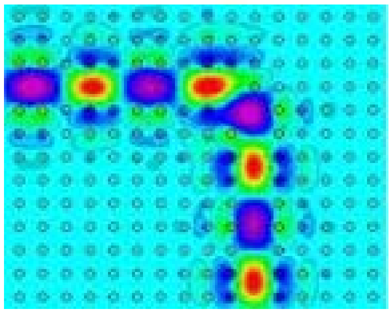
Fast, High-Order Methods in Computational Electromagnetics and Acoustics

Oscar Bruno (Caltech),

McKay Hyde and Fernando Reitich (Minnesota)

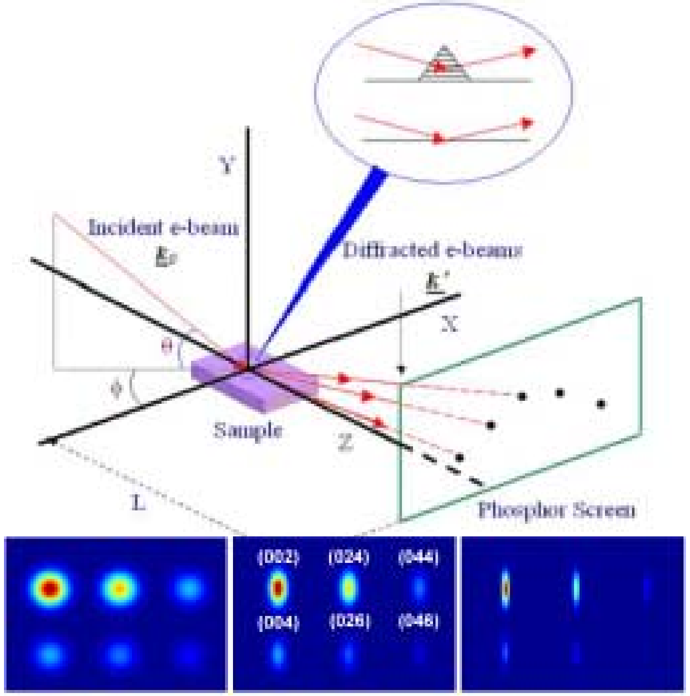
Photonic Crystals



(J. Joannopoulos, MIT)

$$\begin{cases} \nabla \times \vec{\mathcal{E}} = -\mu \dfrac{\partial \vec{\mathcal{H}}}{\partial t} \\ \nabla \times \vec{\mathcal{H}} = \epsilon \dfrac{\partial \vec{\mathcal{E}}}{\partial t} \end{cases}$$

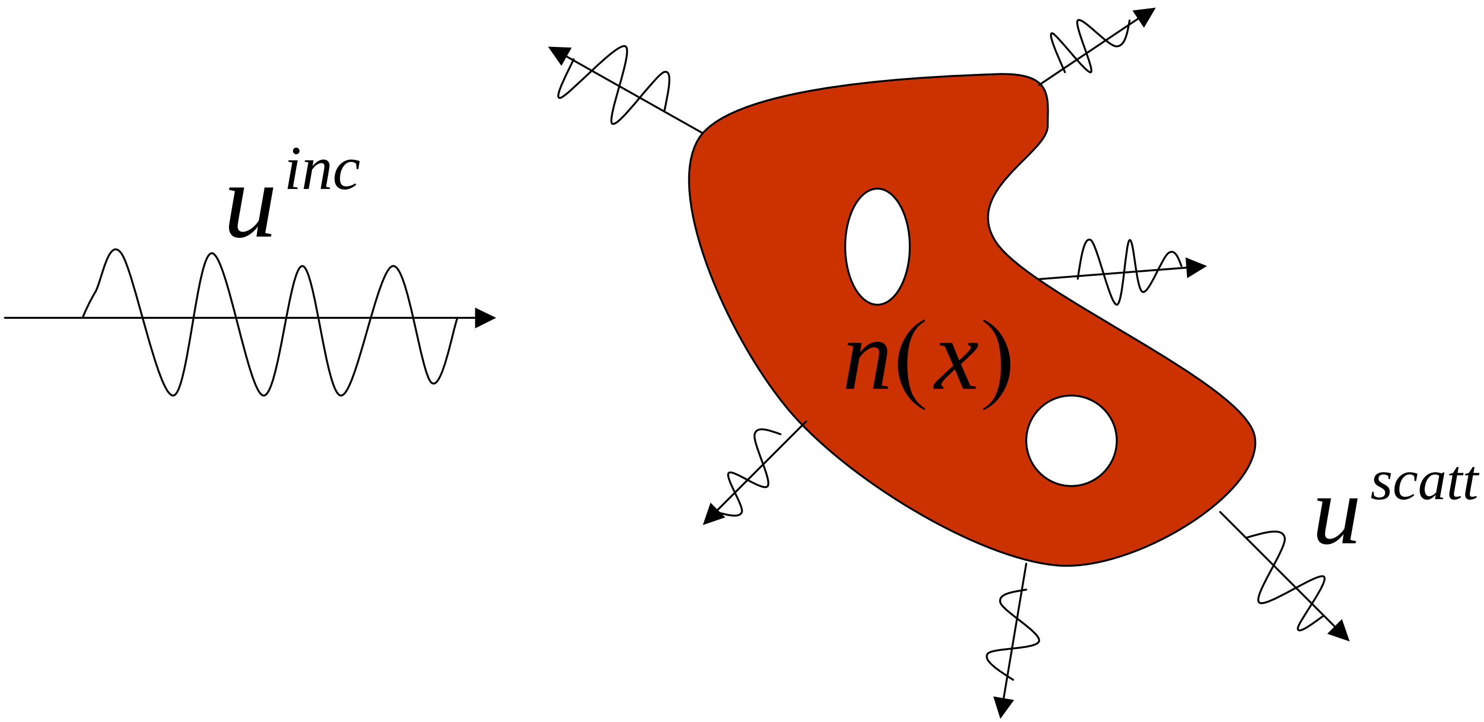
RHEED – Surface structure



(R. Brewer, Caltech)

$$-\frac{\hbar^2}{2m}\Delta\psi + V(x)\psi = E\psi$$

Volumetric Scattering



$$u = u^{inc} + u^{scatt}$$

$$\Delta u + \kappa^2 n^2(x) u = 0$$

$$\Delta u^{inc} + \kappa^2 u^{inc} = 0$$

$$\lim_{r \to \infty} r \left(\frac{\partial u^{scatt}}{\partial r} - i \kappa u^{scatt} \right) = 0$$

