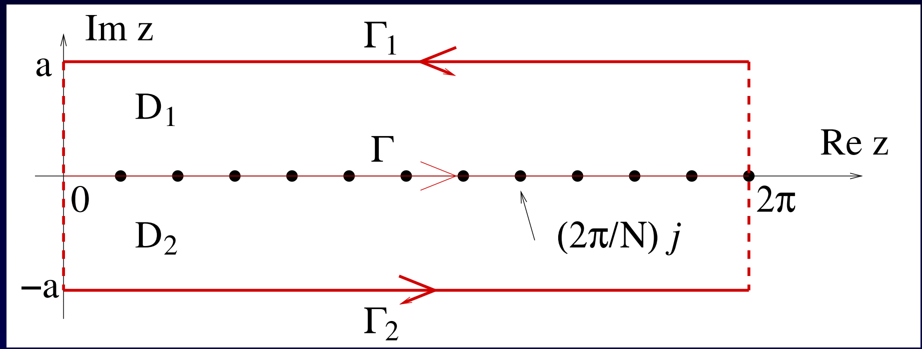

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integrand pure Im on $\mathbb{R}$, so
Re parts antisymmetric $\updownarrow$ add
Im parts symmetric $\updownarrow$ cancel

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

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$\uparrow$ error of our quadrature

