

Diffraction gratings and photonic crystals: numerical analysis of waves

Grad Open House, Apr 2, 2011

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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’
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Study it at grad school = versatile + interdisciplinary + employable

What is numerical analysis?

Theory, Experiment, Computation: third branch of science

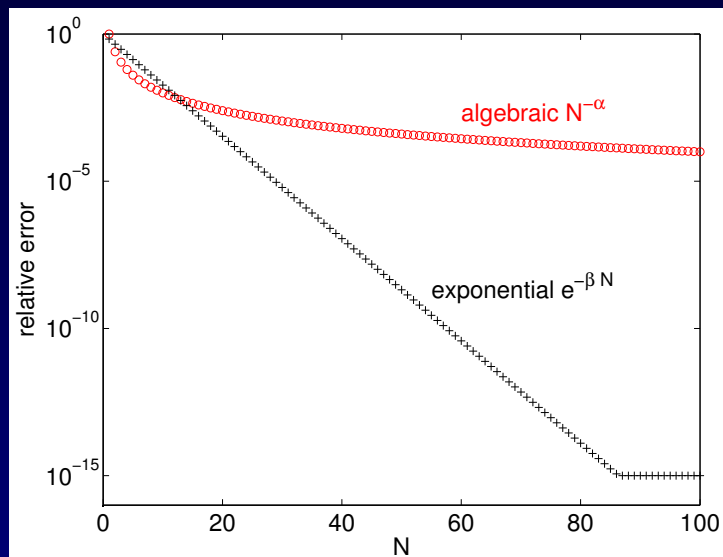
- E.g. in computer, real numbers \mathbb{R} approximated by a finite set F
‘floating point’ binary numbers: e.g. $0.11010111001 \times 2^{-1101}$
rounding $\mathbb{R} \rightarrow F$ causes relative error of 10^{-16} ; how ensure not amplified?

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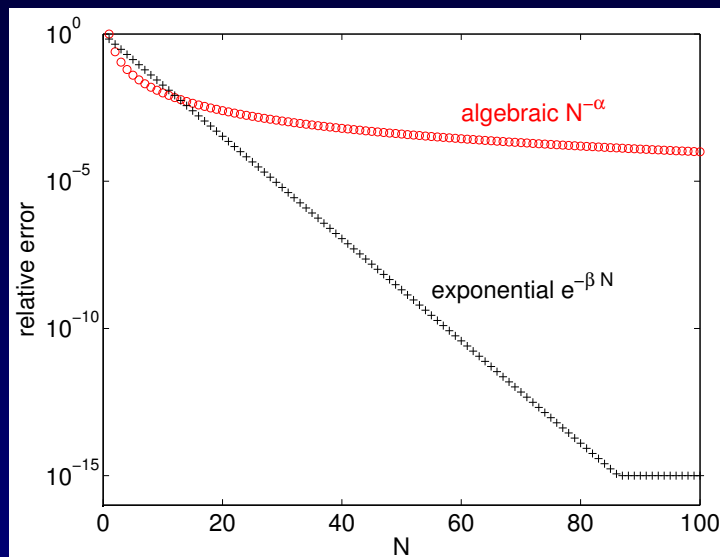
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- Engineering & technology relies on good computational algorithms: insensitive to rounding error, rapid convergence, robust, runs fast

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 $u : \mathbb{R}^2 \rightarrow \mathbb{C}$

u satisfies the Helmholtz PDE $(\Delta + \omega^2)u = 0$

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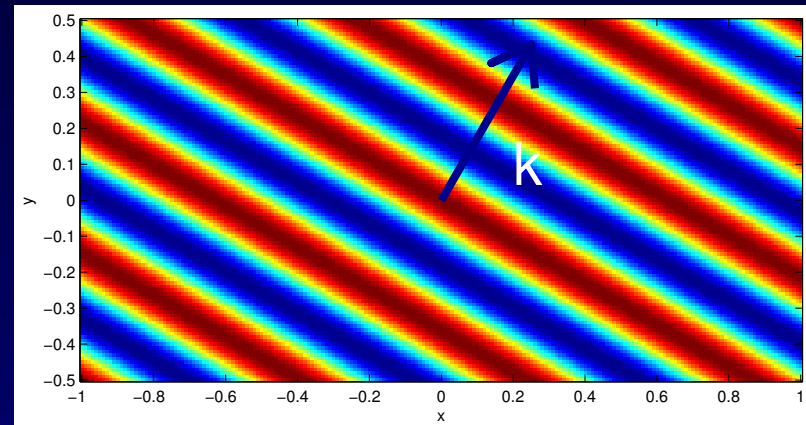
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- E.g. plane wave solution