Lippmann-Schwinger Integral Equation

$$u(x) = u^{inc}(x) - \kappa^2 \int_{\text{supp}\, m} g(x-y)\, m(y)\, u(y)\, dy$$

$u^{scatt}(x)$
Satisfies radiation condition automatically

$g(x) = \dfrac{e^{i\kappa|x|}}{4\pi|x|}$
Satisfies radiation condition

$m(x) = 1 - n^2(x)$
Vanishes outside scatterer

Numerical Solution:

$$u(x_j) + \kappa^2 \sum_{k=0}^{N} g(x_j - x_k)\, m(x_k)\, u(x_k)\, \Delta V = u^{inc}(x_j) \quad \text{for } j = 0, \ldots, N$$

Solve this linear system using an iterative method (GMRES, BiCG, etc.)

Requires $O(N^2)$ per iteration – Must find more efficient integrator

FFT-Based Integration: Trapezoidal Rule

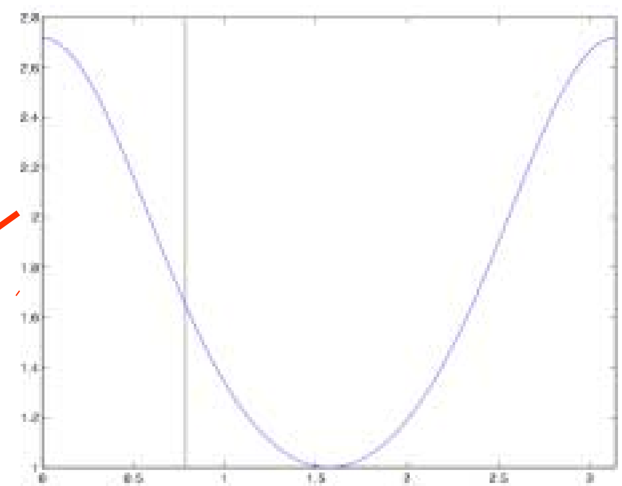
$$\int_0^{1/2} \sqrt{x}\, dx \approx 0.2357 \rightarrow$$

N	Rel. Error	Ratio
1	4.69(-1)	
2	2.04(-1)	2.30
4	8.99(-2)	2.27
8	4.02(-2)	2.24
8192	2.72(-5)	

$$\int_0^{\pi/4} f(x)\, dx \approx 1.8009$$

N	Rel. Error	Ratio
1	4.77(-2)	
2	1.19(-2)	4.03
4	2.95(-3)	4.02
8	7.36(-4)	4.01
8192	7.01(-10)	

$$f(x) = e^{\cos^2(x)}, \quad x \in [0, \pi]$$



smooth and *periodic*

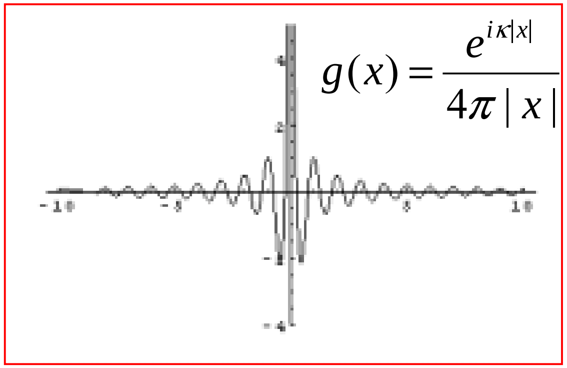
$$\int_0^{\pi} f(x)\, dx \approx 5.5084$$

N	Rel. Error	Ratio
1	5.50(-1)	
2	6.03(-2)	9.12
4	3.10(-4)	1.95(2)
8	7.17(-10)	4.32(5)
16	2.10(-23)	3.42(13)

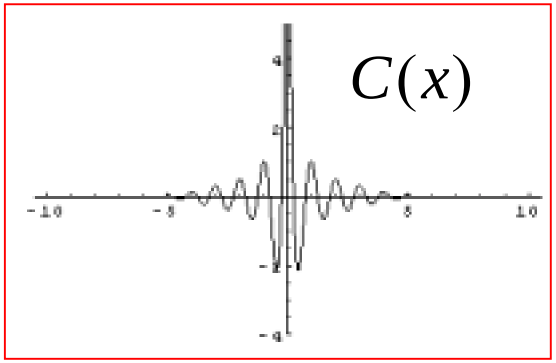
Exponential convergence!

A Fast, High-Order Method for Smooth Scatterers

Decompose the Green's function

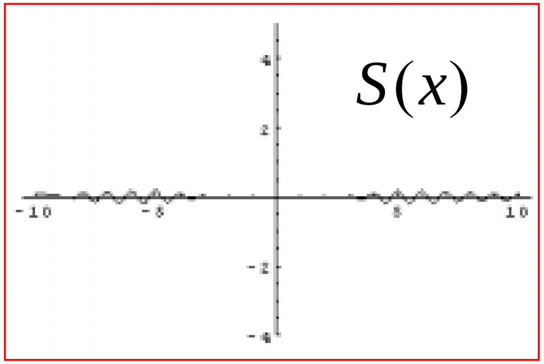


$=$



Singular at $x = 0$, compact support

$+$



Smooth with unbounded support

$$\int g(x-y)\,m(y)\,u(y)\,dy =$$

$$\int C(x-y)\,m(y)\,u(y)\,dy \;+$$

Integral *is smooth and periodic as a function of* x $\Rightarrow$ Fourier Series