$\uparrow$ exp. small $\leq 2/(e^{aN}-1)$

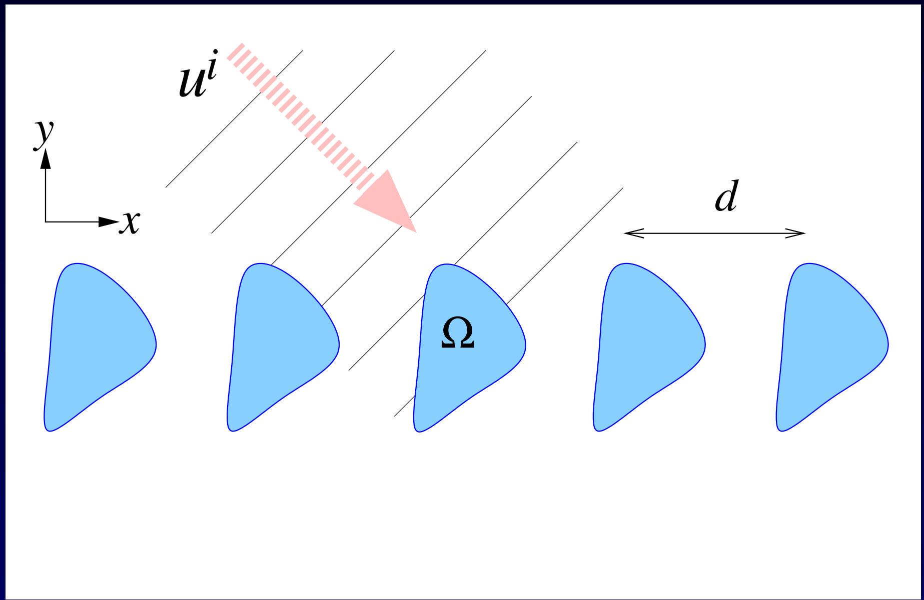
$\uparrow$ bnded in D_1

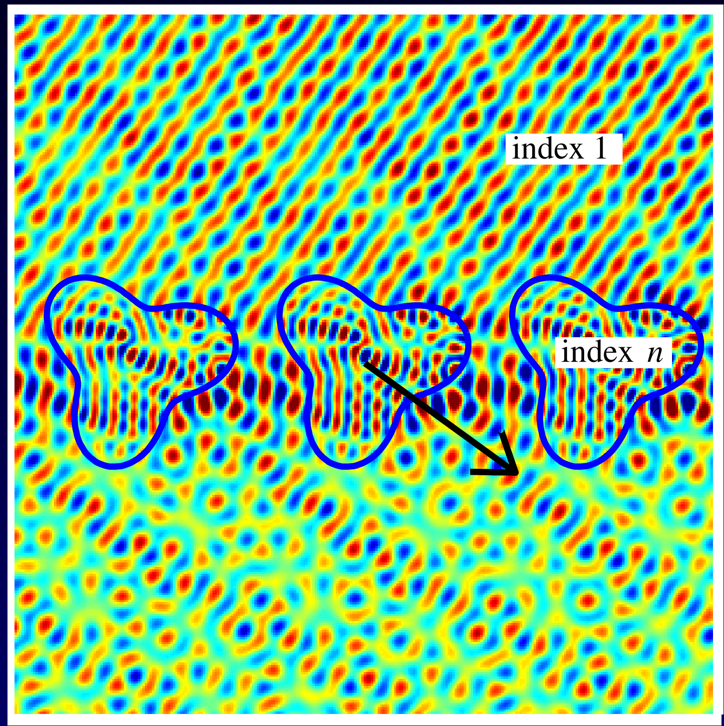
QED

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

Scattering from periodic obstacle grating

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





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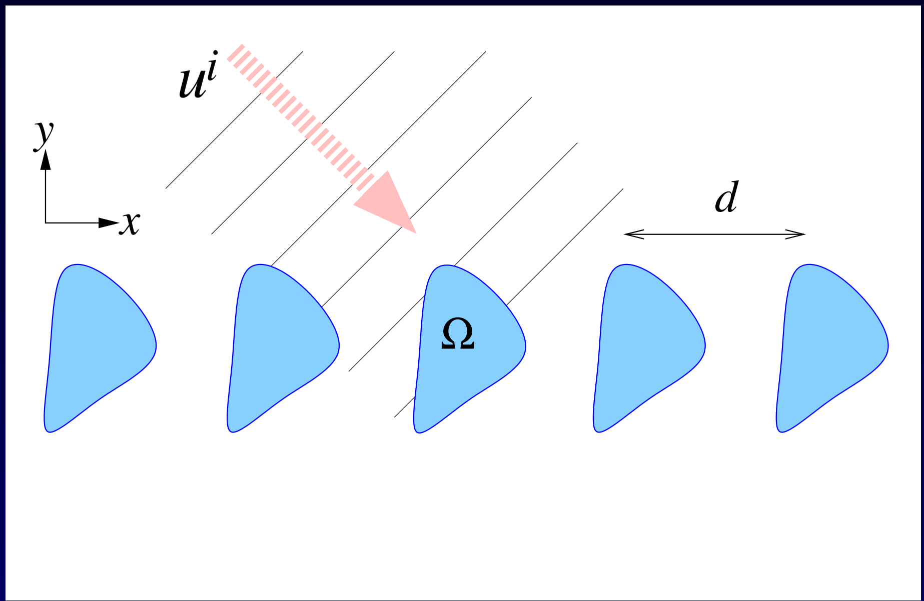

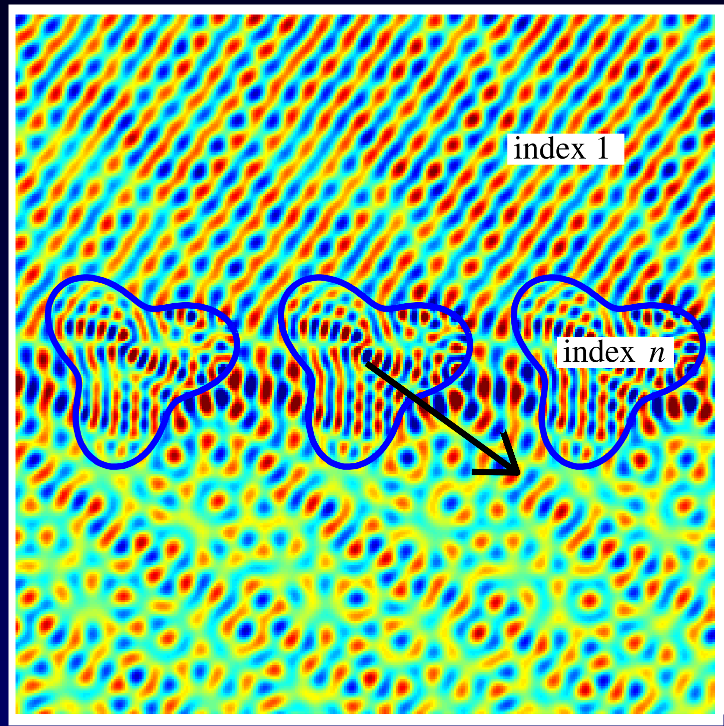

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$$u(x+d,y) \;=\; \alpha u(x,y)$$ Bloch phase α