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

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

traveling waves from distant source



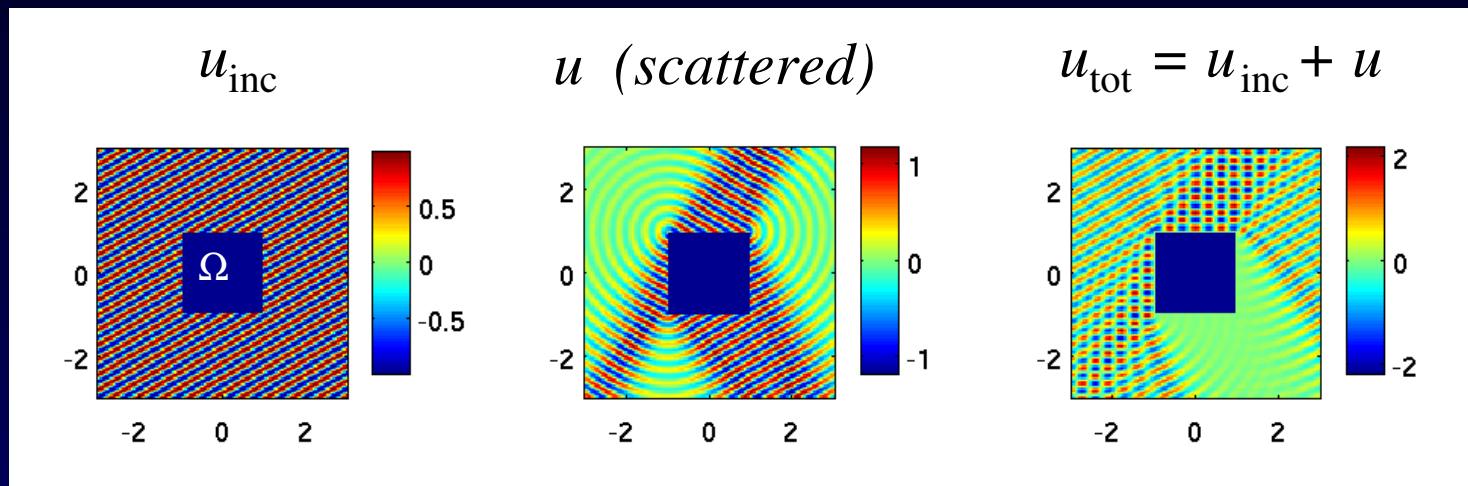
What happens when these waves hit an obstacle? Applications:

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

Scattering of waves

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

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

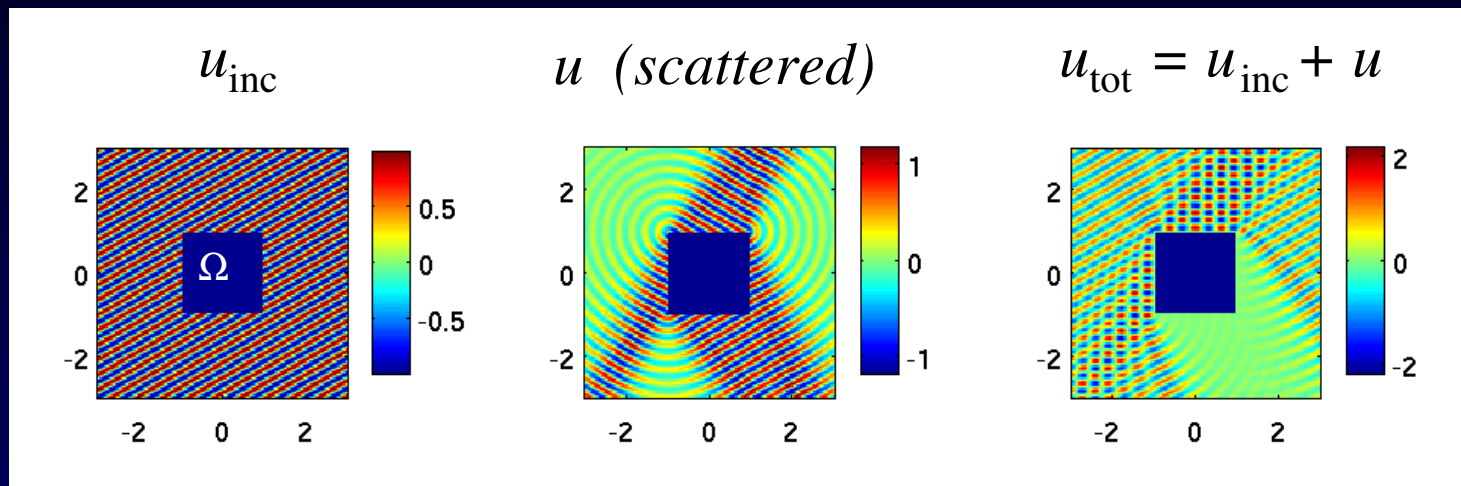


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$$(\Delta + \omega^2)u = 0 \quad \text{in } \mathbb{R}^2 \setminus \overline{\Omega}$$