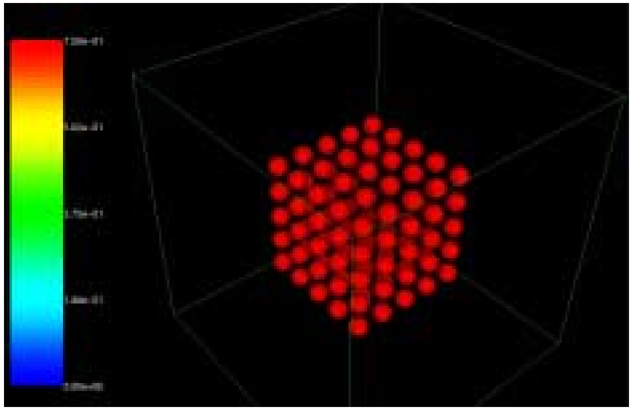
$$\int S(x-y)\,m(y)\,u(y)\,dy$$

Integrand *is smooth and periodic as a function of* y *for each* x $\Rightarrow$ Trap. Rule

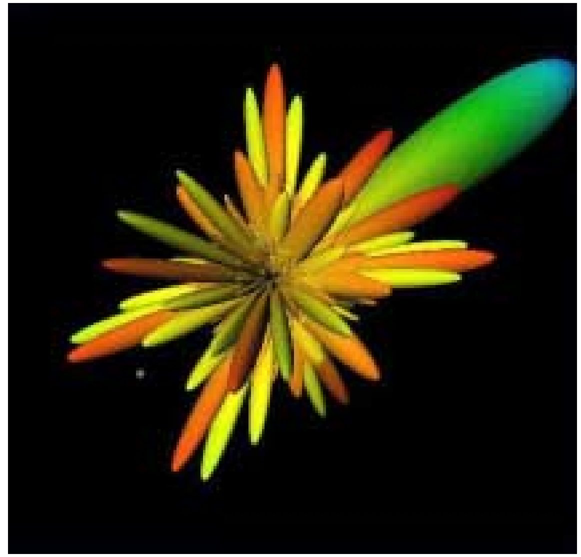
High-Order Accuracy with $O(N \log N)$ complexity!

Superalgebraic Convergence for Smooth Scatterers

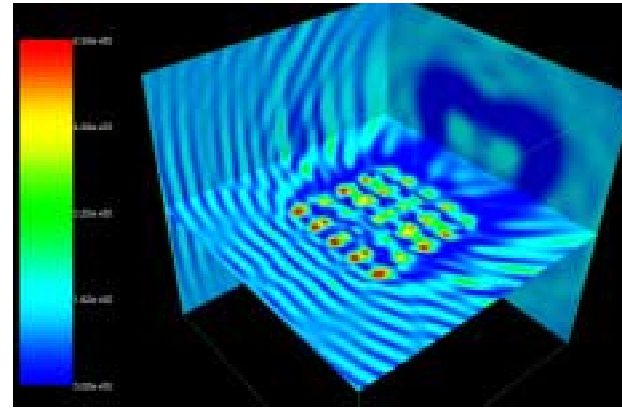
Cubic lattice (5λ x 5λ x 5λ) of smooth, inhomogeneous scatterers (potentials)



Refractive Index Isosurface



Far Field Intensity



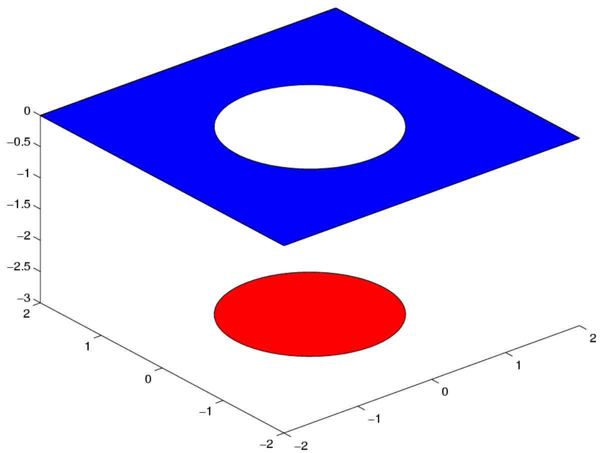
Near Field Intensity

N	Unknowns	Time (32 CPUs)	**Near Field Max Error**	Ratio	**Far Field Max Error**	Ratio
10	1.33K	5.65s	**3.70**		**43.0**	
20	9.26K	6.39s	**1.35**	2.73	**10.6**	4.05
40	68.9K	15.1s	**4.80(-2)**	28.2	**8.66(-2)**	122
80	531K	107s	**8.28(-3)**	5.79	**4.47(-2)**	1.94
160	4.17M	875s	**6.48(-5)**	128	**7.76(-5)**	576

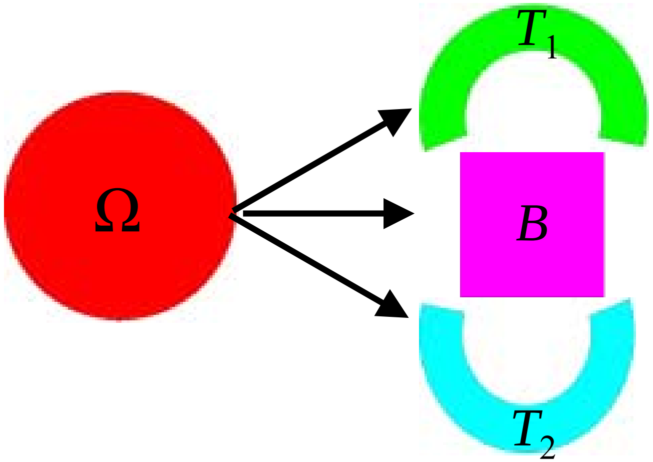
Applications in materials science (e.g. neutron and electron diffraction)

