Accurate and Efficient Numerical Methods for High-frequency 3D Wave Scattering and Periodic Geometries

CIMS Num. Analysis & Sci. Comput. Seminar 2/15/13

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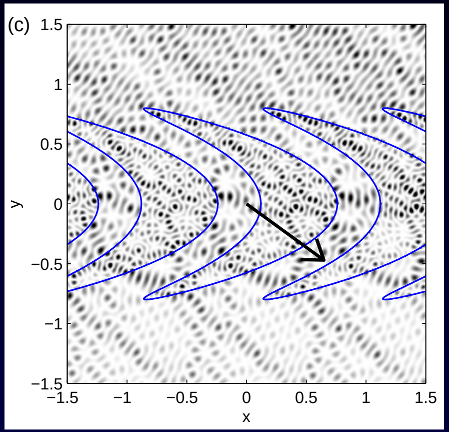
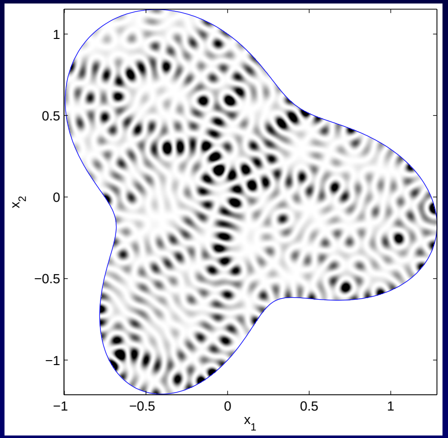
Collaborators: Leslie Greengard (NYU), Andreas Klöckner (NYU), Mike O'Neil (NYU), Zydrunas Gimbutas (NYU), Adrianna Gillman (Dartmouth).

Barnett group research

- numerical methods for scattering of waves
  - time-harmonic (frequency domain)
  - high-order accurate, “fast” algorithms
  - periodic structures, corners, variable media



- eigenvalue problems and quantum chaos
  - fast algorithms for high freq.
  - photonic crystal band structure
  - PDE / numerical analysis



- other applied mathematics: ecology, medical imaging, music

Quantum chaos

Closed cavity (drum) modes

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

Statistics as $j \to \infty$?

- methods $10^3\times$ faster than any other known (B ’06, B–Hassell ’12)
- rigorous error analysis (B ’09, B–Hassell ’11)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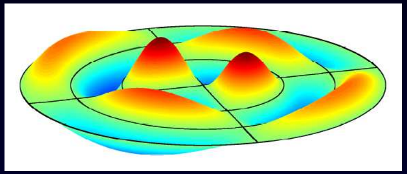
Quantum chaos (see page 41)

Nodal region counts of modes (w/ K. Konrad, snr thesis '12)



ν_j $:=$ # of conn. regions of definite sign in mode j

Thm: $\nu_j \le j$. (Courant '53) $\lim_{j\to\infty} \frac{\nu_j}{j} = r = ?$

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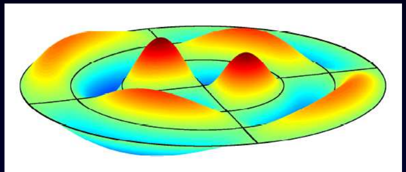

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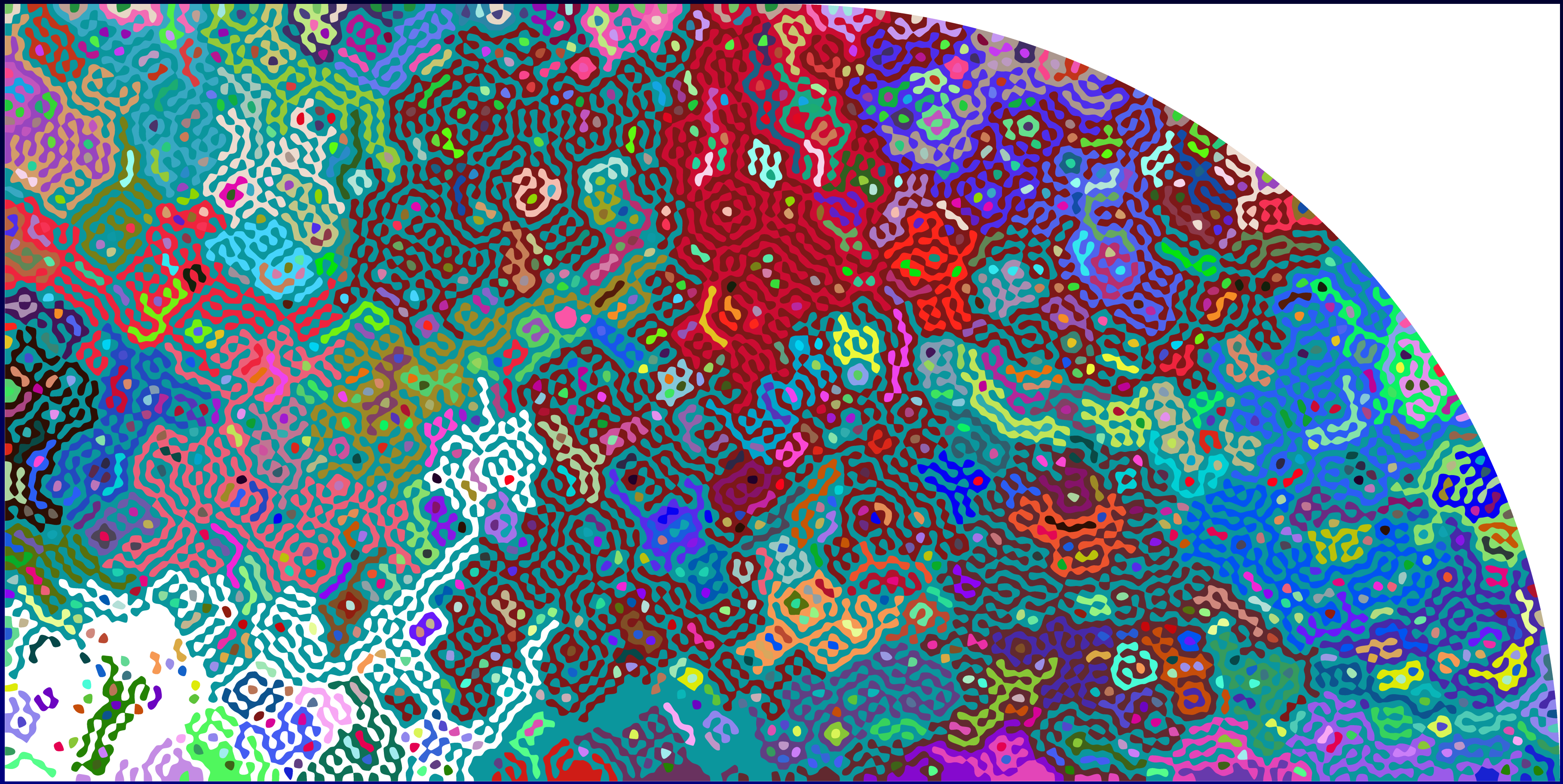


10^9 regions counted. $r \approx 0.0596$ shows conj. 5% off (Bogomolny–Schmit '02)

Today:

- I. New tool for solving high-frequency scattering in 2D and 3D

  accurate near-field evaluation $\rightarrow$ *efficient quadratures*

- II. Robust schemes for solving waves in periodic structures

  low rank property helps solve gratings and crystals

Scattering: motivation & applications

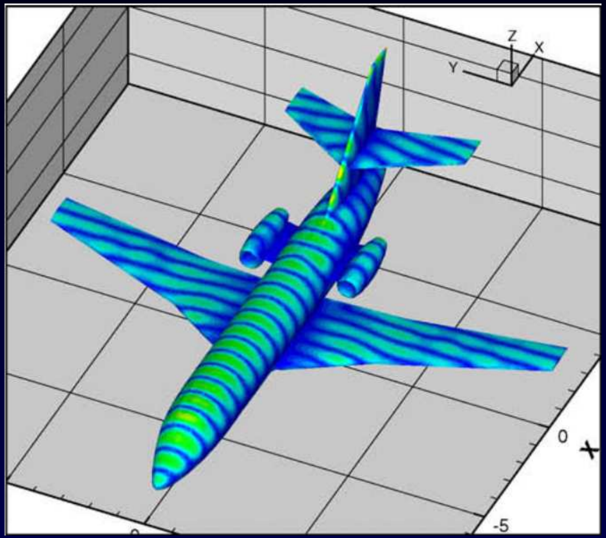
electromagnetics, radar cross section

acoustics, quantum, nanophotonics

devices, lithography, imaging

inverse probs: need good fwd solvers

many involve piecewise-uniform media



(Dolean ’10)

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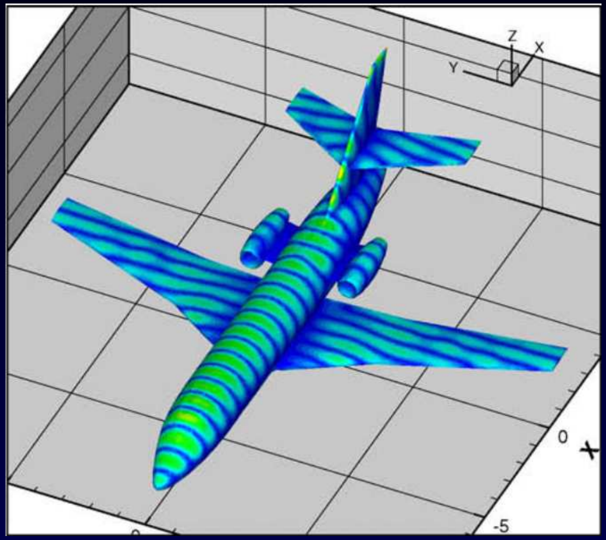

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Need solvers:

- robust — don’t break at certain parameters or geometries
- high-order convergent — reliability, sensitivity anal, optimization
- efficient — optimal complexity: ideally linear in # unknowns

Applications of periodic scattering

Gratings, filters, antennae, photonic crystals, meta-materials, solar…

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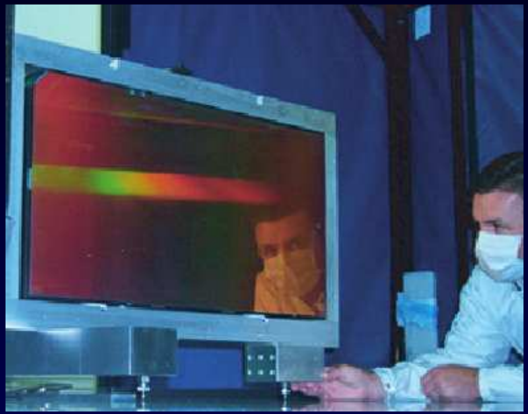

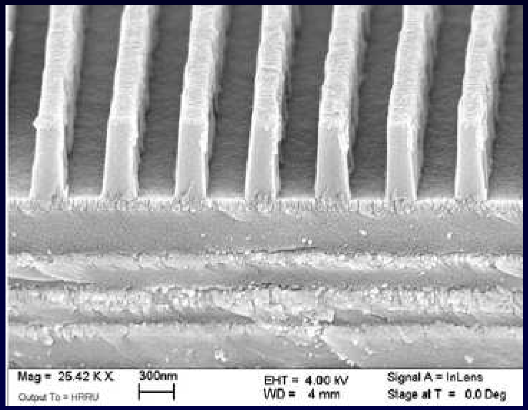

multi-layer dielectric diffraction grating, NIF lasers (LLNL)

2×10^6 periods! (Barty '04)

Applications of periodic scattering

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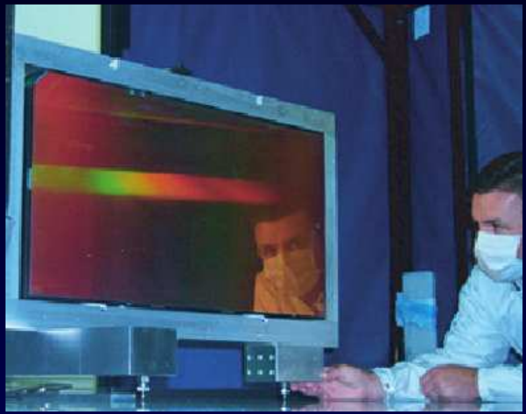

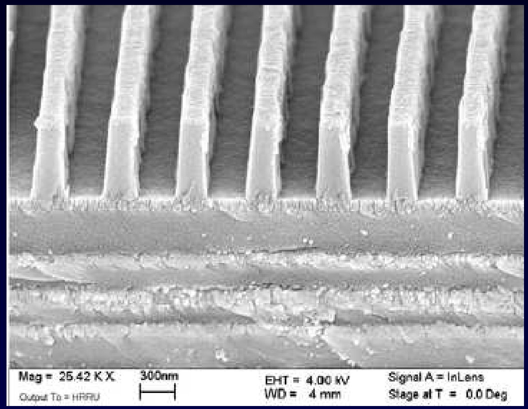

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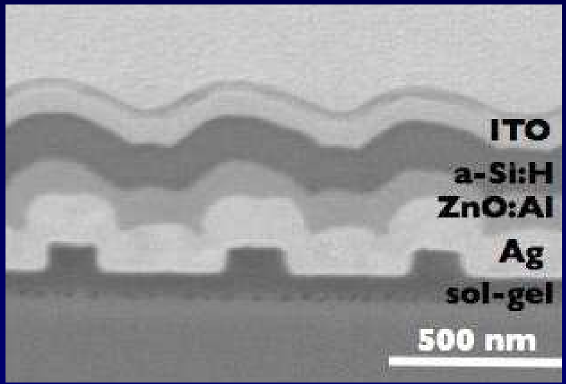
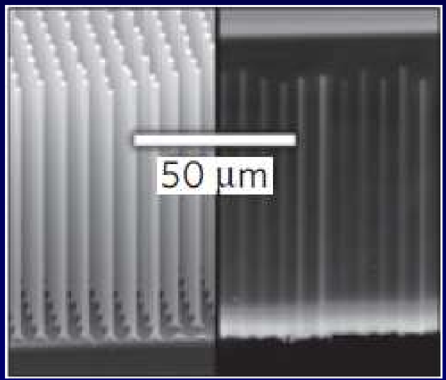


plasmonic solar cell (Atwater '10)



$\updownarrow$ high aspect ratio

Si microwires absorber (Kelzenberg '10)

- Design optimization
- Simulation at $>10^3$ inc. angles, frequencies

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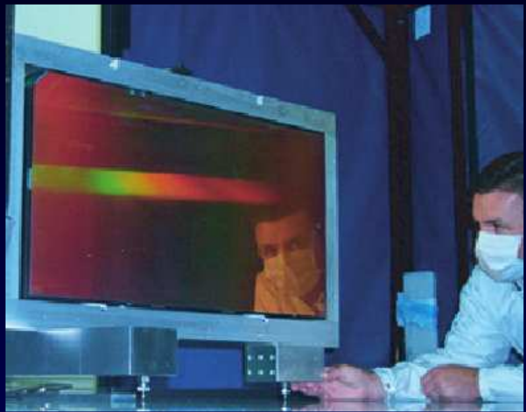
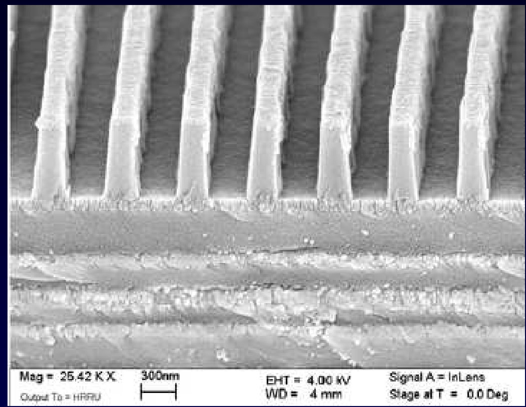
Gratings, filters, antennae, photonic crystals, meta-materials, solar…





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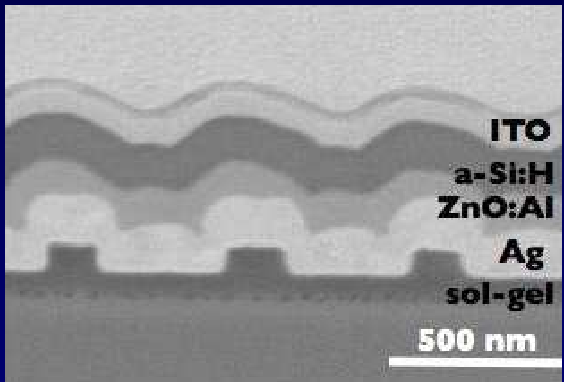

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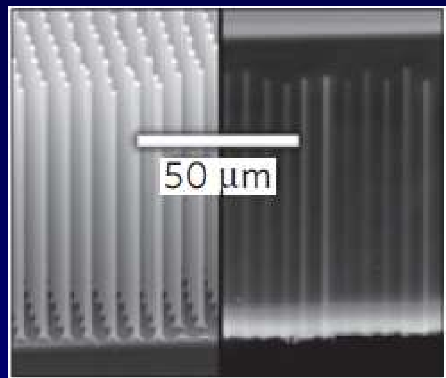