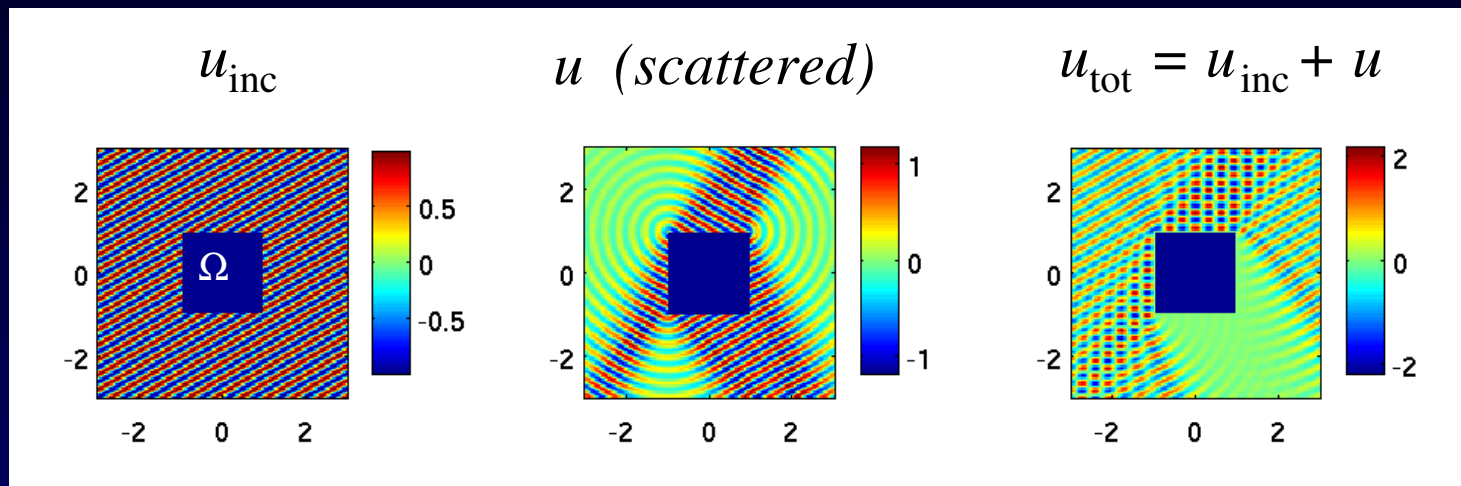
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Note: $\Omega = \text{square}$, is quite hard due to singularities at *corners*: research area!

Tools: potential theory

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

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

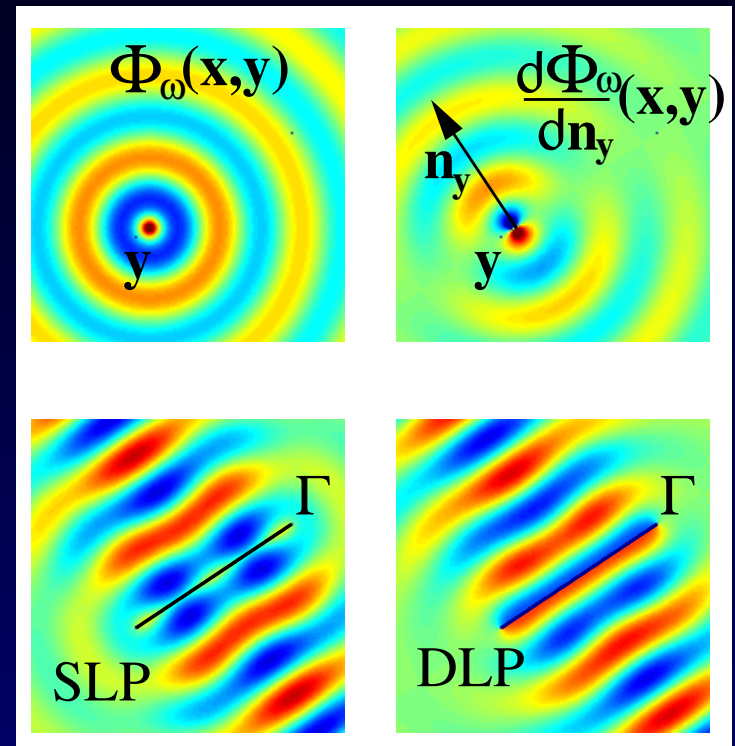
$$v(\mathbf{x}) = \int_{\Gamma} \Phi_{\omega}(\mathbf{x}, \mathbf{y}) \sigma(\mathbf{y}) ds_{\mathbf{y}} := (\mathcal{S}\sigma)(\mathbf{x})$$

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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:

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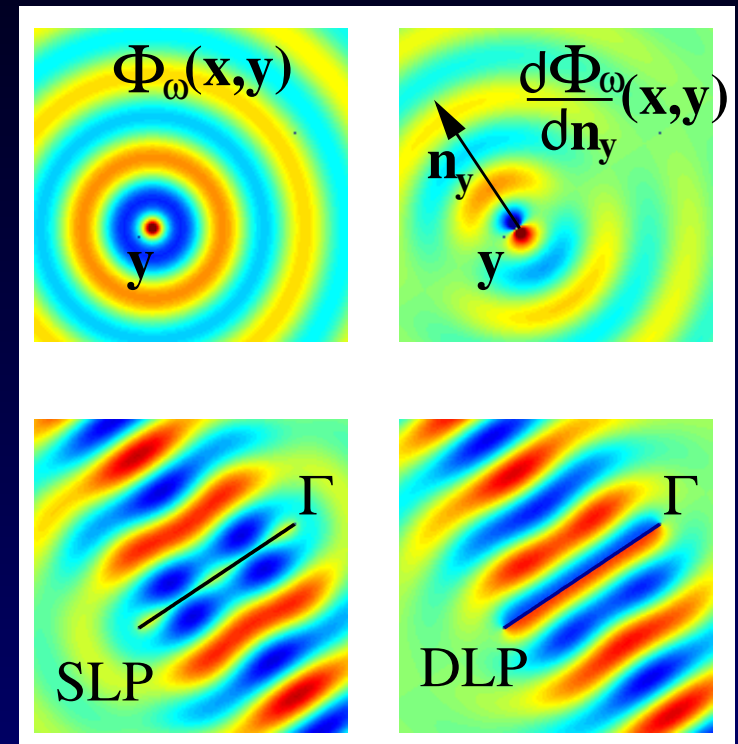
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Jump relation: field limit as $\mathbf{x} \rightarrow \Gamma$ can depend on which side (\pm):

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

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

$$(D\tau)(s) = \int_0^{2\pi} k(s, t)\tau(t)dt \quad 0 \leq t \leq 2\pi \text{ parametrizes } \partial\Omega$$

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

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$$A\tau = b \quad A \text{ matrix} \quad \tau \text{ samples of desired density}$$

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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

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

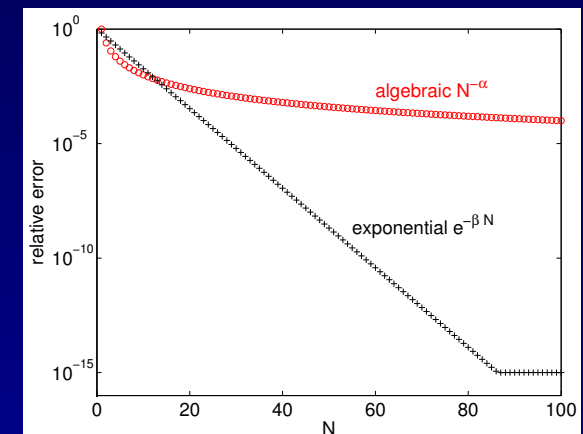
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Theorem (Davis '59): Let f be 2π -periodic, and *real analytic*, meaning $f(z)$ is bounded and analytic in some strip $|\text{Im } z| \leq a$ of half-width $a > 0$. Then there is a const $C > 0$ (indep. of N) such that the error is

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

- 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!



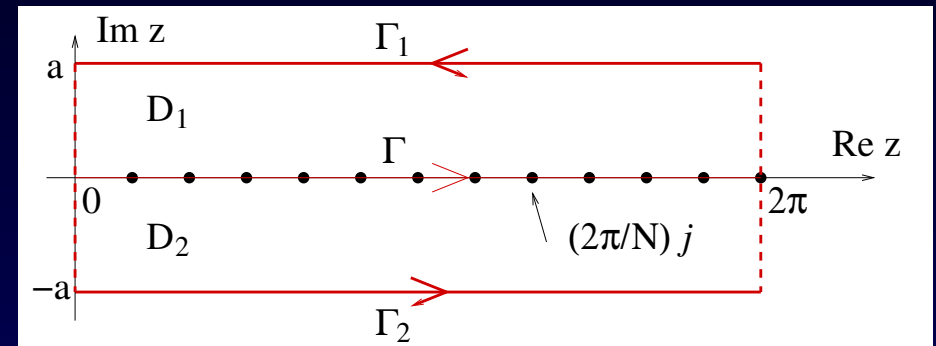
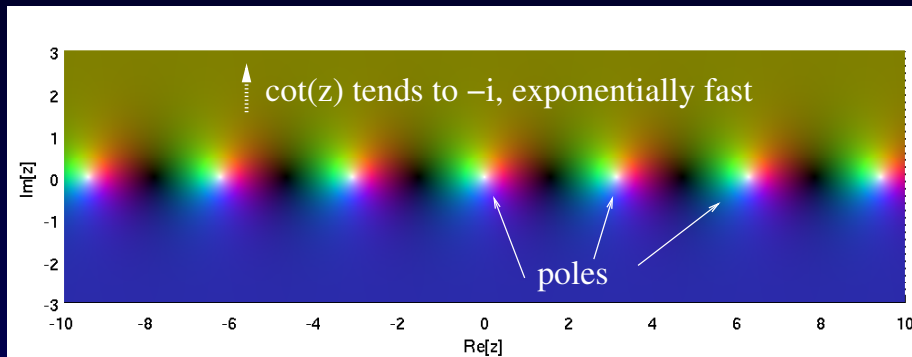
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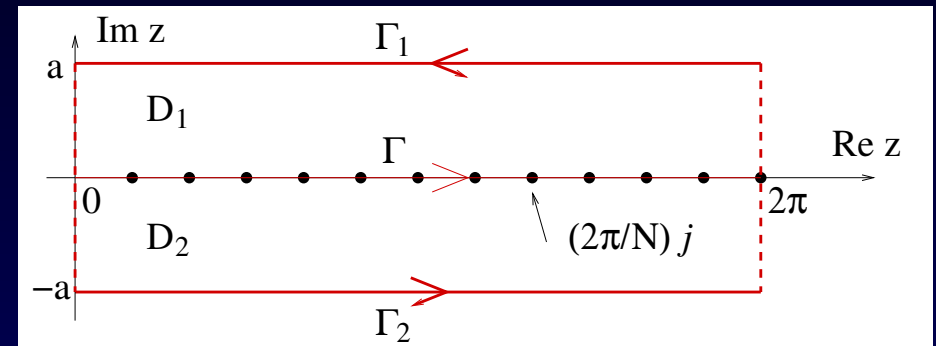
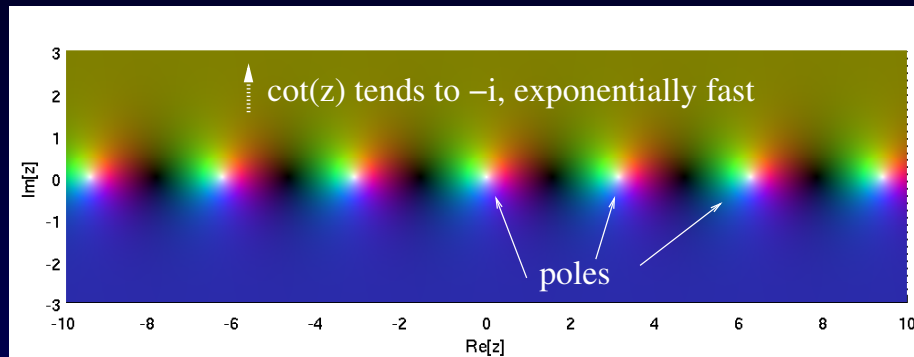
Beautiful cotangent function $\cot(z)$: poles at $\pi j, j \in \mathbb{Z}$, residues 1