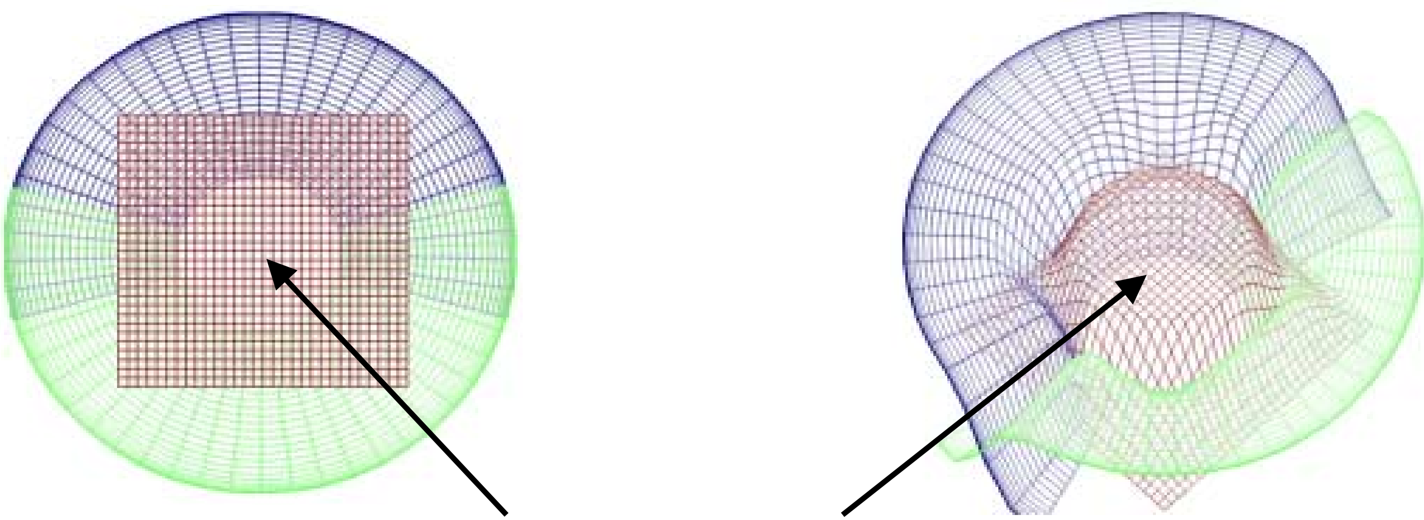
A High-Order Method for Discontinuous Scatterers

Discontinuous $m(x)$



Decompose into thin volume patches and bulk volume patches

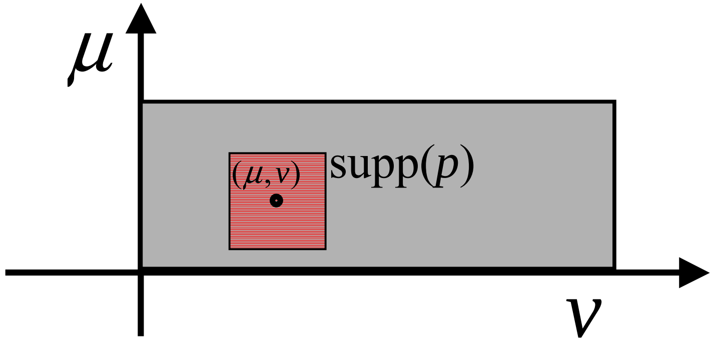




Integrate with Fourier method!

Integration on Thin Volumes

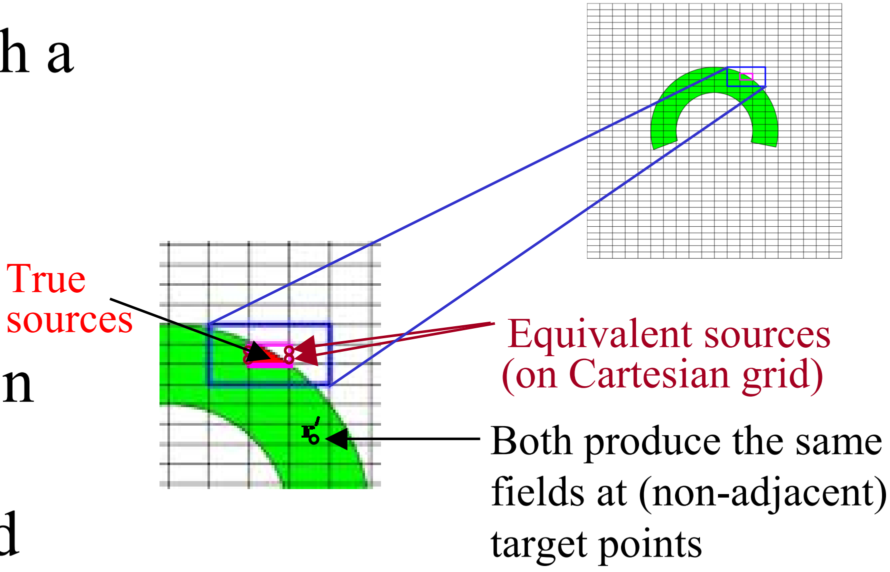
$$\iint_{(\mu',\nu')} g(x(\mu,\nu)-x(\mu',\nu'))\,w(\mu',\nu')\,d\mu'\,d\nu' =$$



Difficulties:

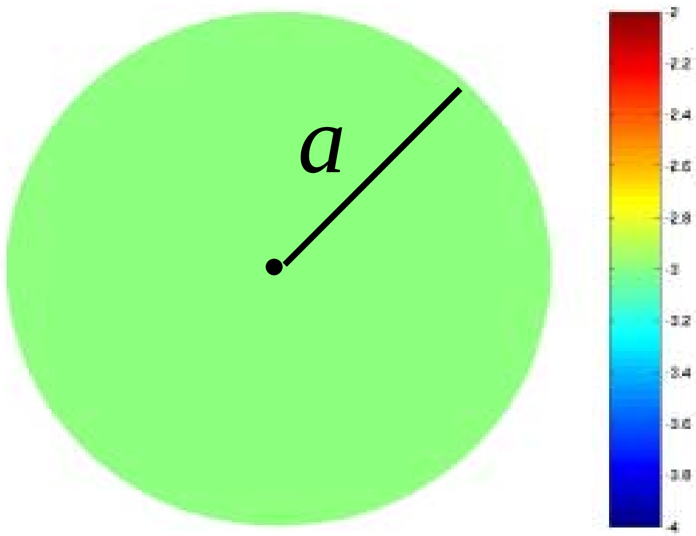
- $g(x)$ is *singular* when x=0
- Direct evaluation is *costly* – $O(N^2)$