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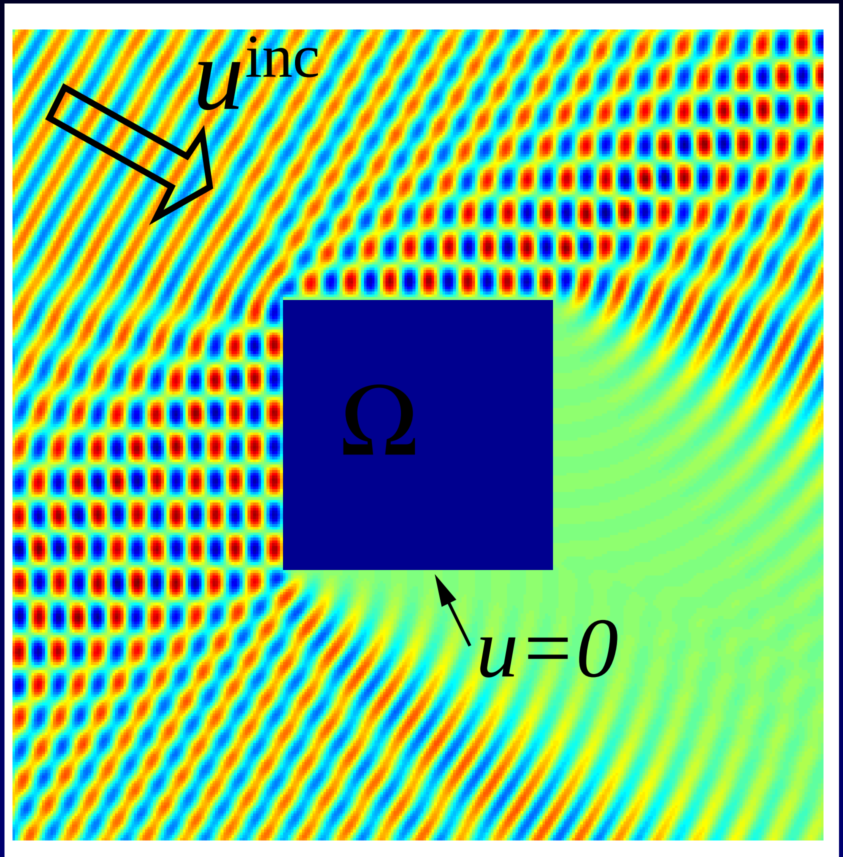
But first some old and new tools for the non-periodic case…

I. Scattering of time-harmonic waves

freq. ω, wavelength $\lambda = \frac{2\pi}{\omega}$ obstacle $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, bdry $\partial\Omega$



plane wave $u^{\text{inc}}(\mathbf{x}) = e^{i\omega\hat{n}\cdot\mathbf{x}}$

physical field $u^{\text{tot}} = u^{\text{inc}} + u$

scattered field u obeys BVP:

$$\begin{aligned}(\Delta + \omega^2)u &= 0 && \text{in } \mathbb{R}^d \backslash \overline{\Omega} \\ u &= -u^{\text{inc}} && \text{on } \partial\Omega\end{aligned}$$

Sommerfeld radiation condition:

$$\frac{\partial u}{\partial r} - i\omega u = o(r^{-(d-1)/2}), \quad r \to \infty$$

$\exists$ unique soln. Sound-soft acoustics / Maxwell TM ($u = E_z$, $\partial\Omega$=PEC)

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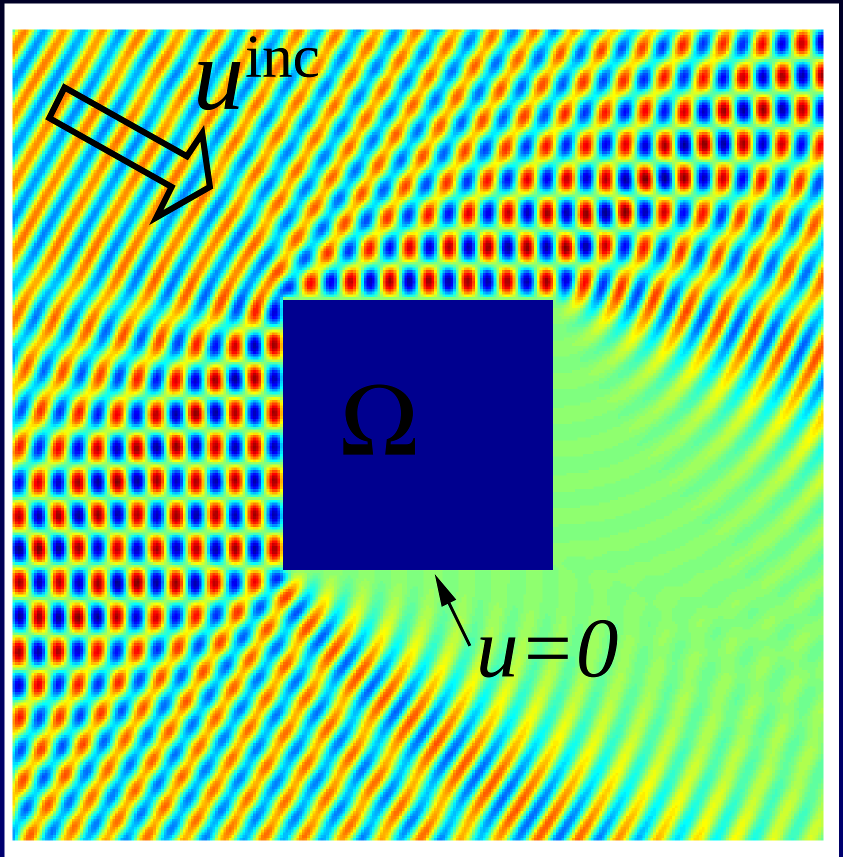

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Errors 10^{-10} (as here) demands high-order … how do this cheaply?

Discretizing: volume vs boundary?

Conventional numerical PDE solution: mesh volume, N unknowns

e.g. finite differencing, finite elements

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Problems:

(1) needs many unknowns per wavelength: $N > O(\omega^d)$

"pollution" (Babuska–Sauter)

(2) meshing expensive (d=3)

(3) must truncate to finite domain w/ approximate rad. cond.

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Fredholm integral equation reminder: given kernel $k(t,s)$ cont. for $s \neq t$

solve for func. τ: $$c\tau(t) + \int_0^{2\pi} k(t,s)\tau(s)ds \;=\; f(t), \quad \forall t \in (0, 2\pi)$$

- if $c = 0$: 1st-kind, ill-posed. Discretize $\rightarrow$ ill-cond. as N grows
- if $c \neq 0$: 2nd-kind, always $\exists$ unique solution; well-cond. indep of N

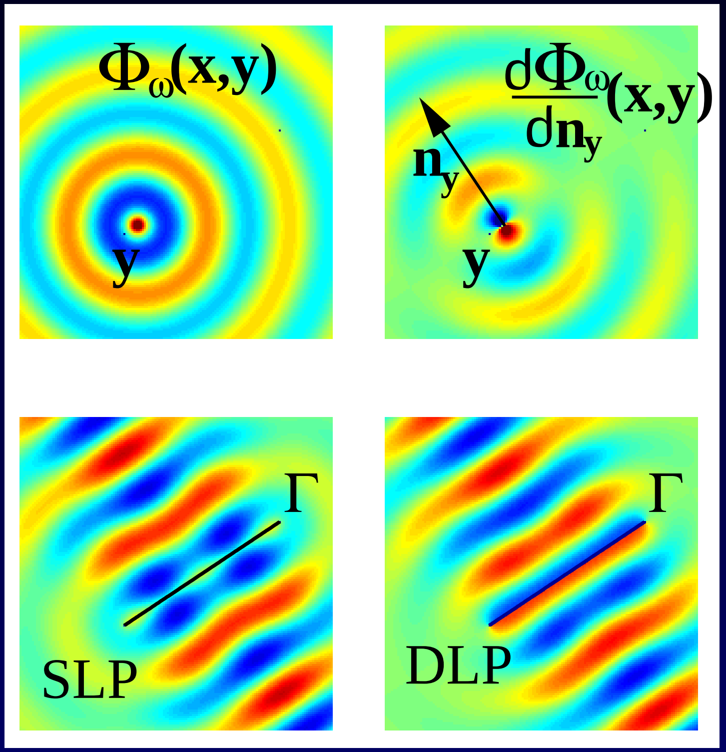
Representing PDE solns: potential theory

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

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

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

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



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

kernel is Helmholtz fundamental soln

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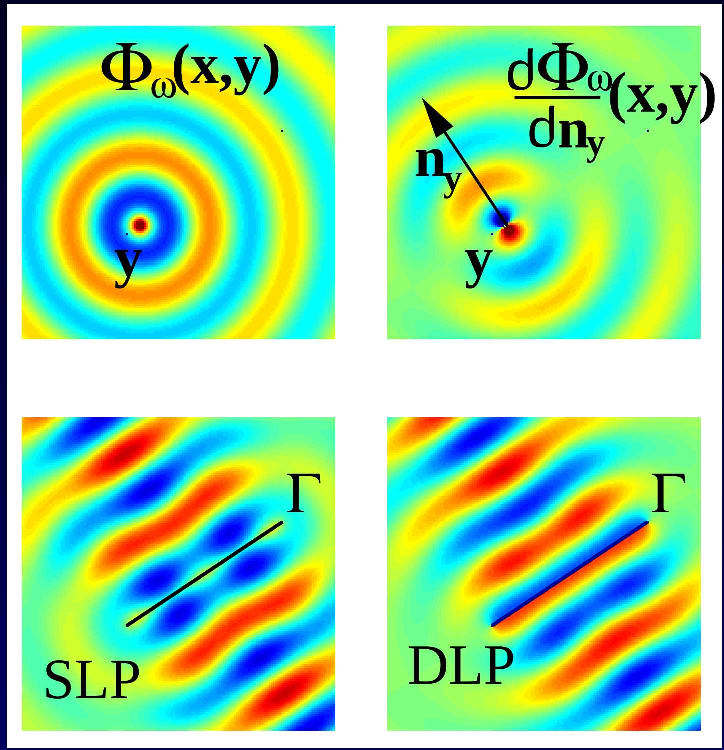

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Jump relations: field limit as $\mathbf{x} \to \Gamma$ can depend on which side ($\pm$):

$v^\pm = S\sigma$ no jump

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

S, D bdry integral ops w/ above kernels, both bounded in $C(\Gamma) \to C^1(\Gamma)$

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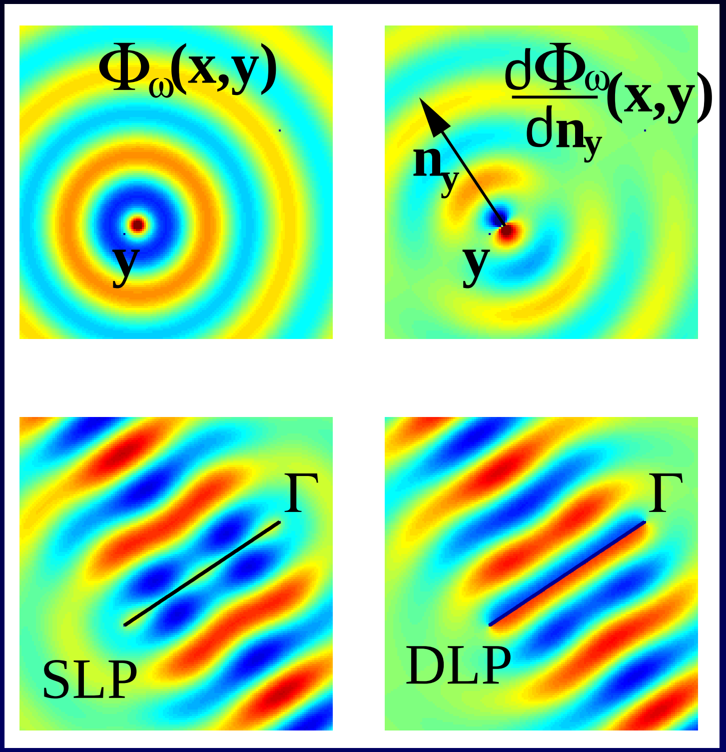

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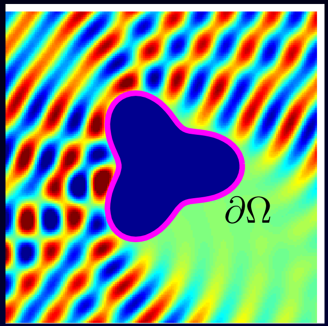
- From now fix $\Gamma = \partial\Omega$ i.e. densities live on obstacle boundary

Single obstacle



scatt. field $u = (\mathcal{D} - i\omega\mathcal{S})\tau$ "combined field repr."

BC & JR: $A\tau := (\frac{1}{2}I + \underbrace{D - i\omega S}_{K,\ \text{kernel } k \text{ weakly singular}})\tau = -u^{\text{inc}}|_{\partial\Omega}$

2nd-kind IE $\nearrow$

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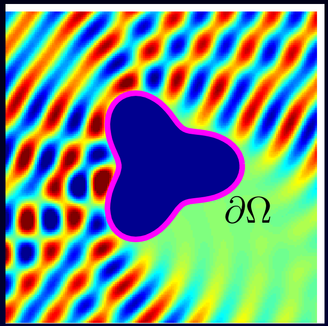

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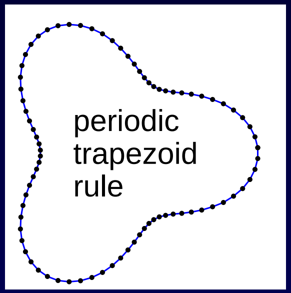
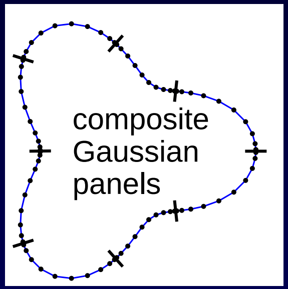
Smooth quadrature: $j = 1, \ldots, N$

nodes $\mathbf{y}_j \in \partial\Omega$, weights w_j





Approx. by dense $N \times N$ linear system:

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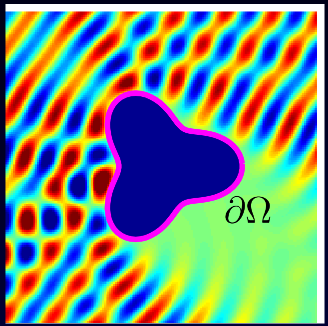

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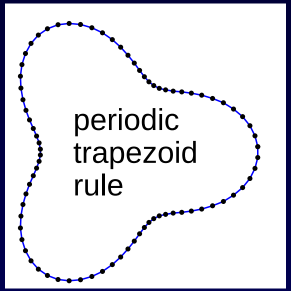

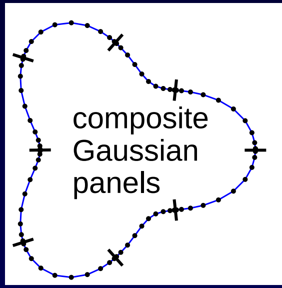

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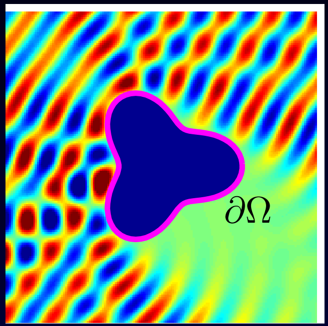

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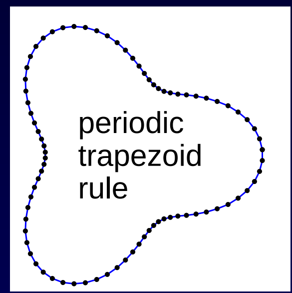

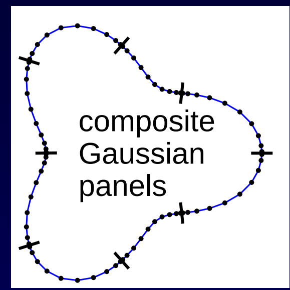

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Distant panels easy: $A_{ij} = k(\mathbf{y}_i, \mathbf{y}_j)w_j$ high-order accurate
Self / neighbor panels hard, esp. in 3D singularity e.g. $k \sim 1/r$ in 3D

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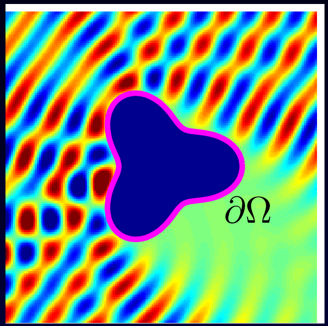