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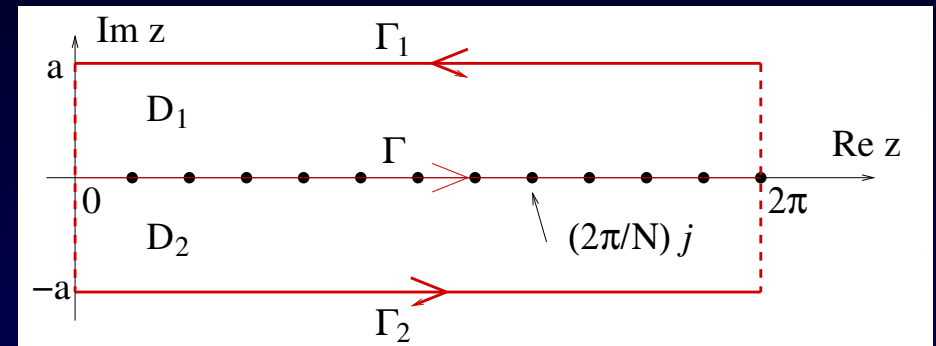
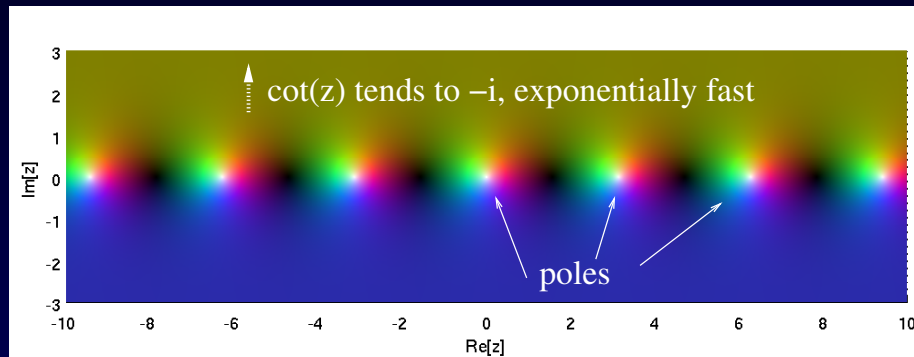


f analytic $\frac{1}{2i} f(z) \cot\left(\frac{N}{2} z\right)$: poles at $\frac{2\pi}{N} j$, residues $\frac{1}{iN} f\left(\frac{2\pi}{N} j\right)$