High-order accuracy achieved through a regularizing change of variables and trapezoidal rule integration

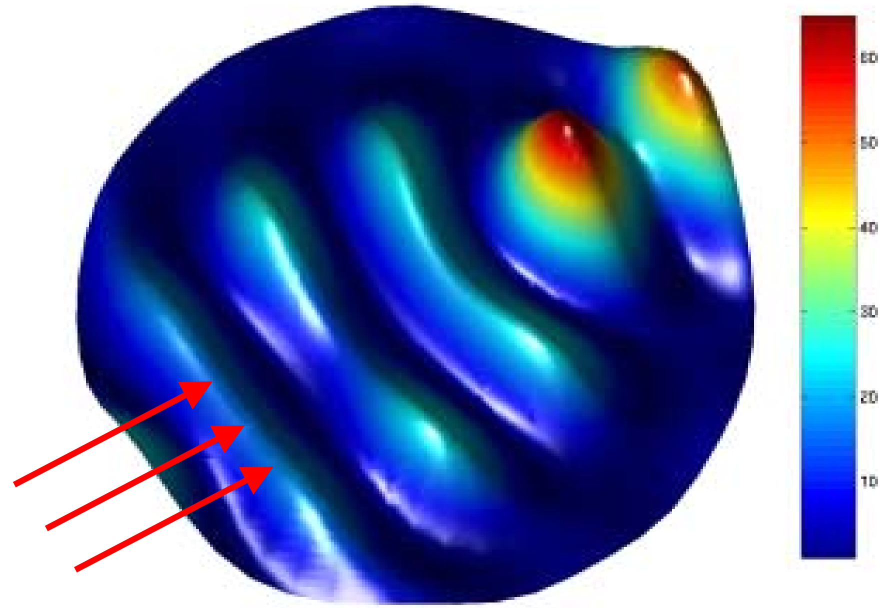


Efficiency achieved by an acceleration scheme based on sparsely distributed equivalent sources on a Cartesian grid ($\Rightarrow$ FFTs!)

Numerical Results



$$m(x) = 1 - n(x)^2$$



Intensity (κ*a*=4)

N	Error (κ*a*=4)
3×16^2	2.3795e-1
3×32^2	1.8715e-3
3×64^2	2.6252e-5
3×128^2	1.3674e-7

κ*a*	N	Time/Iter.
2	3×8^2	0.1s
4	3×16^2	1s
8	3×32^2	7s
16	3×64^2	35s
32	3×128^2	151s
64	3×256^2	688s

Conclusions

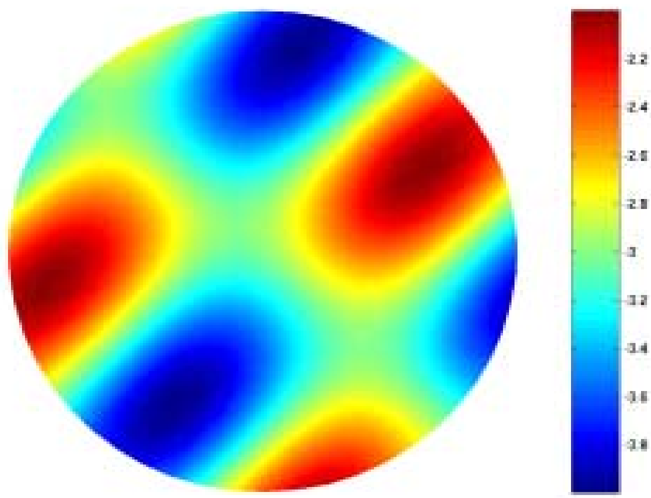
- We have developed a fast, high-order accurate method for scattering by penetrable, inhomogeneous media

- Similar methods could be useful for other problems which admit integral equation formulations (surface scattering, electrostatics, elasticity and fluid dynamics)

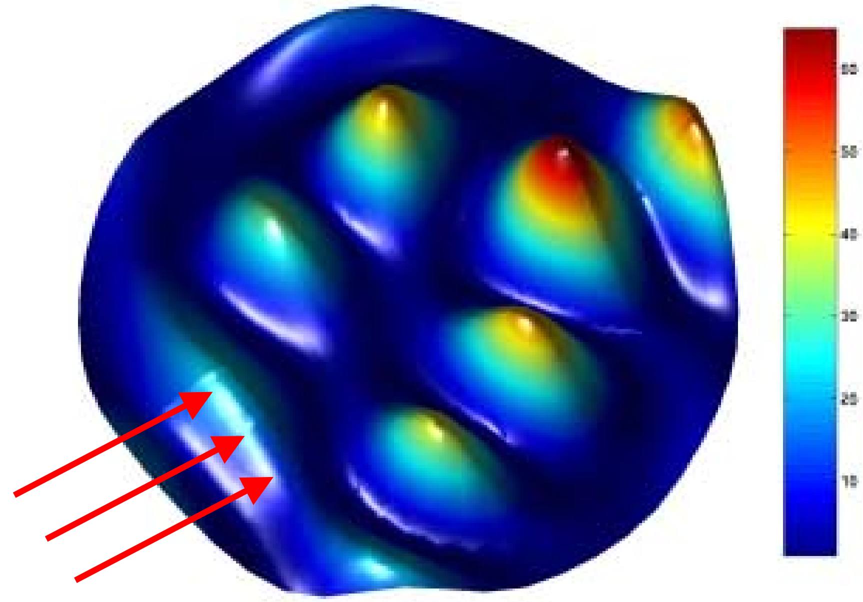
- Soft matter applications: Microscopy, diffractometry, ER/MR fluids, ferroelectrics, liquid crystal displays?