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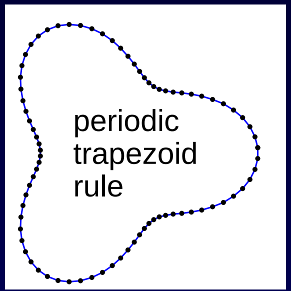

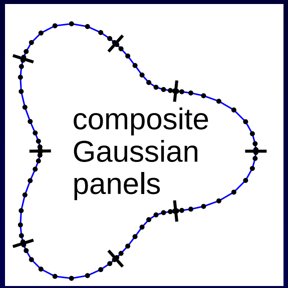

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Exploit: $\boxed{\text{applying } \boldsymbol{A} \ = \ \text{evaluating } u^+ \text{ due to } \boldsymbol{\tau}\text{'s interpolant density}}$

Problem of near-boundary field evaluation

Simpler case: 2D interior Laplace ($\omega = 0$) $\partial\Omega$ param by $Z(s)$, $s \in [0, 2\pi)$

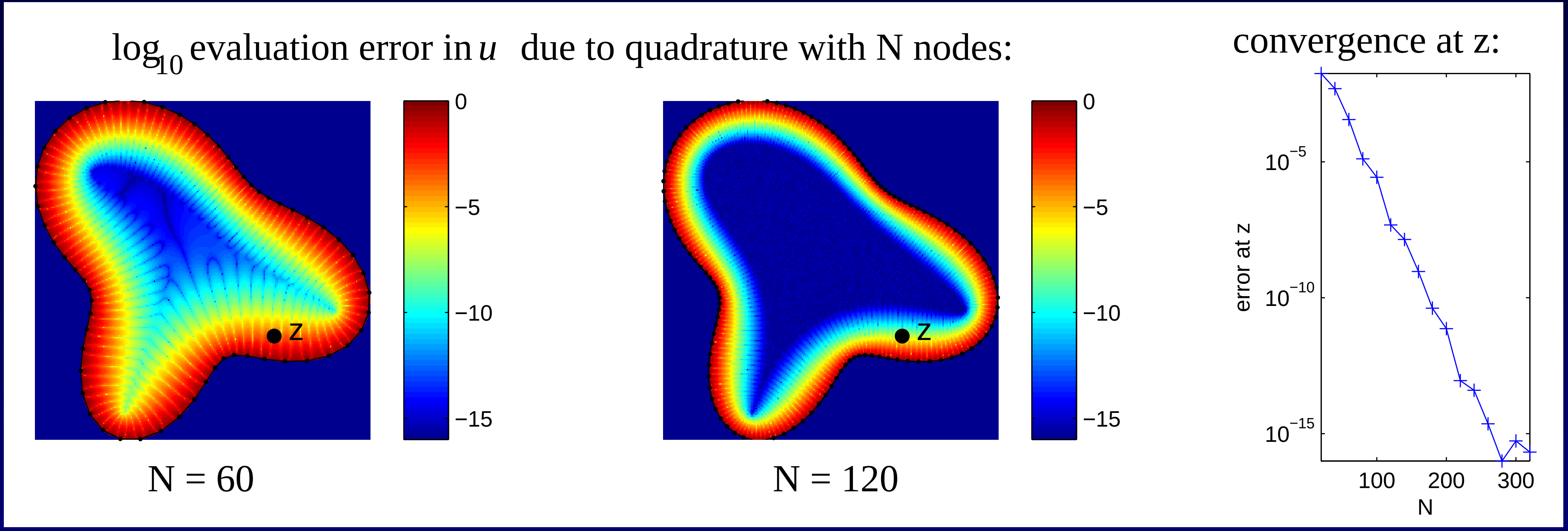
say want eval. $u = \mathcal{D}\tau$ $u = \operatorname{Re} v$, $v(z) = \frac{i}{2\pi} \int_{\partial\Omega} \frac{\tau(y)}{z - y} dy$

Problem of near-boundary field evaluation

Simpler case: 2D interior Laplace ($\omega = 0$) $\quad$ $\partial\Omega$ param by $Z(s)$, $s \in [0, 2\pi)$

say want eval. $u = \mathcal{D}\tau$ $\qquad u = \operatorname{Re} v, \quad v(z) = \dfrac{i}{2\pi}\displaystyle\int_{\partial\Omega} \frac{\tau(y)}{z-y}dy$

Use periodic trapezoid rule (N nodes uniform in param s) :

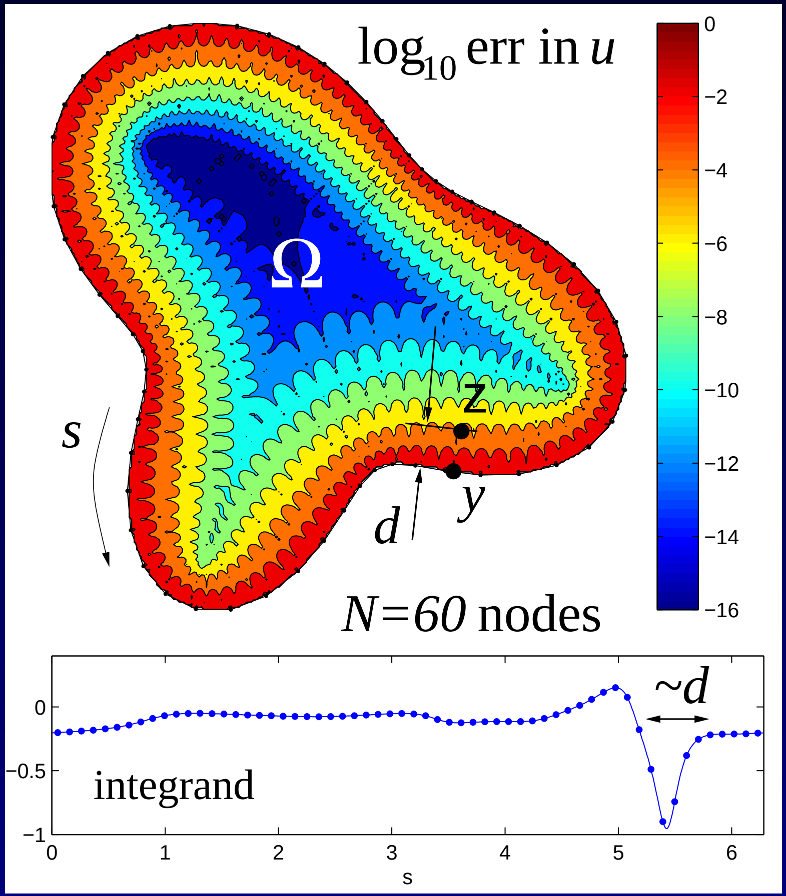


- exponential convergent, but rate arbitrarily slow as $z \to \partial\Omega$

  Thm (B '12): rate = dist. of $Z^{-1}(z)$ from real axis in complex s plane

Why is close evaluation hard?

$$u = \mathrm{Re}\, v, \qquad v(z) = \frac{i}{2\pi}\int_{\partial\Omega}\frac{\tau(y)}{z-y}dy,$$ approx. by N-node quadr



target $z \to \partial\Omega$: integrand non-smooth

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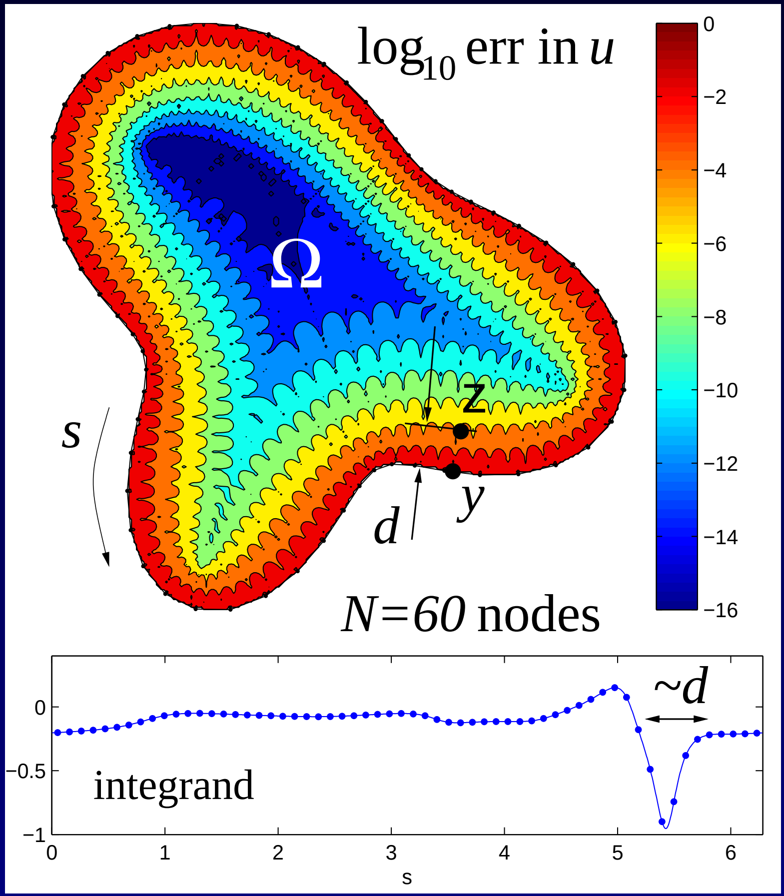

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- adaptive quad? v. slow as $z \to \partial\Omega$ done afresh for each target point

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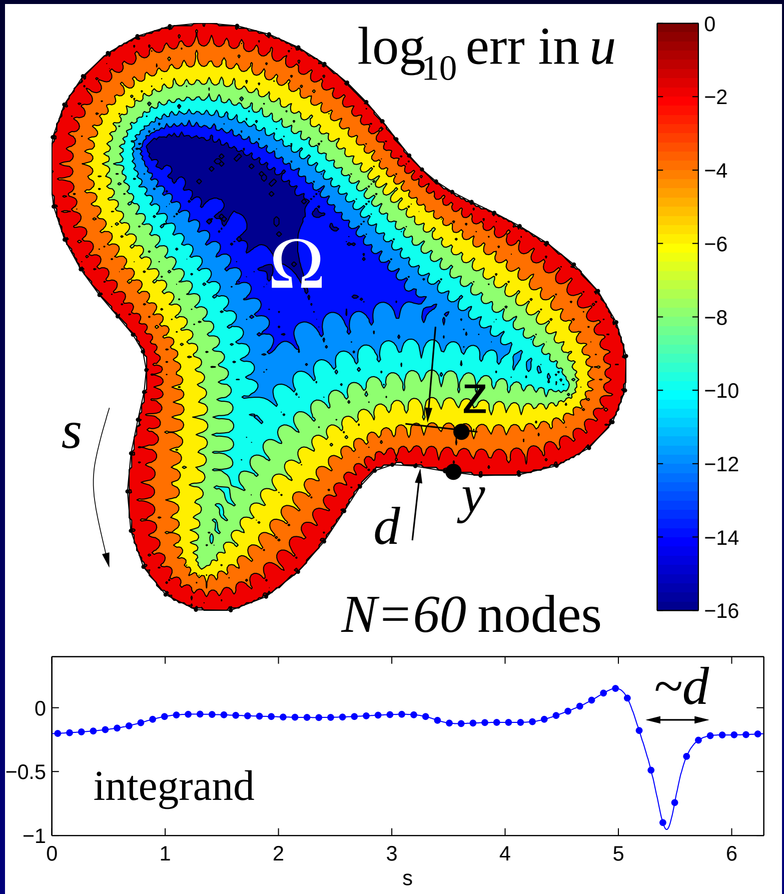

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2D case recently solved efficiently

(Helsing–Ojala '08, Helsing '12)

But want scheme which generalizes simply to 3D …

Quadrature By eXpansion (QBX)

(B '12)

(Klöckner-B-Greengard-O'Neil '12)

τ, $v|_{\partial\Omega}$ analytic $\Rightarrow$ v extends analytically some dist. outside Ω

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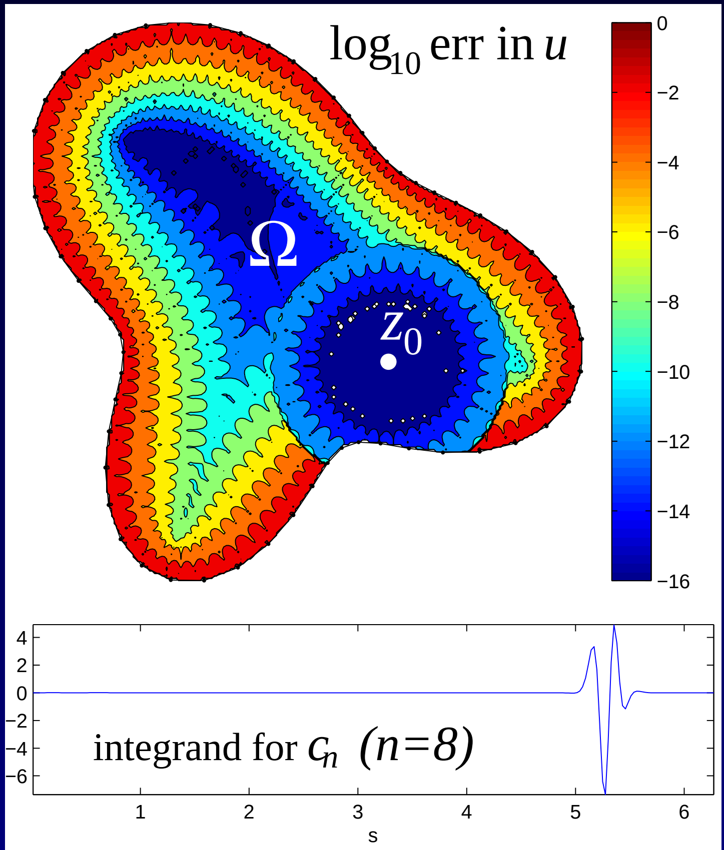
Taylor exp. $v(z) = \sum_{n=0}^{\infty} c_n (z - z_0)$ rad. of conv. ρ takes you beyond $\partial\Omega$



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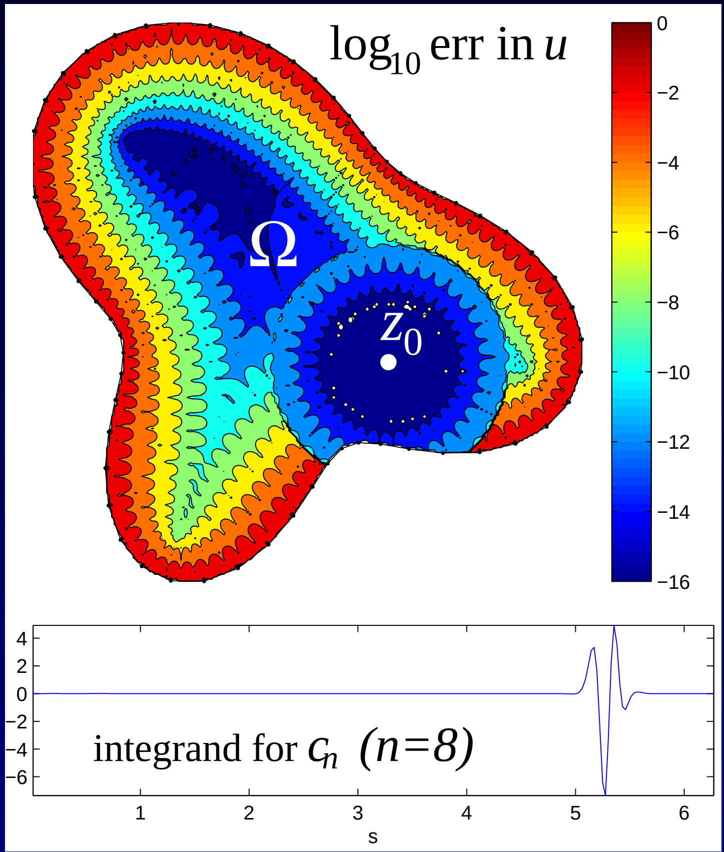

- pick center z_0 about $2.5h$ from $\partial\Omega$
- eval. p terms via Cauchy,

$$c_n = \frac{v^{(n)}(z_0)}{n!} = \frac{i}{2\pi} \int_{\partial\Omega} \frac{\tau(y)}{(z-y)^{n+1}} dy$$

integrand more osc. $\Rightarrow$ need βN nodes, $\beta \approx 4$
interpolate τ from original N

- eval. Taylor exp. in $|z - z_0| \leq R < \rho$
- repeat for z_0's all around $\partial\Omega$