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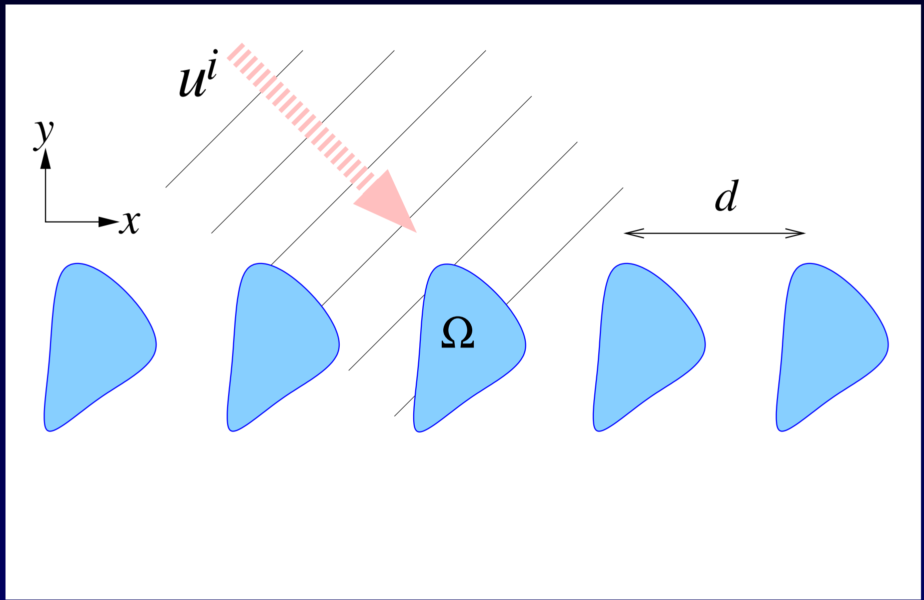

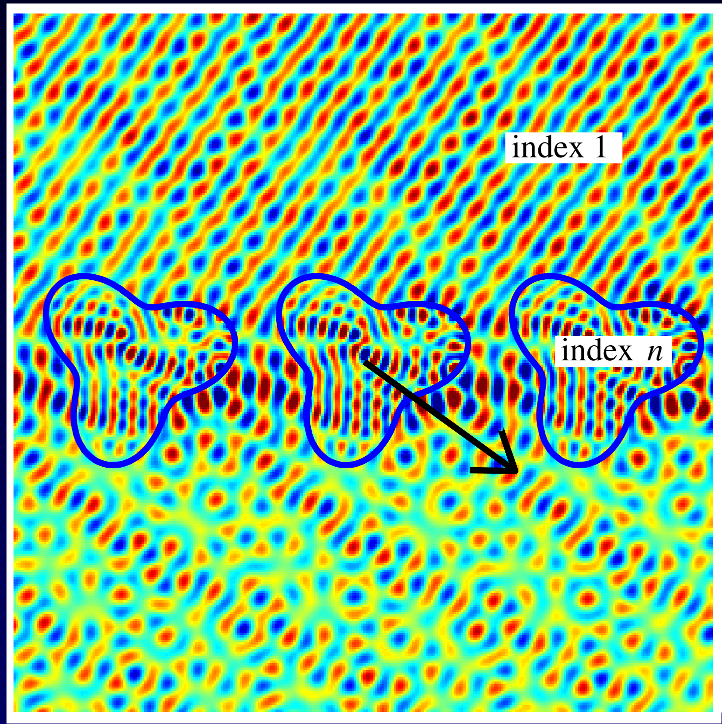

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- Research: *robust* way to 'periodize' integral equations in 2D (3D?)