END

Numerical Results: *Accuracy*



$$m(x) = 1 - n(x)^2$$



Intensity (κa=4)

N	Near Field Error
3 x 16^2	2.4827e-1
3 x 32^2	2.5092e-3

Numerical Results: *Parallelization*

Most trivial parallelization scheme: Only computation of adjacent interactions is divided among the processors

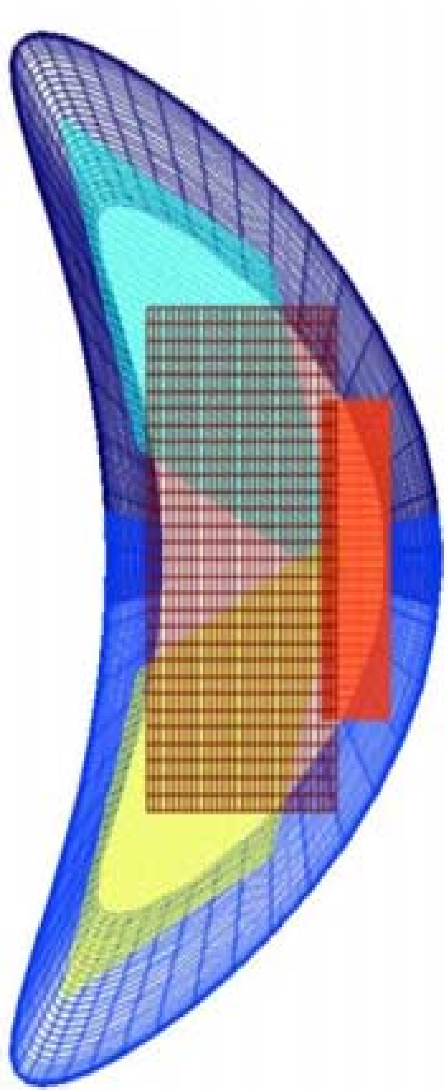
Example: Beowulf cluster with ethernet interconnect

N	Number of Proc.	Time/Iteration
3×128^2	1	1254s
3×128^2	2	685s
3×128^2	4	328s
3×128^2	8	154s
3×128^2	16	89s
3×128^2	32	59s
3×128^2	64	43s
3×128^2	128	40s