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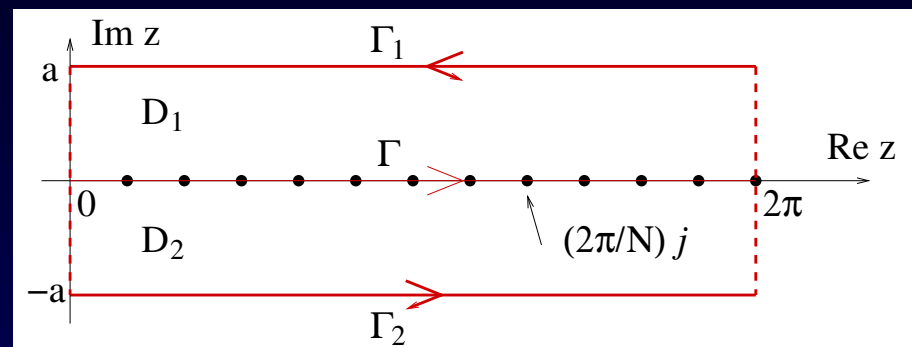
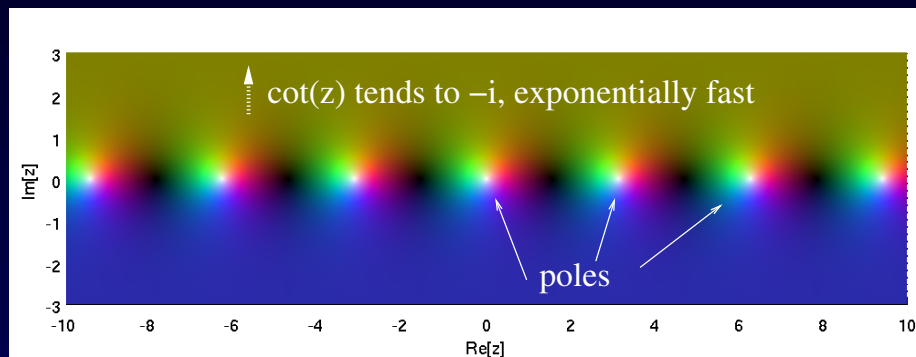
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integrand pure Im on \mathbb{R} , so

Re parts antisymmetric \updownarrow add

Im parts symmetric \updownarrow cancel

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↑
error of our quadrature

↑
exp. small $\leq 2/(e^{aN} - 1)$

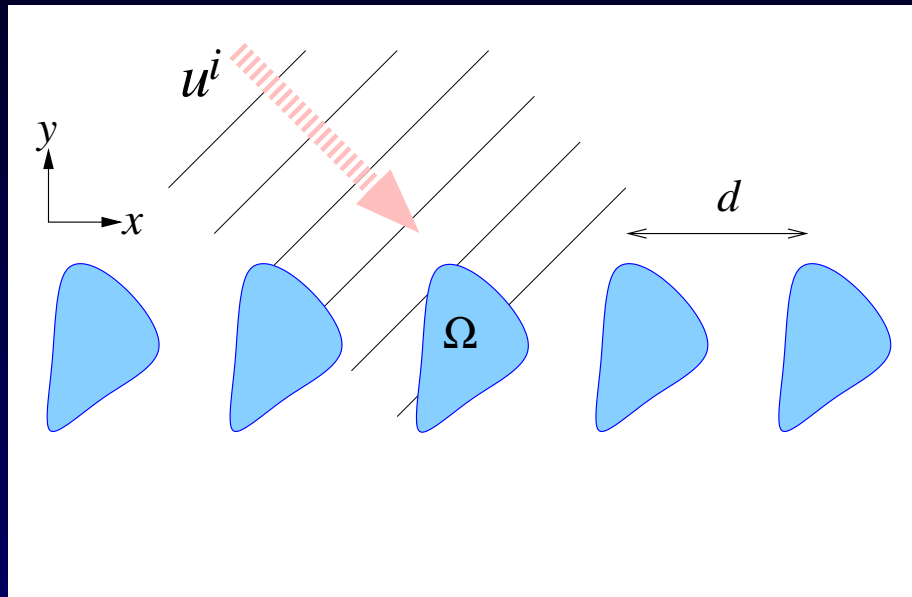
↑
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QED