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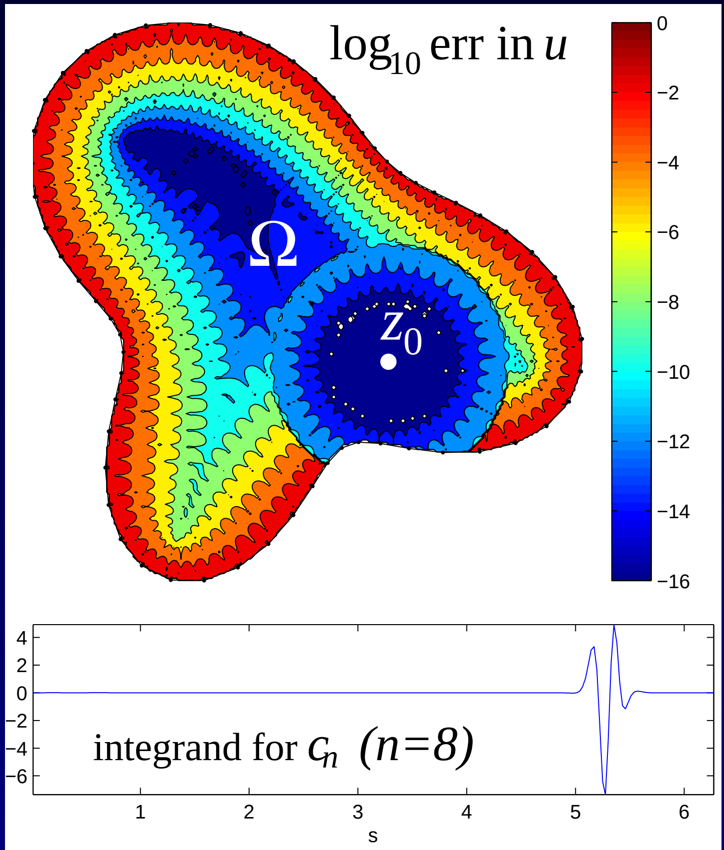

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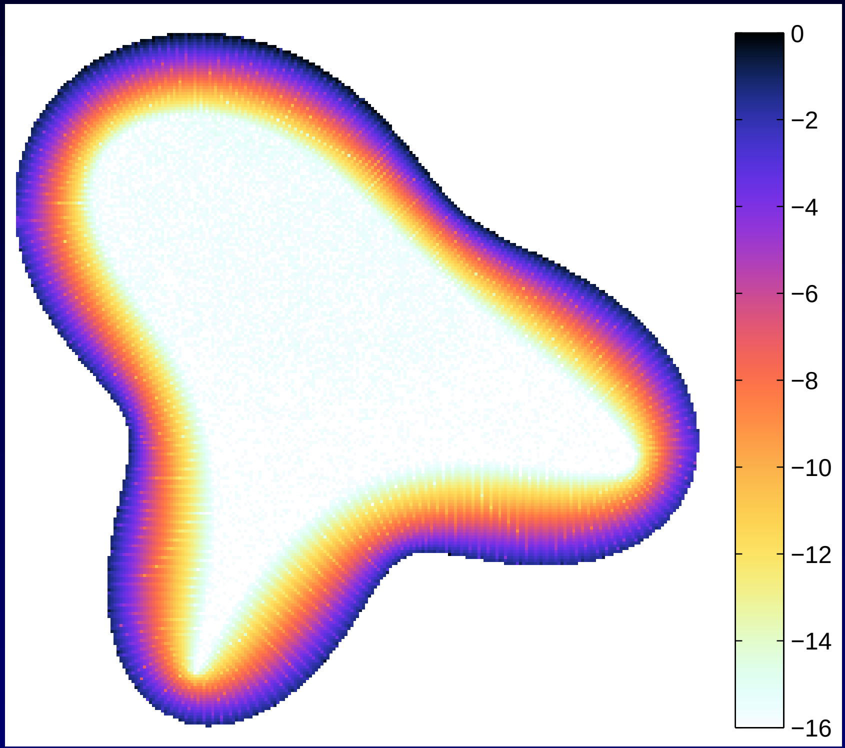
Thm. (B) error $\le C\left(\frac{R}{\rho}\right)^p + Cp\left(\frac{C\beta}{p}\right)^p e^{-C\beta}$ asymp. exponential conv. in p, β

QBX for close eval: interior Laplace BVP

As before, double-layer rep. $u = \mathcal{D}\tau$ exact soln $u(x, y) = e^y \cos x$

$\log_{10}$ relative err, $N = 130$



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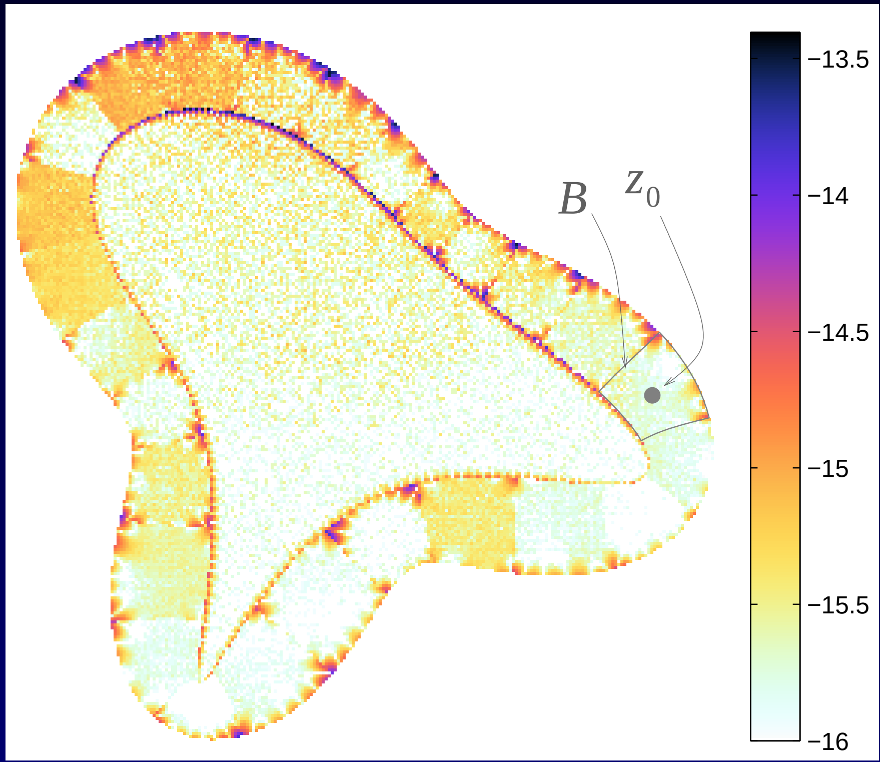

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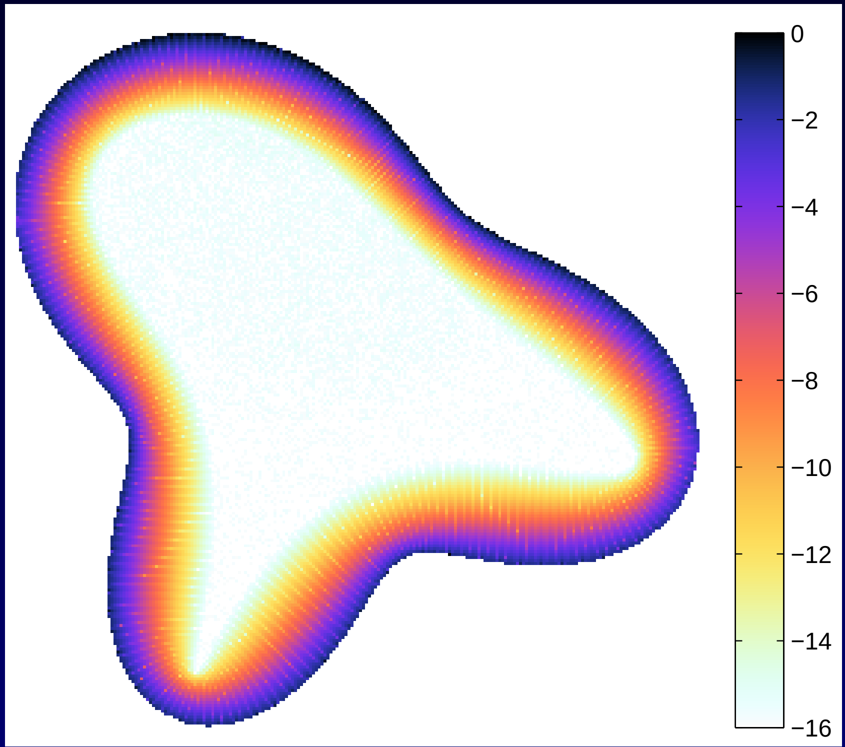

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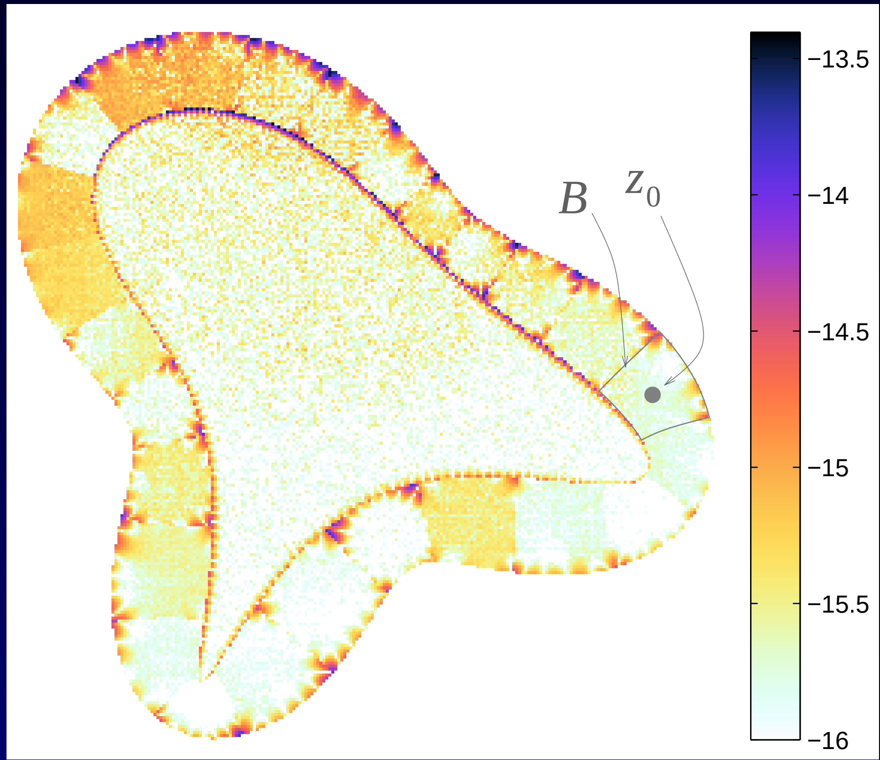

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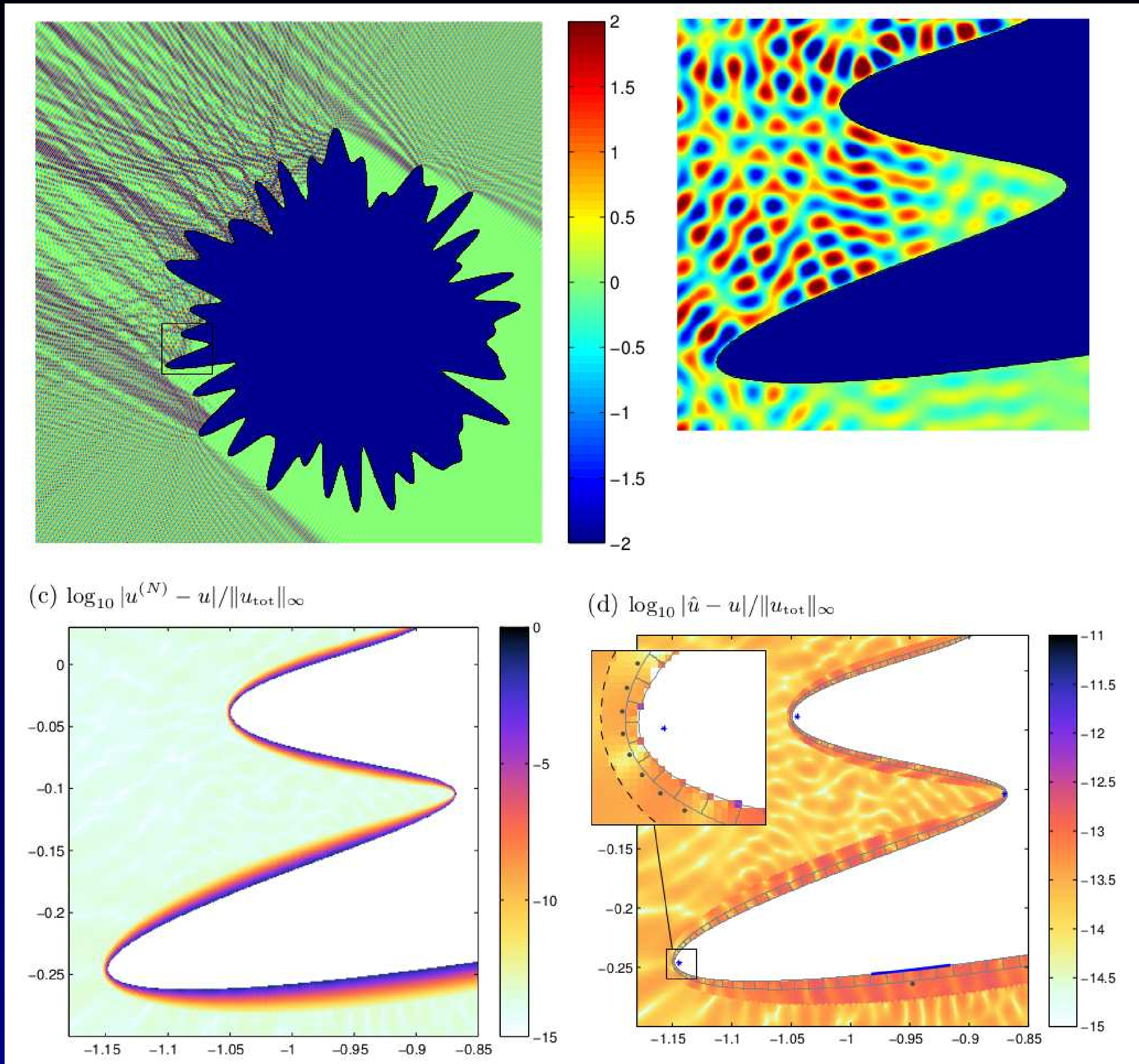
Helmholtz ($\omega>0$):

- Taylor $\to$ local expansion $\sum_{|n|<p} c_n J_n(\omega r) e^{in\theta}$
- Cauchy $\to$ Graf's addition theorem



QBX, high freq. close eval. for Helmholtz

100 λ diam.

700 λ perimeter

N=9000 unknowns

fill + solve   87 sec

FMM eval in 24 sec
   (8×10^6 pts)

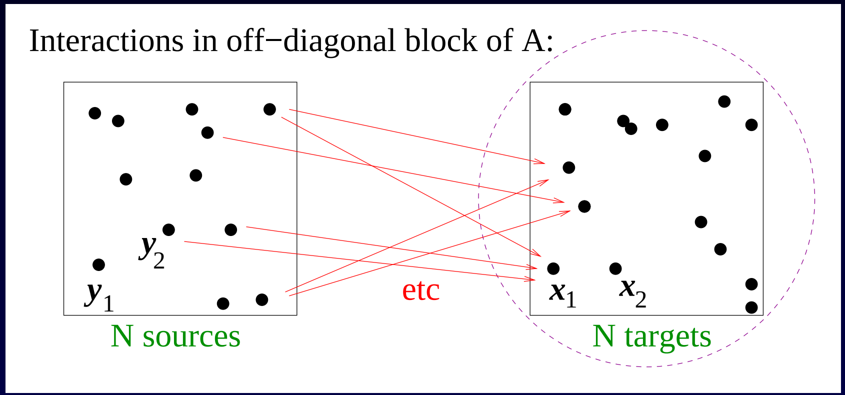
QBX in 28 sec
   (2×10^5 pts)

rel. error $< 10^{-11}$

(B ’12)

Fast algorithms for evaluation & applying A

Kernels (Green's funcs) special between "distant" boxes:



$$A_{ij} = k(\mathbf{x}_i, \mathbf{y}_j)$$

N^2 elements

$$\text{rank}(A) \;:=\; \{\#\text{ sing. vals. } > 10^{-16}\} \;=\; ?$$

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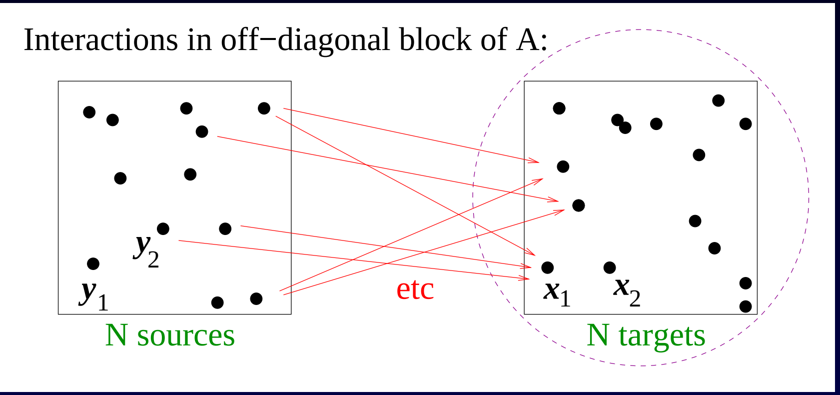