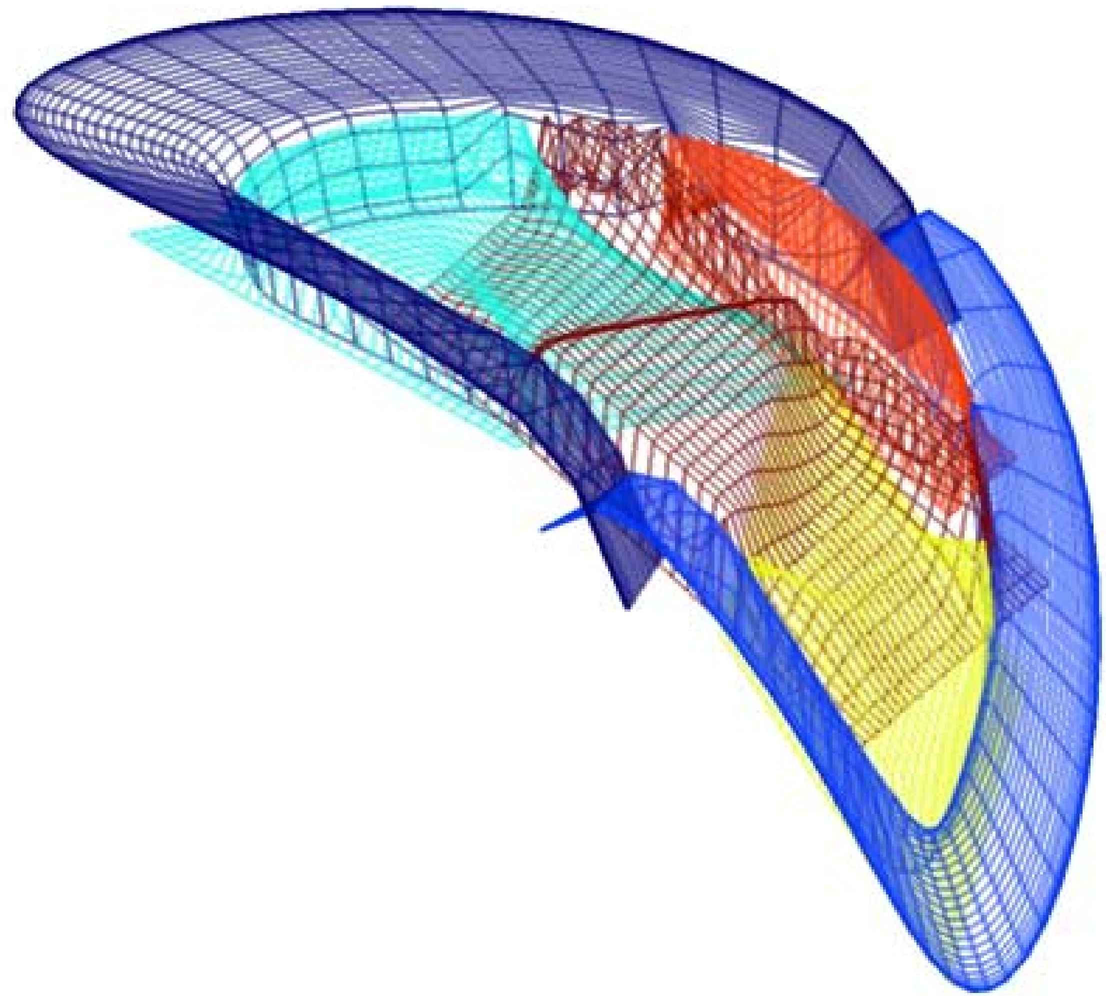
Communication begins to dominate

Complex Scatterers

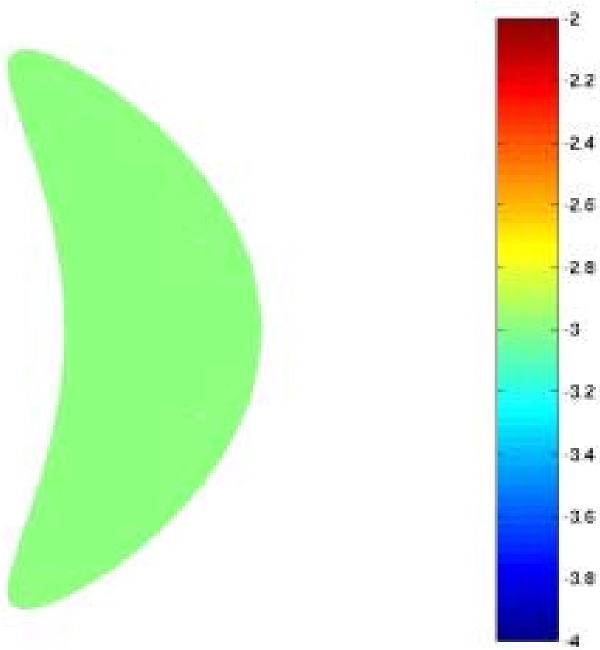
Patches

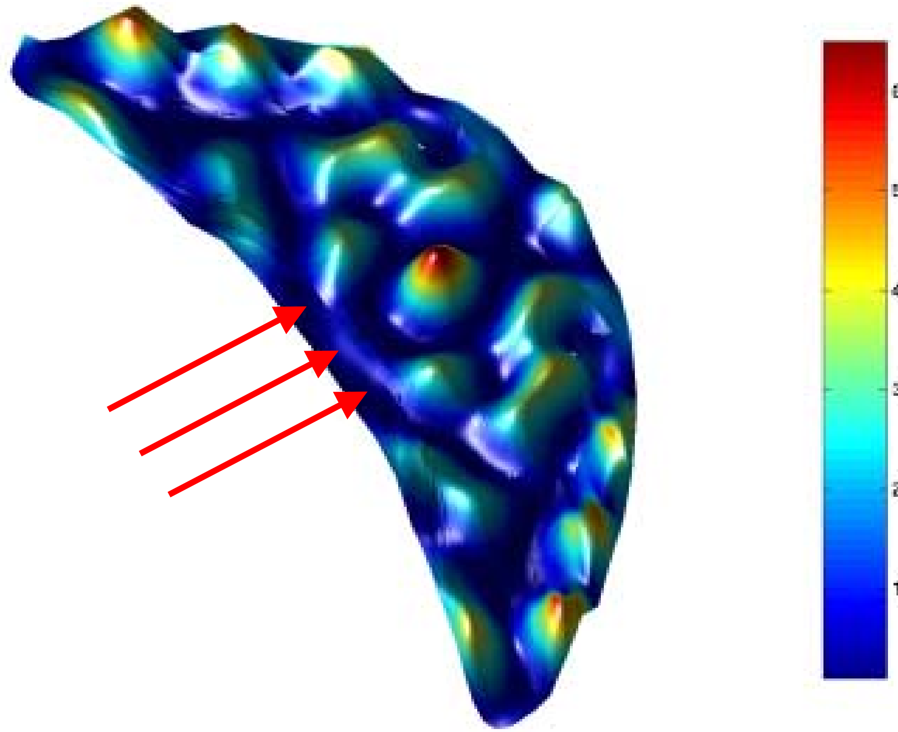


Partition of unity



Complex Scatterers



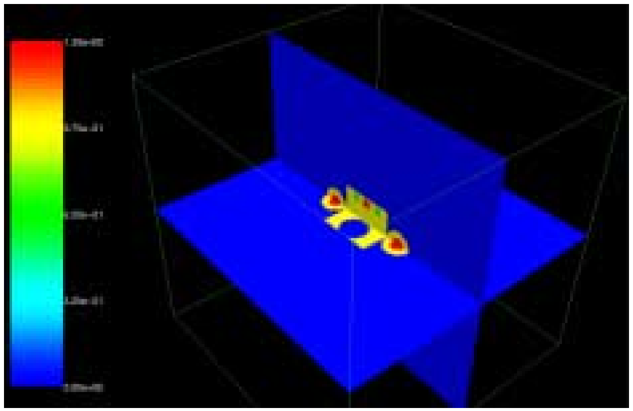


$m(x) = 1 - n(x)^2$

Intensity (κa=4)

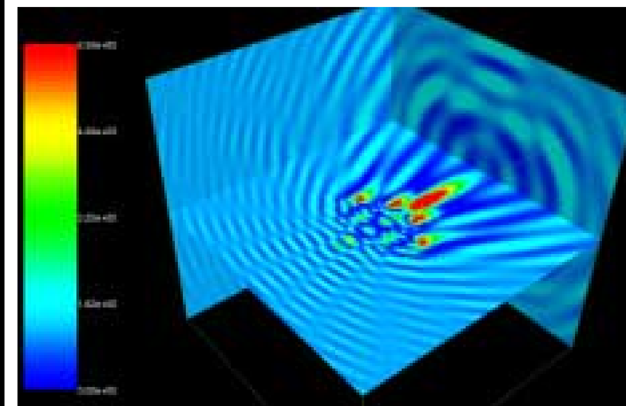
Complex Scatterer

Scatterer composed of a cube, layered spheres, and inhomogeneous components



Refractive Index (2.5λ x 5λ x 2.5λ)

Far Field Intensity



Near Field Intensity

N	Unknowns	Time x CPUs	**Near Field Max Error**	Ratio	**Far Field Max Error**	Ratio
8 x 16 x 8	1.38K	4.39s x 1	**3.98**		**13.6**	
16 x 32 x 16	9.54K	10.8s x 4	**0.554**	7.17	**1.45**	9.37
32 x 64 x 32	70.8K	59.5s x 4	**2.99(-2)**	18.5	**7.02(-2)**	20.6
64 x 128 x 64	545K	96.0s x 32	**3.37(-3)**	8.87	**1.03(-3)**	68.1
128 x 256 x 128	4.28M	781s x 32	**4.04(-4)**	8.34	**8.64(-5)**	11.9

Remark 5. The last theorem proves the convergence of the discretized approximated kernel which is used numerically. Unfortunately, because of roundoff errors, this convergence is not numerically attained...