MOVIE 1

Applications of periodic scattering problems

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

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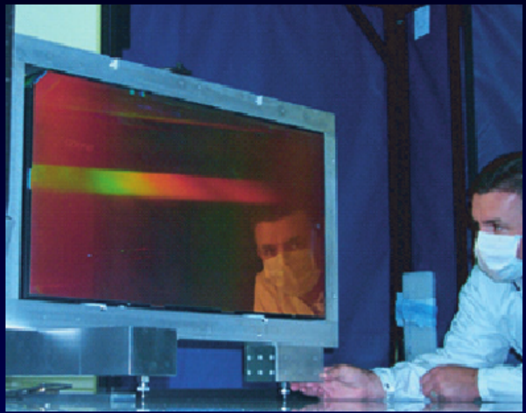
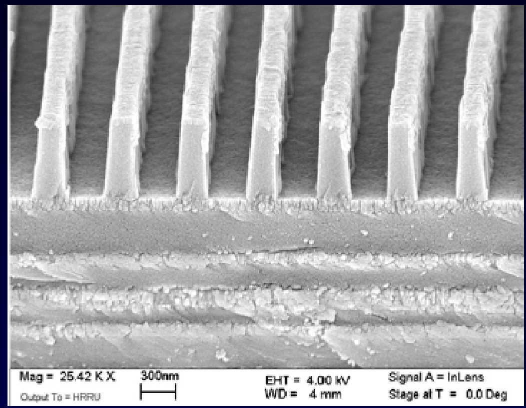


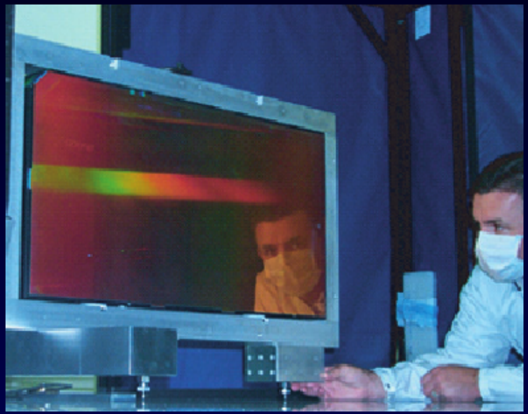


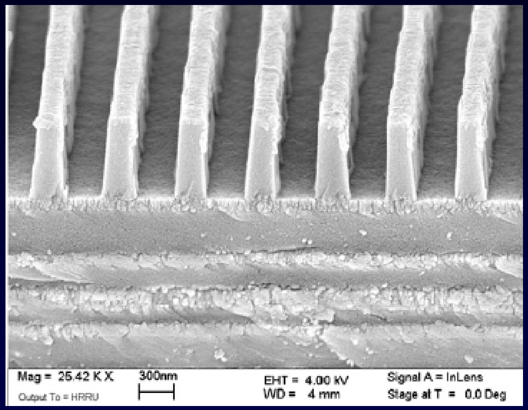
multi-layer dielectric diffraction grating, NIF lasers (LLNL)

2×10^6 periods! (Barty '04)

Applications of periodic scattering problems

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





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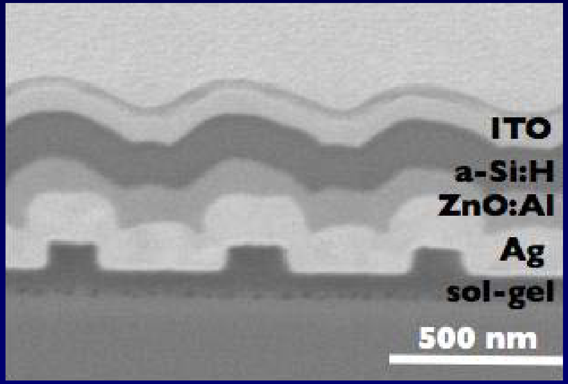
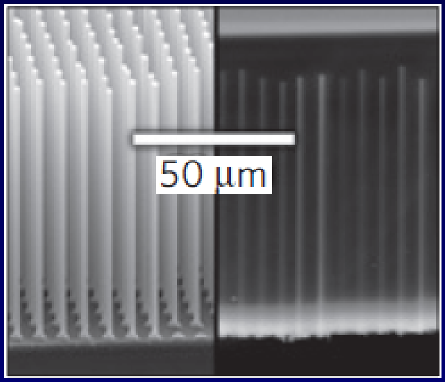


plasmonic solar cell (Atwater '10)



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

Enjoy your visit!