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≈ 20, indep of N ! $\quad$ low rank

Proof? $\quad u|_{\text{targets}} \approx$ loc. exp. in ball

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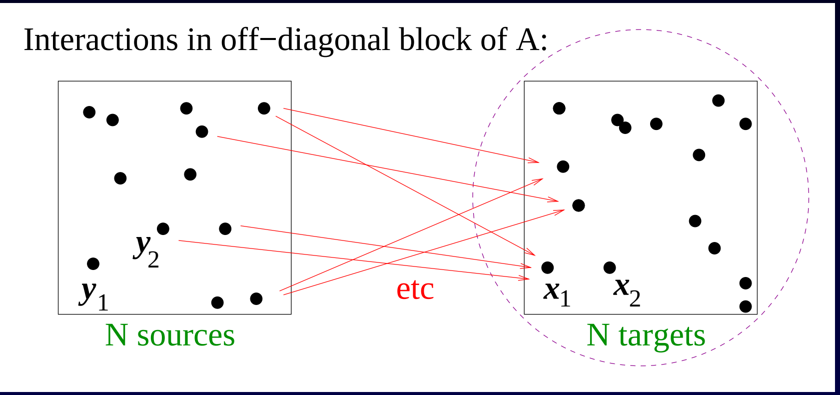

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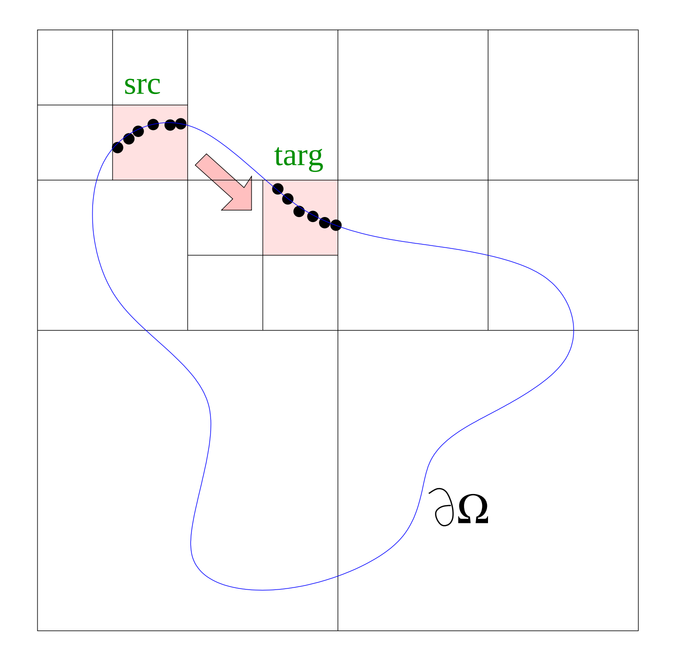
Fast Multipole Method (FMM): (Greengard–Rokhlin '87)



does dense matrix-vector prod. in $O(N)$

hierarchical subdivision (quad-tree)

distant interactions: LE's & multipoles

combine MP up tree, split LE down tree

Summary of panel-based $O(N)$ scattering solver

(1) For each target panel, use QBX to precompute A_{ij} for
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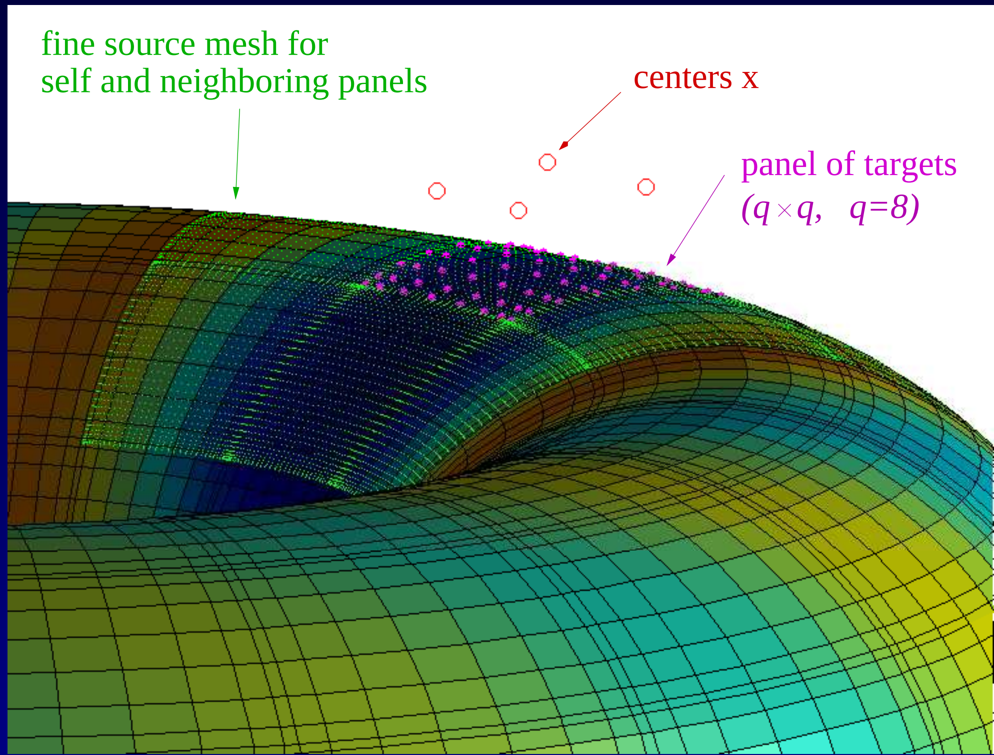
3D: panels $q \times q$ Gauss nodes

Local expansion $u(r,\theta,\phi) =$

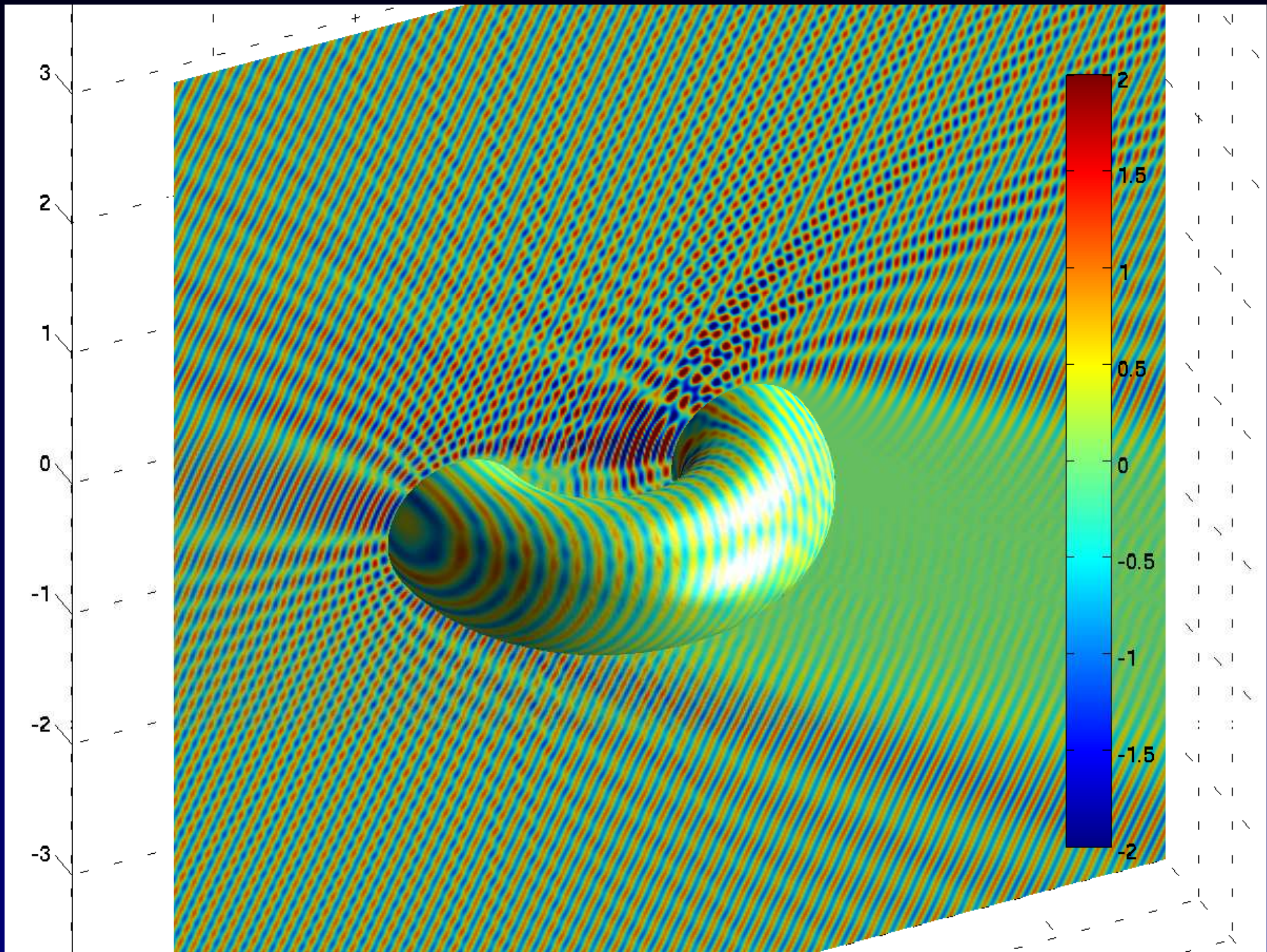
$$\sum_{|n|\le p} \sum_{m=-n}^{n} c_{nm} j_n(\omega r) Y_n^m(\theta,\phi)$$

spherical harmonic addn thm



- $p+1$ th order proven, $\tau \in W^{p+3+\epsilon,2}$ (Epstein–Greengard–Klöckner ’12)

3D high-freq. torus scattering result



30λ diameter
($1800\ \lambda^2$ surf. area)

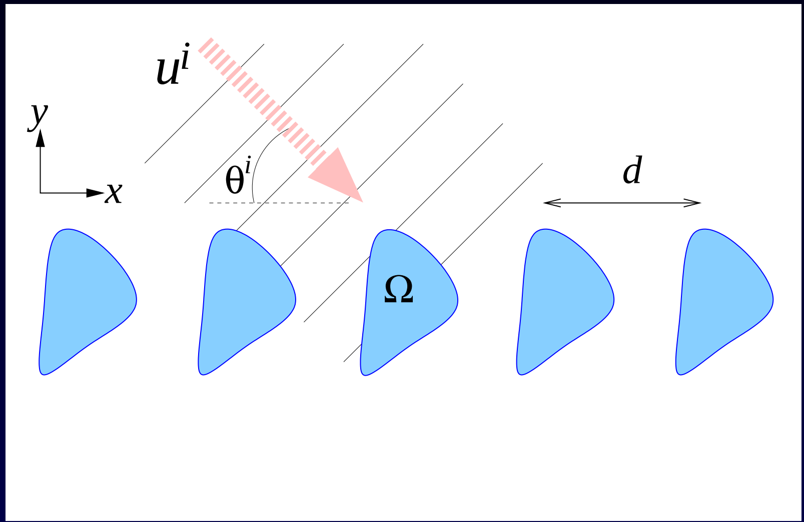
$N \approx 145000$
q=8, p=10, β=4.5

QBX quad 1.2 hr
GMRES 1 hr (57 its)
laptop (4-core i7)

relative error 10^{-5}

- FEM/FDTD at this high accuracy & freq. prohibitive
- Corners also handled in 2D;   3D edges/corners ongoing work . . .

II. Quasi-periodic scattering from grating



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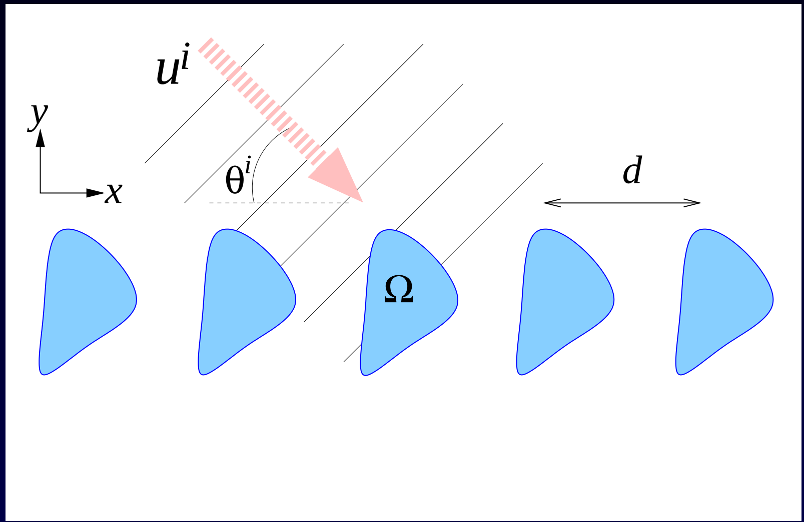

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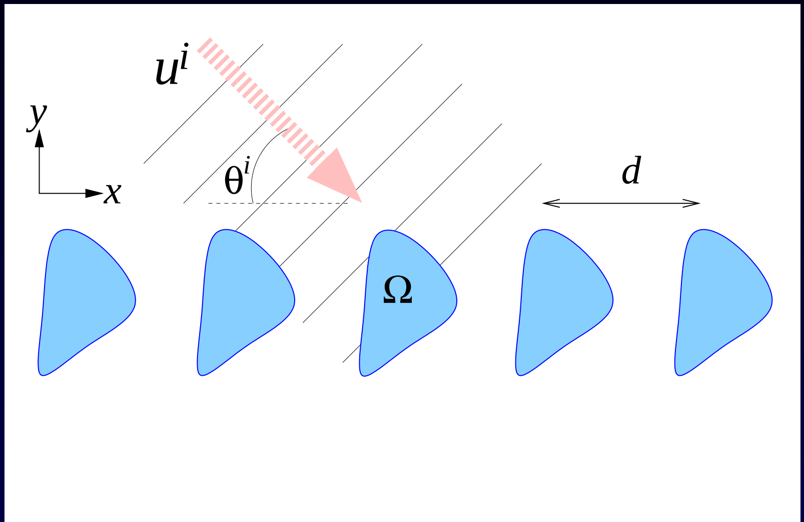

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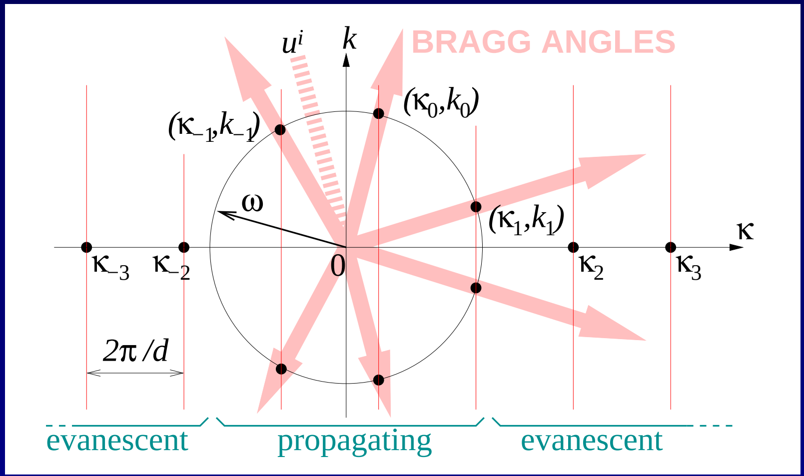
Rayleigh–Bloch radiation condition for u:



set of QP plane waves, x-wavenumbers

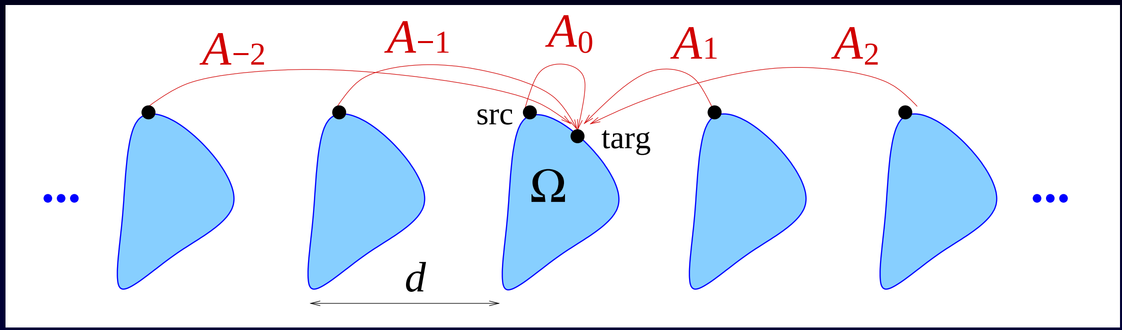
$$\kappa_n := \kappa^i + 2\pi n/d$$

Only outwards-prop. or decaying:

$$u(x, y > y_0) = \sum_{n\in\mathbb{Z}} a_n e^{i(\kappa_n x + \sqrt{\omega^2 - \kappa_n^2}\, y)}$$

$$u(x, y < y_0) = \sum_{n\in\mathbb{Z}} b_n e^{i(\kappa_n x - \sqrt{\omega^2 - \kappa_n^2}\, y)}$$