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

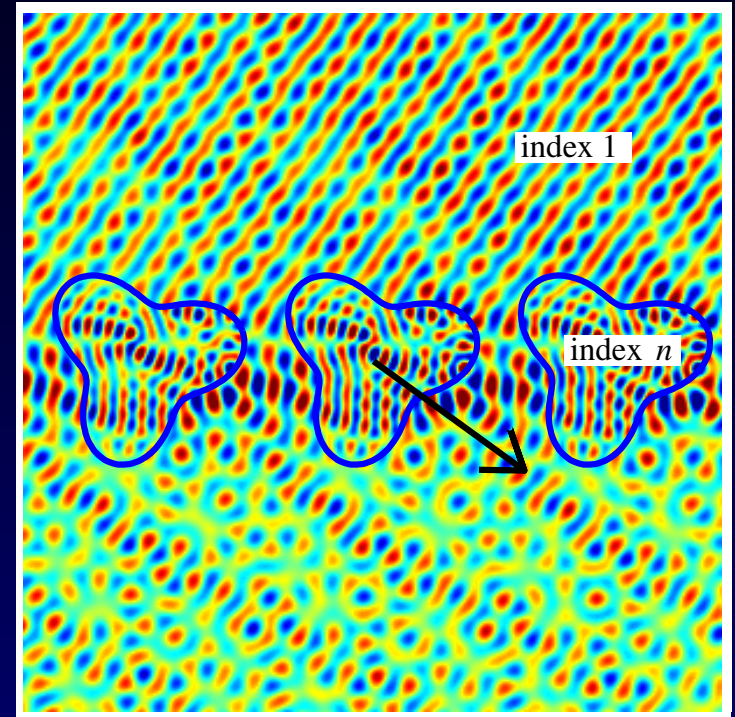
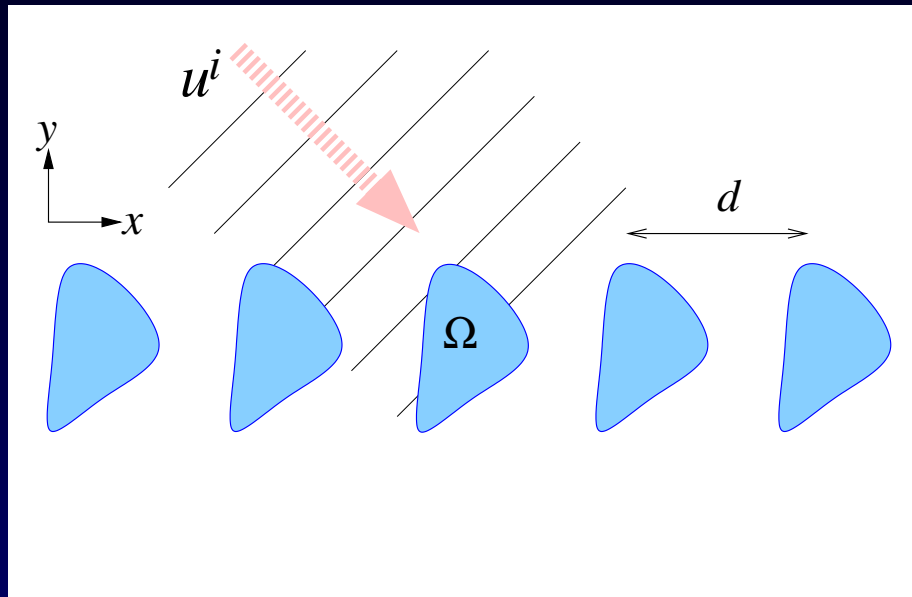
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lattice of obstacles (hint: you don't want to discretize an ∞ long boundary!)



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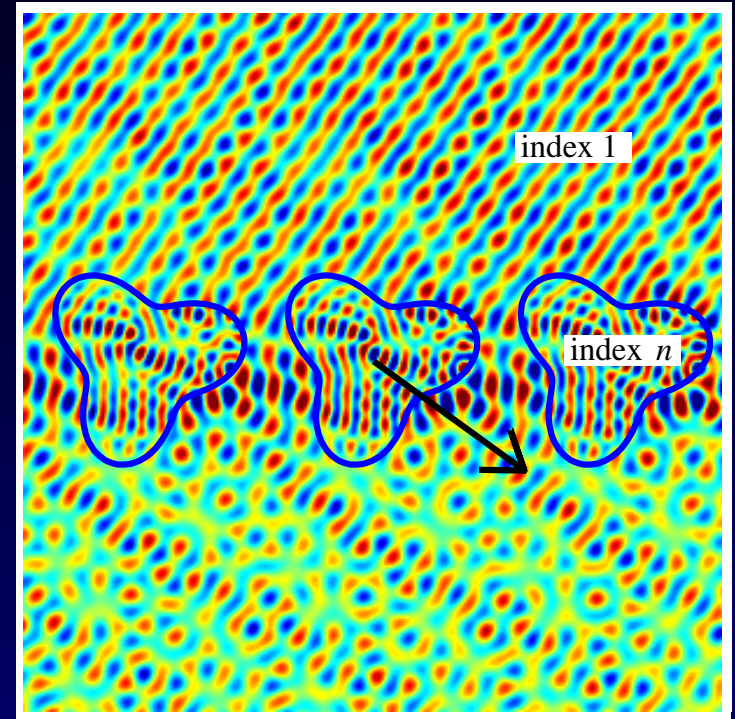
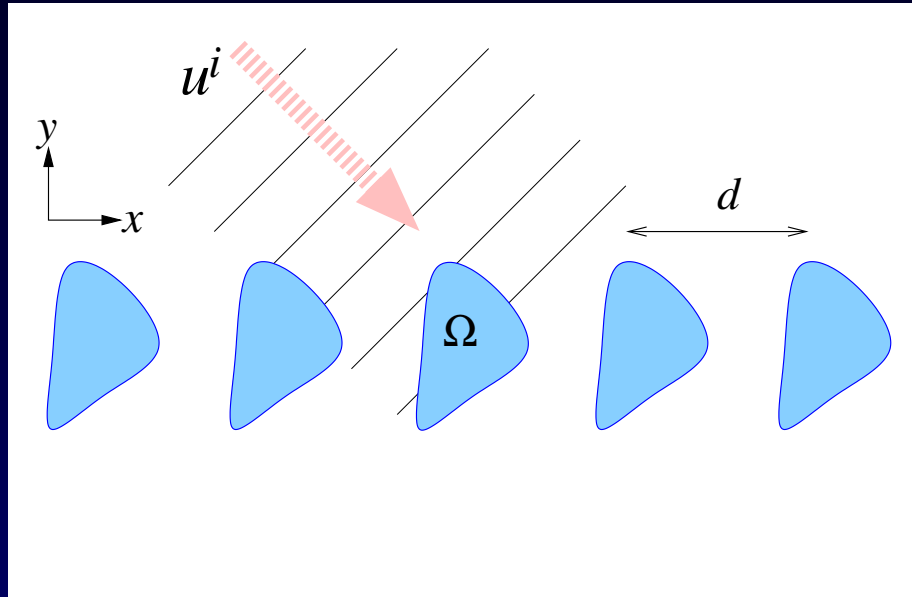