Standard way to periodize integral equations



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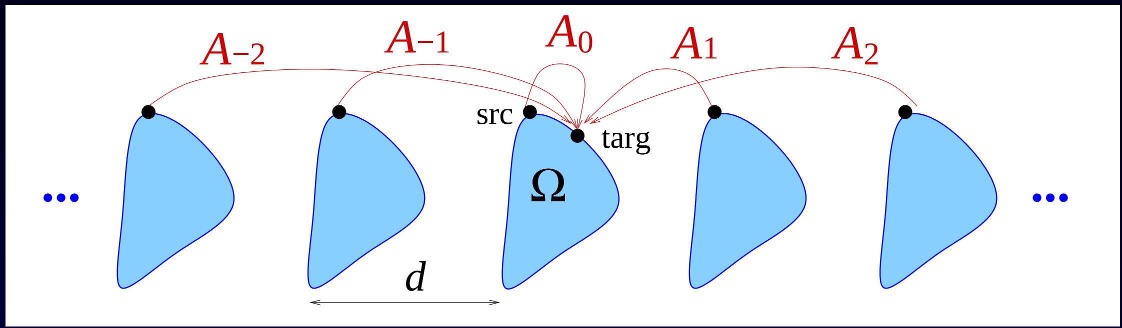

Replace free-space kernel $G(x,y) := G(x,y;\mathbf{0})$ by

$$G_{\mathrm{QP}}(x,y) := \sum_{n\in\mathbb{Z}} \alpha^n G(x, y-nd)$$

- replaces A by $A_{\mathrm{QP}} := \sum_n A_n$

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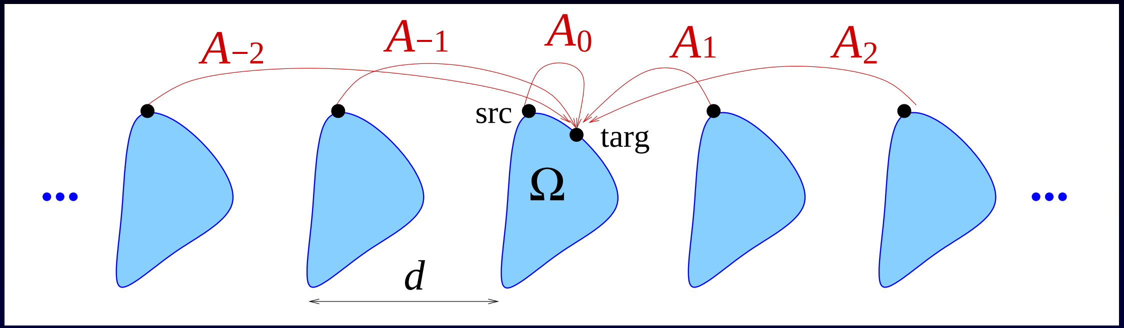

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Issues:

(1) G_{QP} slow to evaluate accurately (e.g. lattice sums)

much effort spent! (McPhedran, Linton, Kurkcu–Reitich, Bruno,...)

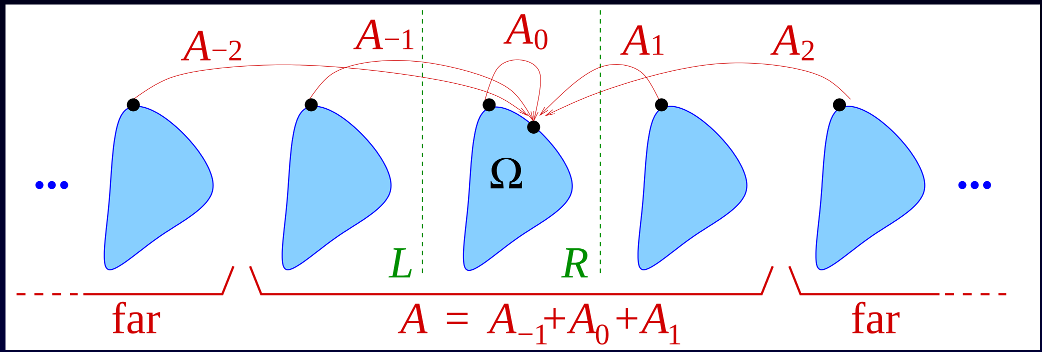
(2) Large-scale problems: never want to fill N^2 entries of dense A_{QP}

need something else if want fast algorithms

(3) G_{QP} doesn't exist at, blows up near, "Wood anomalies": not robust!

(ω, θ^i) params where one or more Bragg angles along the grating (Wood 1902)

New low-rank periodizing scheme (B–Greengard ’11)



replace “far” effect on u by basis $\sum_{m=1}^{M} c_m \varphi_m$

each φ_n solves Helmholtz eqn

far $\Rightarrow$ low rank $\Rightarrow$ M small

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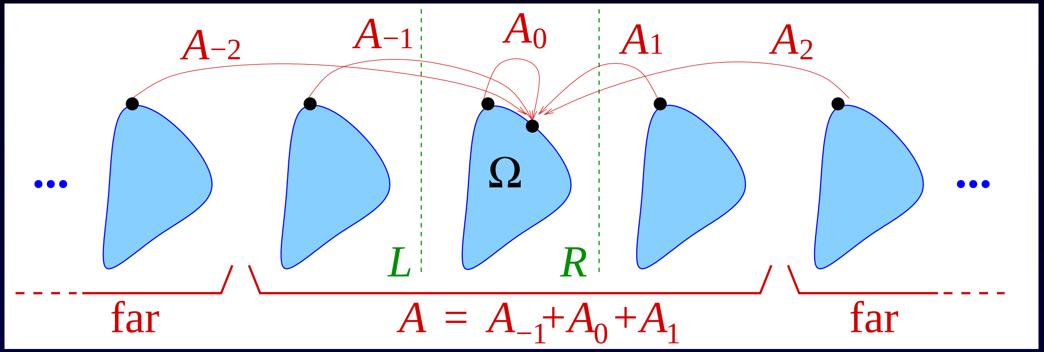

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Must now impose QP on walls: $u_R - \alpha u_L = 0$, $u_{n,R} - \alpha u_{n,L} = 0$

2×2 block linear sys:

$$\begin{bmatrix} A & B \\ C & Q \end{bmatrix} \begin{bmatrix} \tau \\ \boldsymbol{c} \end{bmatrix} = \begin{bmatrix} -u^{\text{inc}}|_{\partial\Omega} \\ 0 \end{bmatrix}$$

$\leftarrow$ usual BC on $\partial\Omega$

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cures 3 issues: robust, good w/ FMM, all free-space G, no lattice sums

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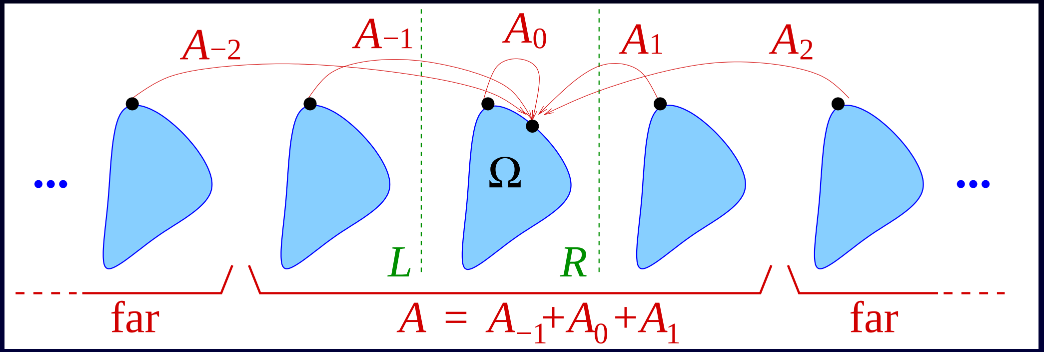

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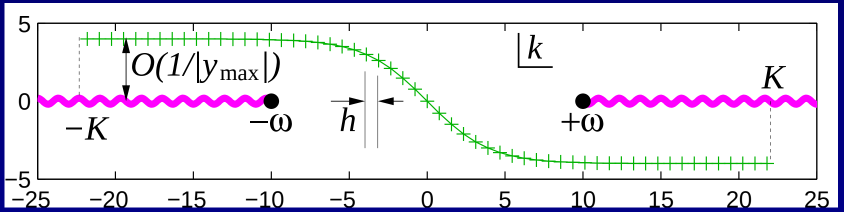
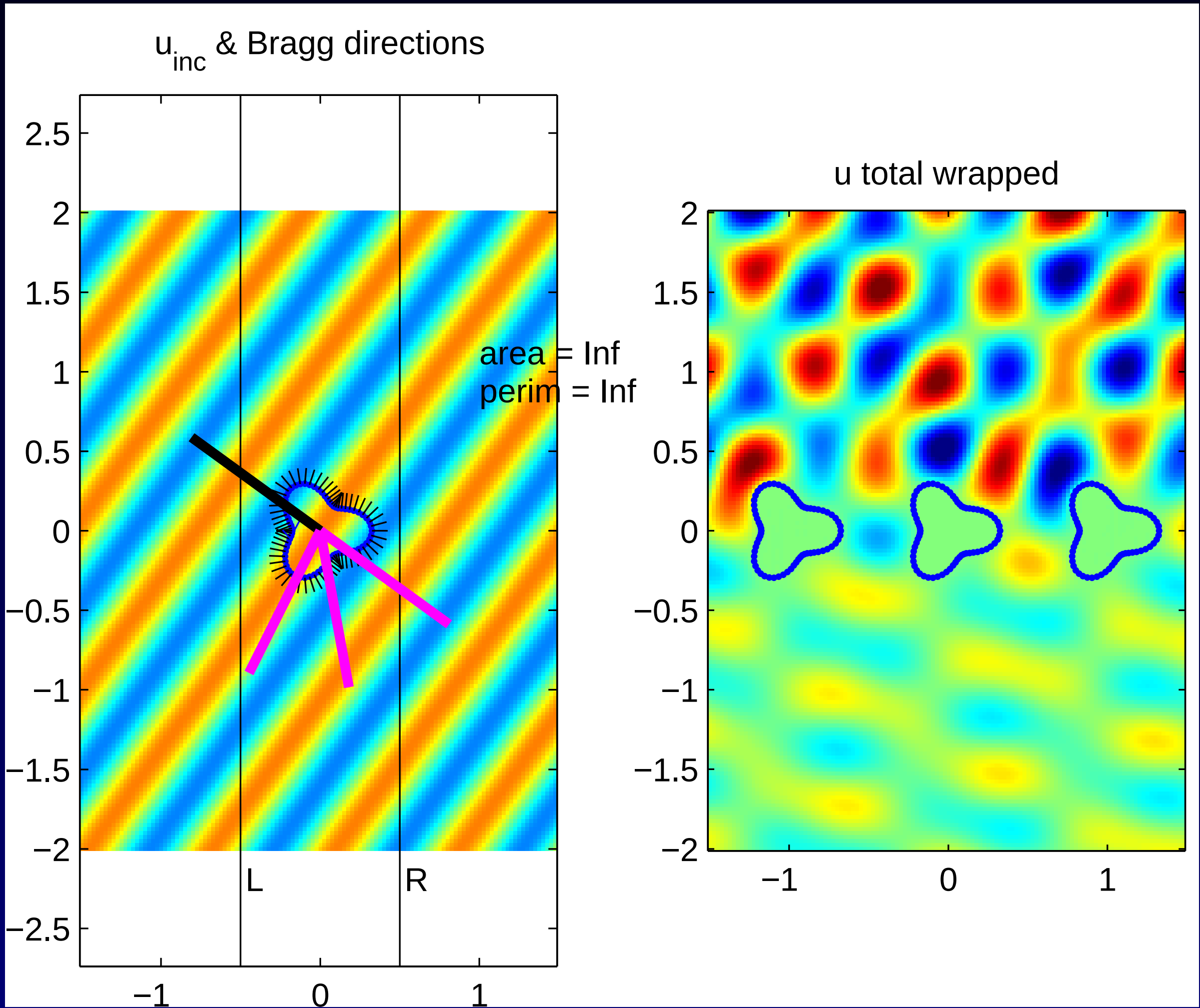
L, R unbounded $\Rightarrow$ Fourier transform $y \leftrightarrow k$, on Sommerfeld contour:



$$G(x,y) = \frac{i}{4\pi} \int_{-\infty}^{\infty} e^{iky} \frac{e^{i\sqrt{\omega^2-k^2}\,|x|}}{\sqrt{\omega^2-k^2}}\, dk$$

k-quadrature exponentially convergent in M nodes (φ_m = complex plane waves)

Small demo (10-line code in MATLAB toolbox `MPSpack`, B–Betcke ’09)



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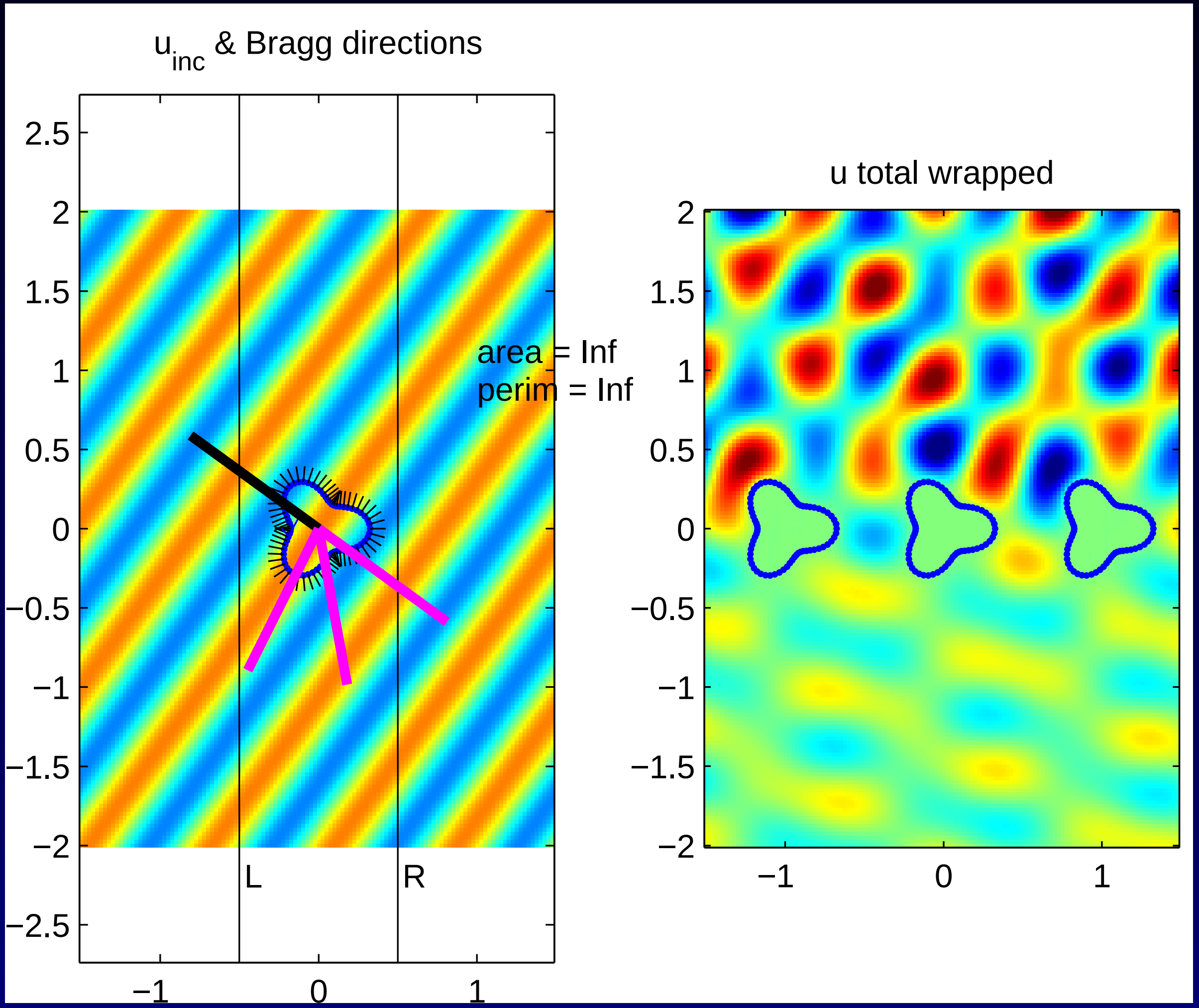
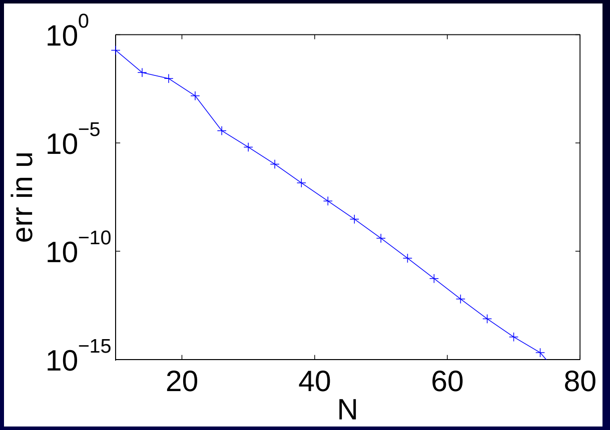
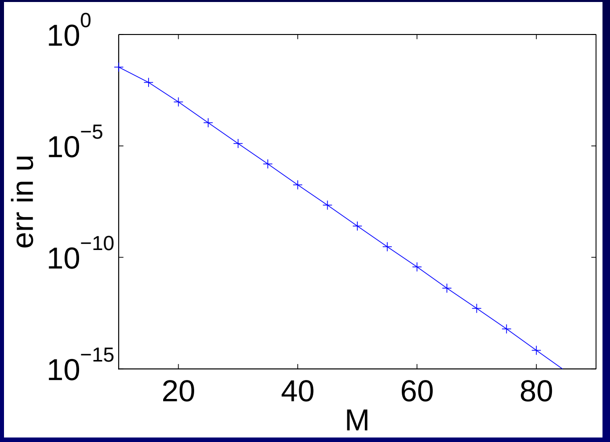