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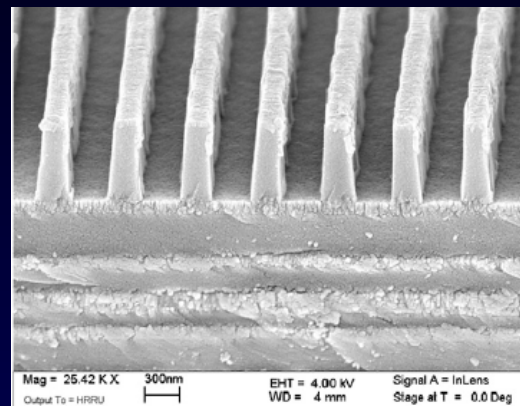
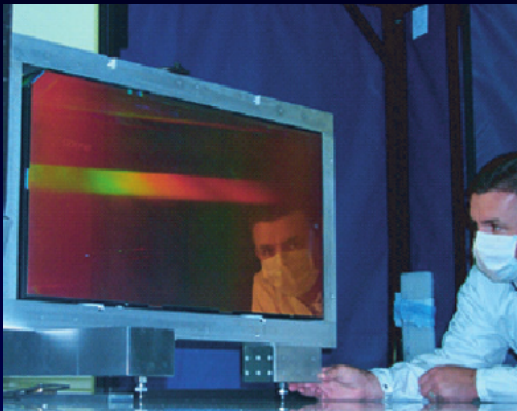
- Research: *robust* way to 'periodize' integral equations in 2D (3D?)

Applications of periodic scattering problems

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

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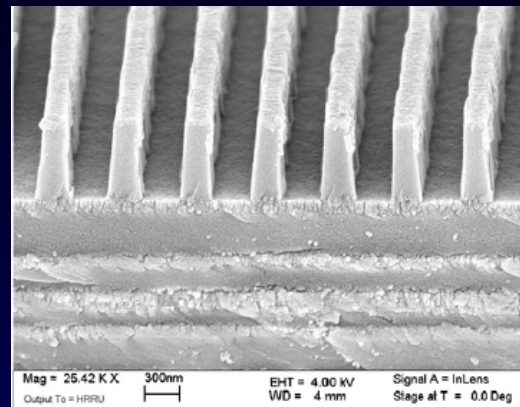
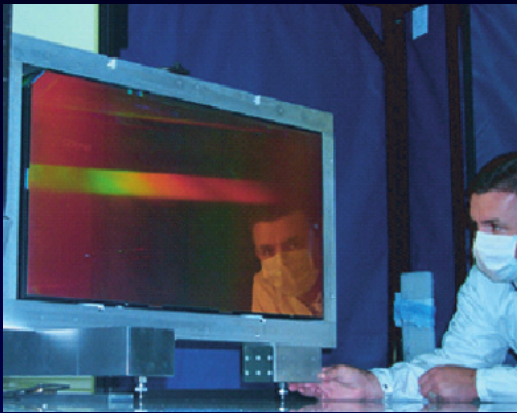
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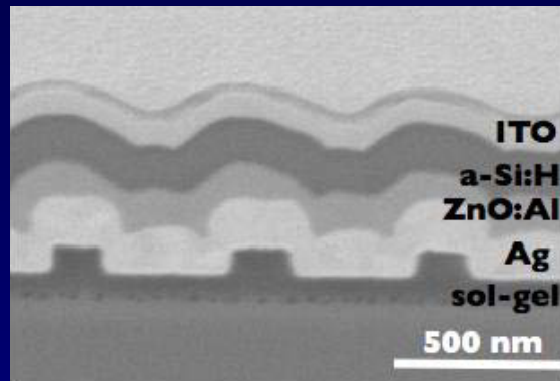
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grating, NIF lasers (LLNL)
 2×10^6 periods! (Barty '04)

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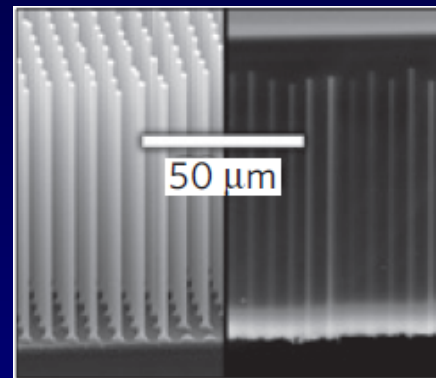
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plasmonic solar cell (Atwater '10)



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!