Exponential convergence:





$d = 1.6\lambda$ $N = 70$ $M = 80$ error 10^{-14} $t_{\text{fill+dense solve}} = 0.04$ s (laptop)

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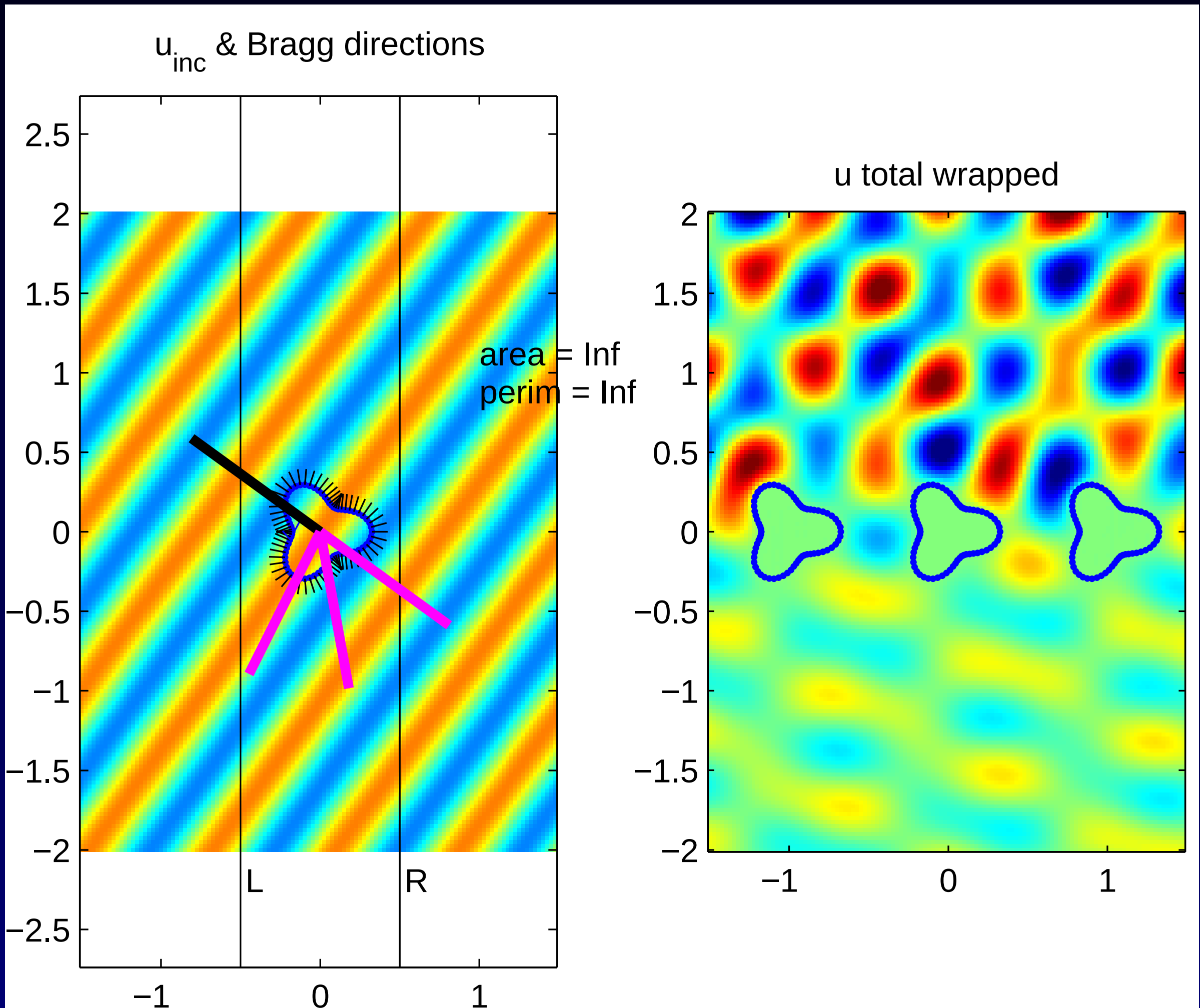

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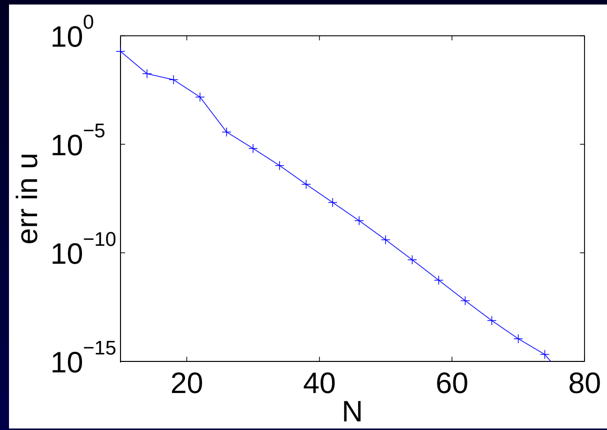

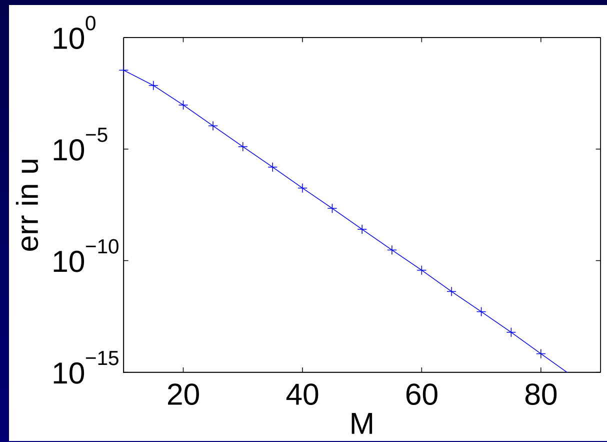

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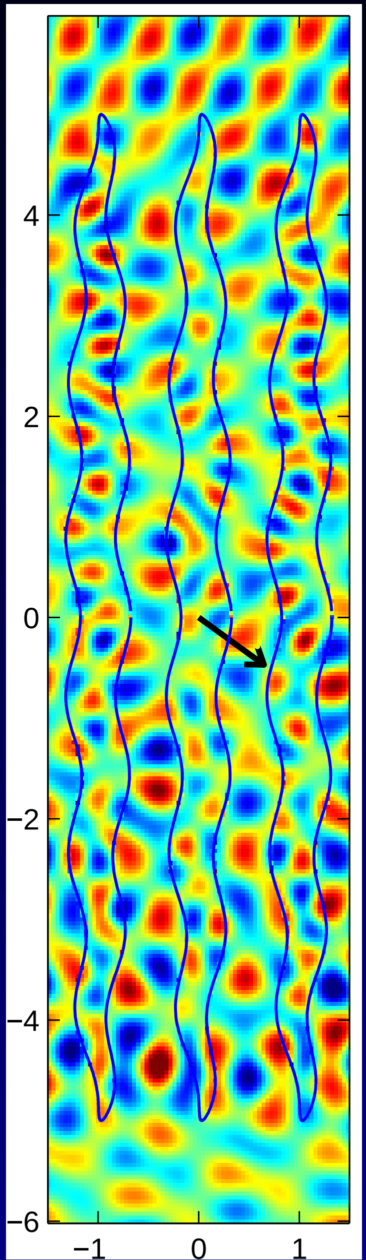
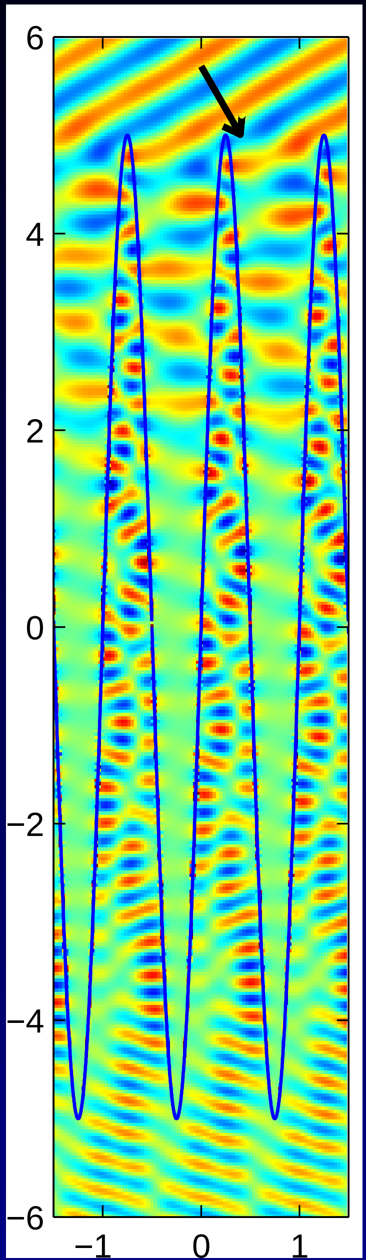
MOVIE 1

Dielectrics, interfaces, high aspect ratios





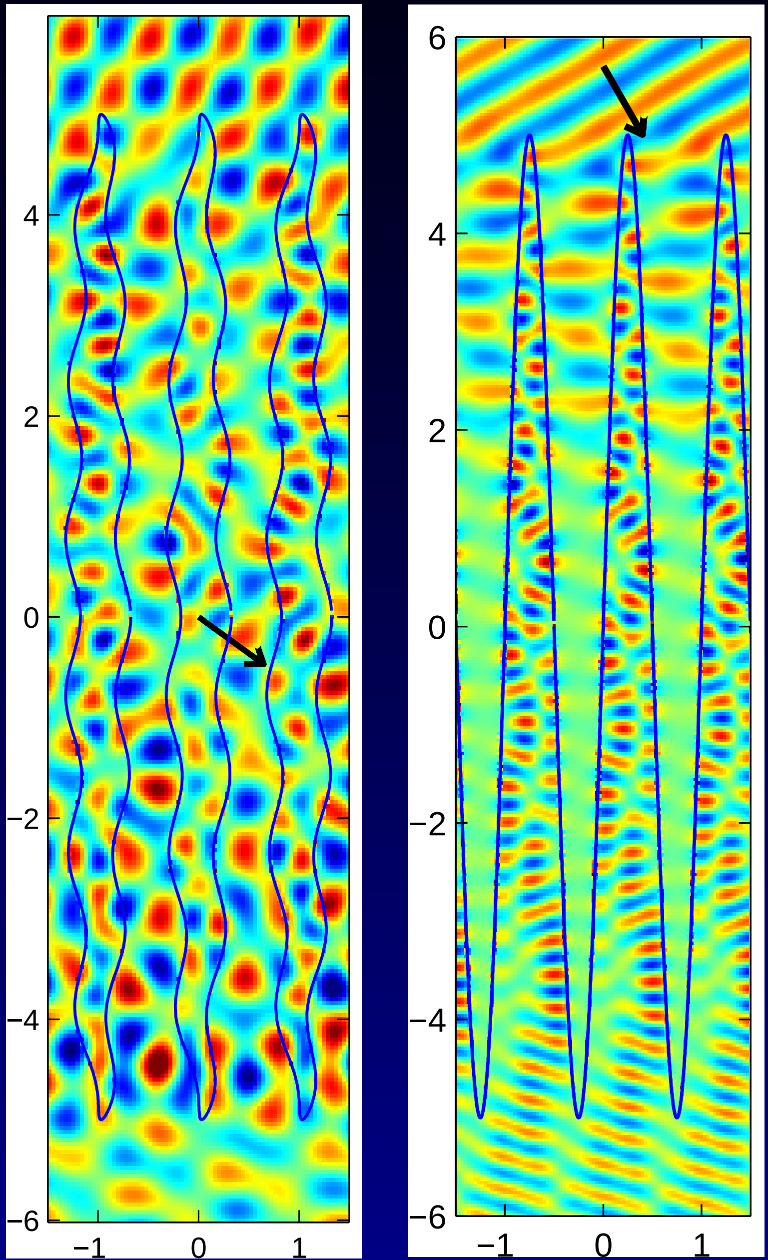
$$
\begin{aligned}
(\Delta + \omega^2)u &= 0 \qquad \text{outside} \\
(\Delta + n^2\omega^2)u &= 0 \qquad \text{inside}
\end{aligned}
$$

$$
\left.\begin{aligned}
u^+ - u^- &= -u^i \\
u_n^+ - u_n^- &= -u_n^i
\end{aligned}\right\} \text{ on } \partial\Omega
$$

transmission

(TM Maxwell)

Dielectrics, interfaces, high aspect ratios



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$$\left.\begin{aligned} u^+ - u^- &= -u^i \\ u_n^+ - u_n^- &= -u_n^i \end{aligned}\right\} \text{on } \partial\Omega$$

transmission (TM Maxwell)

2nd kind rep: (Müller ’69, Rokhlin ’83)

$$u = \begin{cases} \mathcal{D}\tau + \mathcal{S}\sigma & \text{inside} \\ \mathcal{D}_i\tau + \mathcal{S}_i\sigma & \text{outside} \end{cases}$$

A now 2×2; must periodize both layers

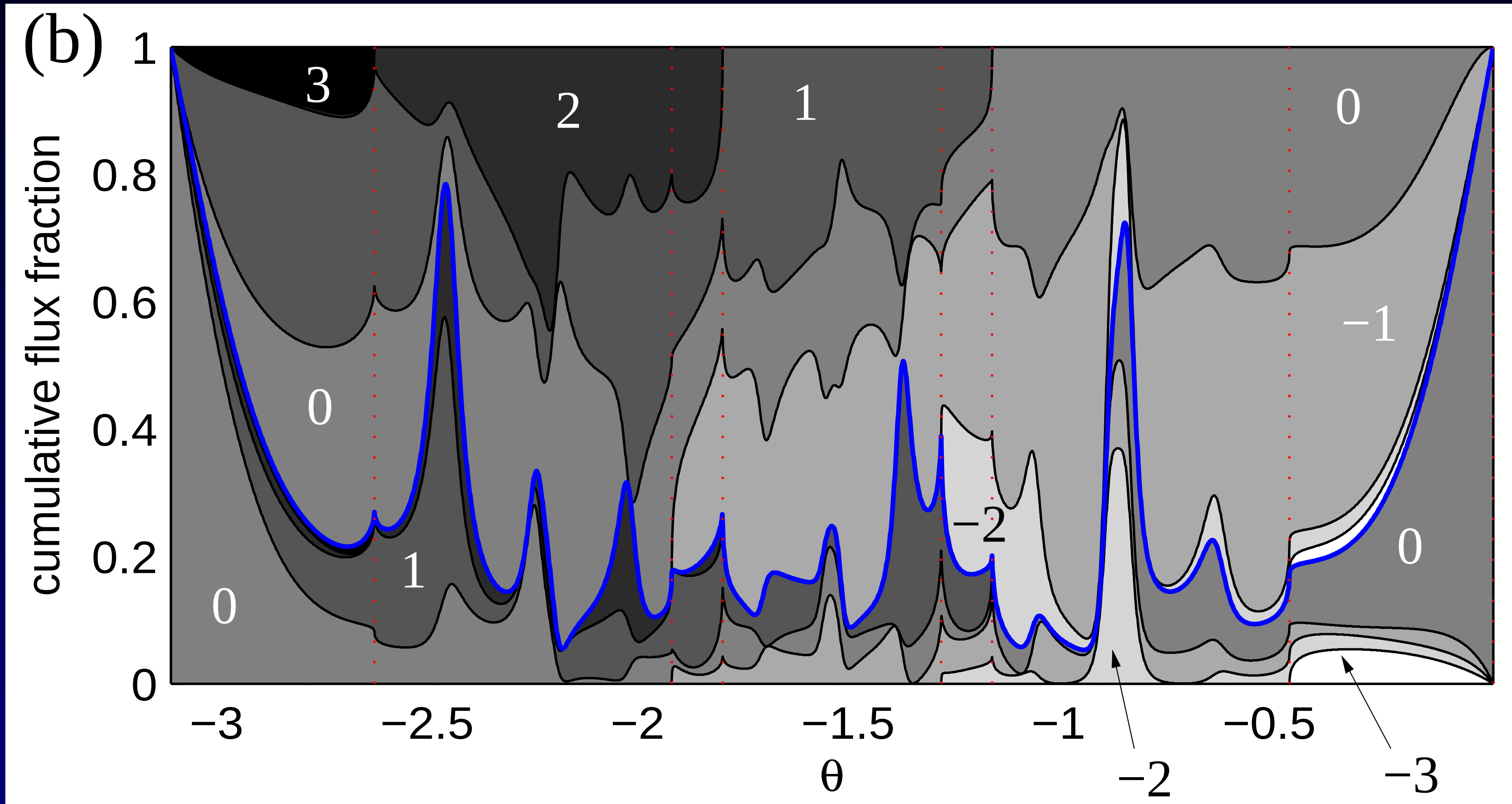
High aspect easy $M \sim N \sim$ height

unlike lattice sums (Nishimura ’08)

32λ tall $N=700$ $M=300$ err 10^{-8} 4 s

Applications care about multiple incident angles

Power fractions scattered into each transmitted/reflected Bragg order:



$d = 1.6\lambda$ diel. obst. error 10^{-12} 3000 angles in 8 mins

- square-root type cusps at each Wood anomaly (dotted red)

Fast direct periodic scattering solver (Gillman–B '12)

Iterative methods not ideal:

- start afresh for each RHS $\boldsymbol{f} = -u^{\text{inc}}|_{\partial\Omega}$
- resonances, complex geom $\to$ many iters

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Direct solve possible in $O(N)$:

nested compressed rep. of $\boldsymbol{A}^{-1}$

exploits low-rank offdiag. blocks

can then apply $\boldsymbol{A}^{-1}$ v. cheaply

(Hackbusch, Rokhlin–Martinsson)

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Direct soln of periodic 2×2 sys:

$$\begin{aligned} \boldsymbol{c} &= (Q - CA^{-1}B)^{-1}A^{-1}\boldsymbol{f} \\ \boldsymbol{\tau} &= A^{-1}(\boldsymbol{f} - B\boldsymbol{c}) \end{aligned}$$

cf (Ho-Greengard ’12) redoes A_{QP}^{-1}

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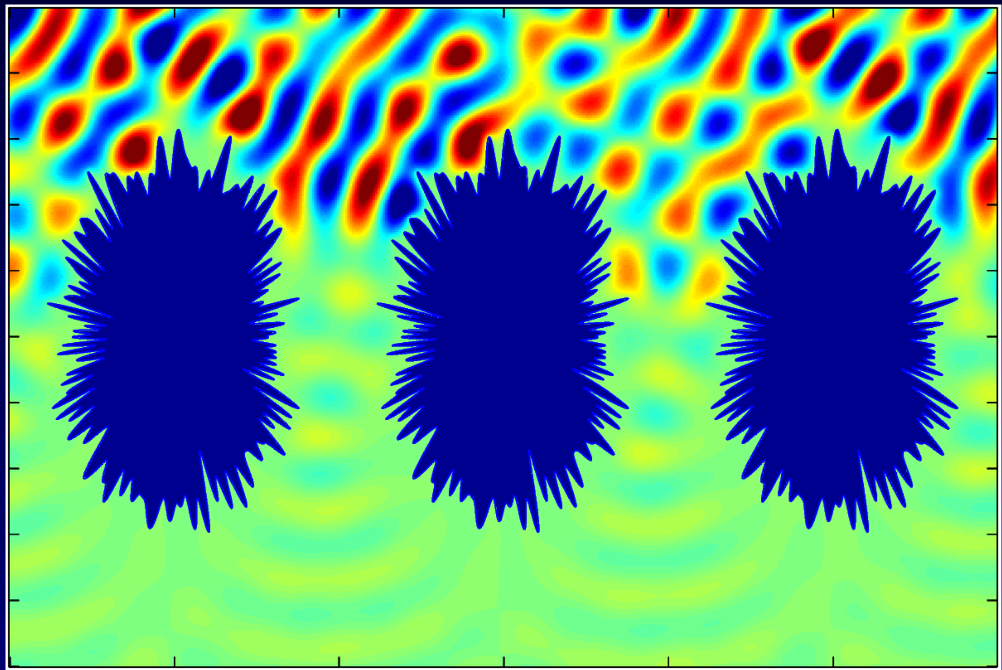
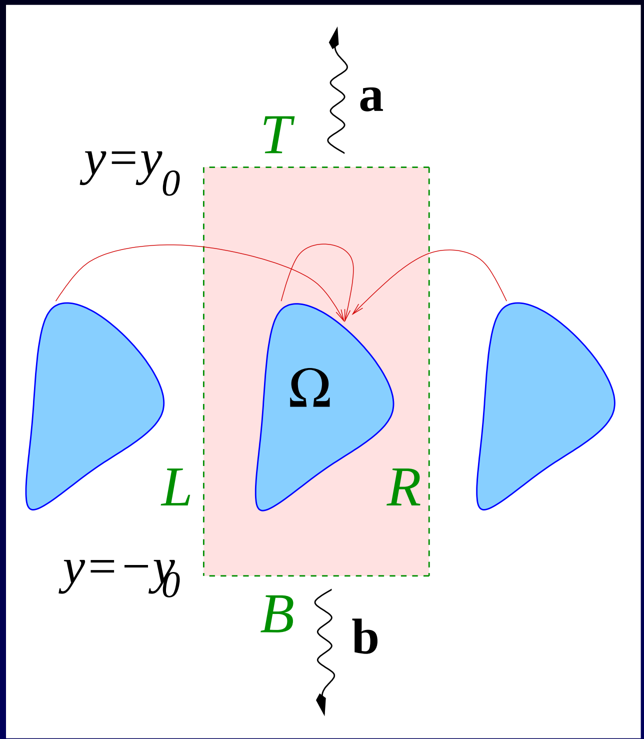


E.g.: rough obstacle, Wood's

needs $N = 10^5$ for error 10^{-10}

- 4 min for A^{-1}, 6 sec per θ^i: 600$\times$ faster than even FMM + GMRES

Towards 3D: simpler "box scheme" & folding up



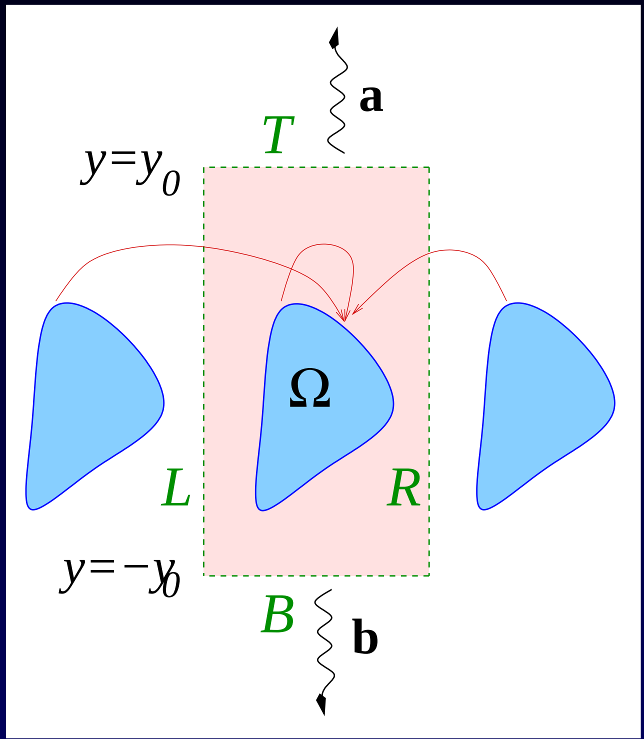
in box: $u = (\mathcal{D} - i\omega\mathcal{S})\tau + \sum_{m=1}^{M} c_m \varphi_m$

near CFIEs   loc. exp.

above & below: $u =$ radiating Rayleigh–Bloch

$$
\begin{array}{l}
\text{BC:} \\
\text{L−R QP:} \\
\text{T cont:} \\
\text{B cont:}
\end{array}
\left[\begin{array}{cc|c|c}
A & B & & \\
\hline
C & Q & & \\
C_T & Q_T & P_T & \\
C_B & Q_B & & P_B
\end{array}\right]
\left[\begin{array}{c}
\boldsymbol{\tau} \\
\hline
\mathbf{c} \\
\hline
\mathbf{a} \\
\hline
\mathbf{b}
\end{array}\right]
=
\left[\begin{array}{c}
\mathbf{f} \\
\hline
0 \\
\hline
0 \\
\hline
0
\end{array}\right]
$$

Towards 3D: simpler “box scheme” & folding up



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$$\begin{array}{l} \text{BC:} \\ \text{L−R QP:} \\ \text{T cont:} \\ \text{B cont:} \end{array} \begin{bmatrix} A & B & & \\ C & Q & & \\ C_{\mathrm{T}} & Q_{\mathrm{T}} & P_{\mathrm{T}} & \\ C_{\mathrm{B}} & Q_{\mathrm{B}} & & P_{\mathrm{B}} \end{bmatrix} \begin{bmatrix} \boldsymbol{\tau} \\ \mathbf{c} \\ \mathbf{a} \\ \mathbf{b} \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

- Q not square, exp. ill. cond: bad to iterate on whole sys!

Eliminate QP unknowns: block Schur w/ small pseudoinverse

$$\begin{bmatrix} A & B \\ C & Q \end{bmatrix} \begin{bmatrix} \tau \\ \boldsymbol{c} \end{bmatrix} = \begin{bmatrix} \boldsymbol{b} \\ 0 \end{bmatrix} \quad \Leftrightarrow \quad \underbrace{(A - BQ^{\dagger}C)}_{A_{\mathrm{QP}}}\tau = \boldsymbol{f}$$

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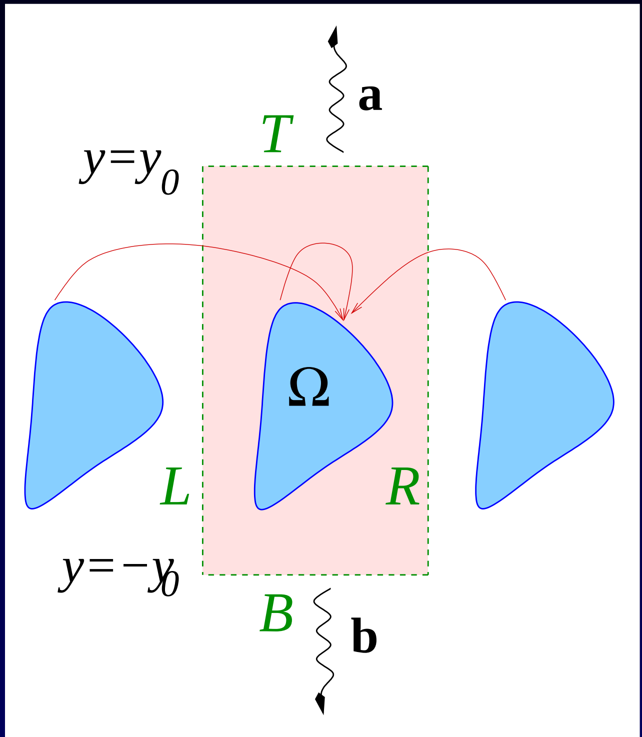

in box: $u = (\mathcal{D} - i\omega\mathcal{S})\tau + \sum_{m=1}^{M} c_m \varphi_m$

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A & B & & \\
\hline
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\hline
C_{\mathrm{T}} & Q_{\mathrm{T}} & P_{\mathrm{T}} & \\
\hline
C_{\mathrm{B}} & Q_{\mathrm{B}} & & P_{\mathrm{B}}
\end{array}\right]
\left[\begin{array}{c}
\boldsymbol{\tau} \\
\hline
\mathbf{c} \\
\hline
\mathbf{a} \\
\hline
\mathbf{b}
\end{array}\right]
=
\left[\begin{array}{c}
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\hline
0 \\
\hline
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\hline
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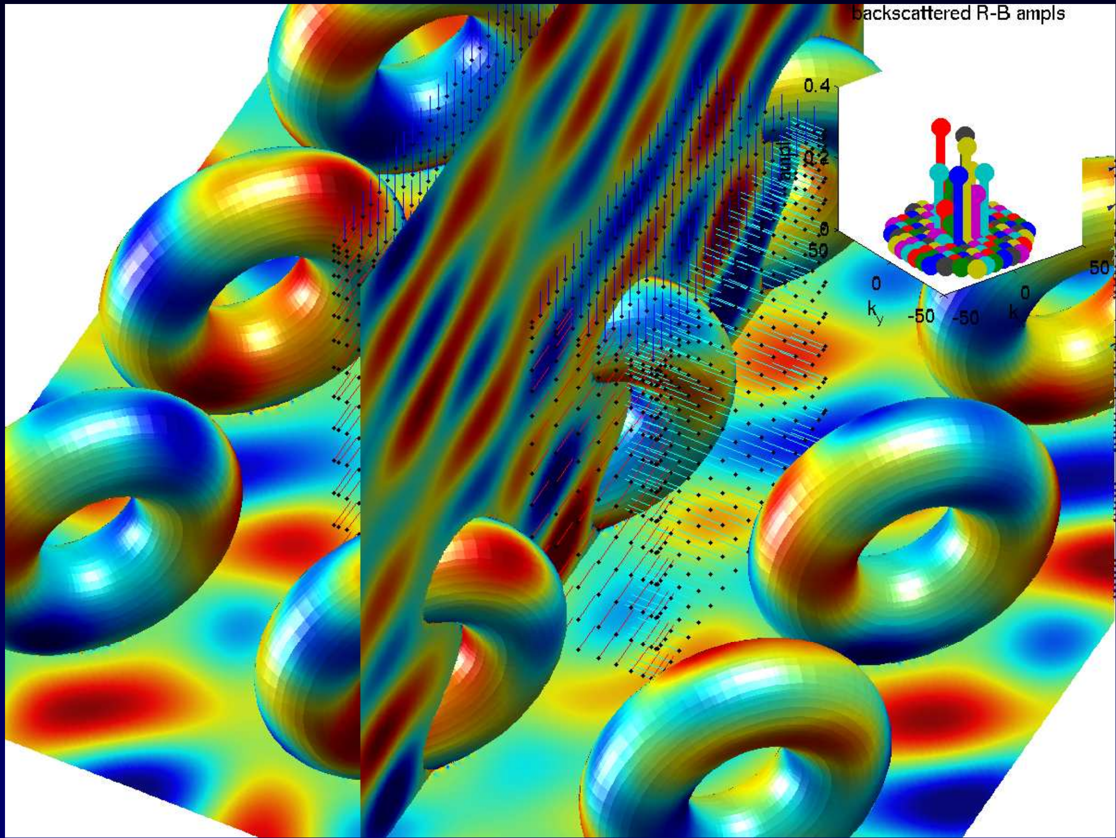
$$

- robust @ Wood's? Dirichlet/impedance half-space A_{QP} always exists

Prelim. results: 3D bi-periodic scattering

φ_m basis = 3D loc. exp. Match QP (4 faces) & rad. cond. (2 faces)



Dirichlet obstacles

$d = 2.4\lambda$

$N = 4032$ (small)

QBX 20 s

$Q^\dagger$ 5 sec (4000×1339)

31 its 60 s

error (flux) 10^{-5}

- $O(N)$ scheme: small dense lin. alg. replaces messy lattice sums!
- high aspect simple via $\varphi_m =$ plane waves
- Apps: modeling photonic crystal slab, metamaterials

Conclusions

Accurate, efficient, analysis-based scattering solvers, optimal $O(N)$ work

- QBX: high-order quadrature to apply IE ops on surfaces
  – simple new idea: use local expansion near boundary

- Periodic problems: use low-rank property of distant interactions
  – only free-space G, robust at Wood's, works with fast solvers

Ongoing/future: multilayer dielectrics, Neumann BC, Maxwell,
solar cells (w/ J. Liu), periodic Stokes

B, *subm.* SIAM J. Sci. Comp.
Klöckner–B–Greengard–O'Neil, *subm.*
Gillman–B, *subm.* J. Comput. Phys.
B–Greengard, BIT Numer. Math. (2011)

http://math.dartmouth.edu/∼ahb

funding: NSF DMS-1216656

code: (try it!)
`MPSpack` toolbox for MATLAB
http://code.google.com/p/mpspack