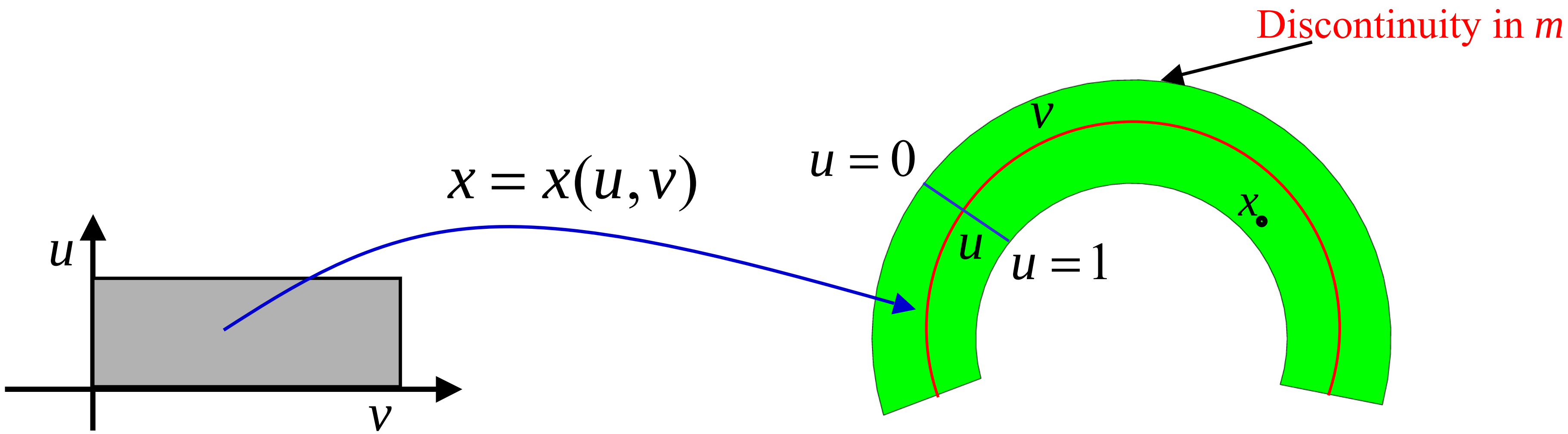
$$G(x;x') \approx G_N^D(x;x0) := \frac{1}{2\pi N_T} \sum_{n_T=1}^{N_T} e^{(ik(x-z_i)\cdot U(\theta_{n_T}))} \cdot e^{(-ik(x'-z_j)U(\theta_{n_T}))} \cdot \left[\sum_{m=-N}^{N} e^{(im(\theta_{n_T}-arg(z_i-z_j)))} K_{|m|}(-ik|z_i - z_j|) \right] \quad (6)$$

$$\left(\theta_{n_T} = \frac{2\pi}{N_T} n_T \right)$$

The main difficulty we face in studying Rokhlin's method lies in the fact that, even if from a theoretical point of view (see Theorems 2, 4, 6 and 7) the greater N the more accurate the approximation, N must (in numerical simulations) belong to a fixed range of integers. If N is too small, the overall accuracy is not good, which is quite logical. But if N is too large, then (6) is not numerically accurate... Hopefully, there is a range of integer values N such that the accuracy of Rokhlin's formula (6) is quite good...

*C. Labreuche, "A convergence theorem for the fast multipole method for 2-dimensional scattering problems", Math. Comp. **67**, 553-591[1998]*

Resolving Edge Discontinuities

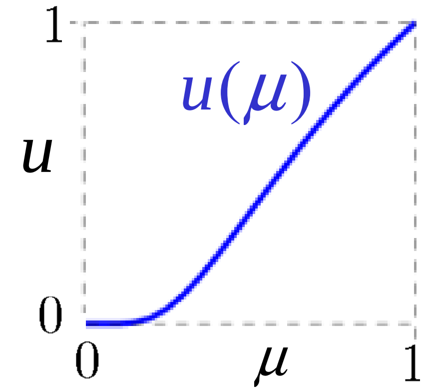


$$\int_{T_1} g(x-y)\underbrace{\psi_{T_1}(y)m(y)u(y)}_{\varphi(y)}dy = \iint_{(u',v')} g(x-x(u',v'))\,\varphi(u',v')\,J(u',v')\,du'dv'$$

"Regularize" at $u = 0$:

$$x = x(u(\mu),v) \equiv x(\mu,v)$$

$$J(\mu',v') = J(u(\mu'),v')\left.\frac{du}{d\mu}\right|_{\mu=\mu'}$$



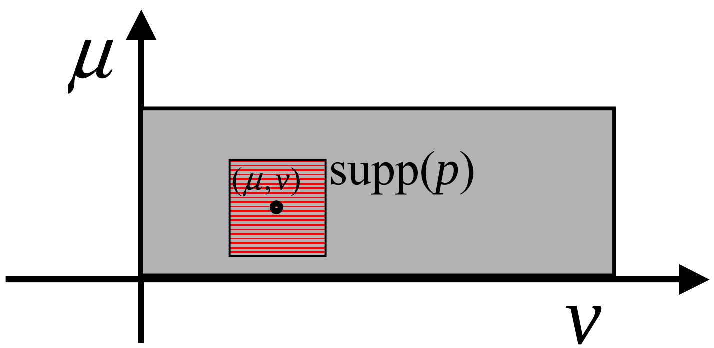
$\Rightarrow w(\mu',v') \equiv \varphi(\mu',v')\,J(\mu',v')$ is smooth and periodic!

Integration on Thin Volumes

$$\iint_{(\mu',v')} g(x(\mu,v)-x(\mu',v'))\,w(\mu',v')\,d\mu'\,dv' =$$

Difficulties:

- $g(x)$ is *singular* when $x=0$
- Direct evaluation is *costly* – $O(N^2)$



$$= \iint_{\text{supp}(p)} g(x(\mu,v)-x(\mu',v'))\,p(\mu',v')\,w(\mu',v')\,d\mu' dv'$$

Singular $\Rightarrow$ Regularize with change of variables

$$+ \iint_{(\mu',v')} g(x(\mu,v)-x(\mu',v'))\big(1-p(\mu',v')\big)w(\mu',v')\,d\mu' dv'$$

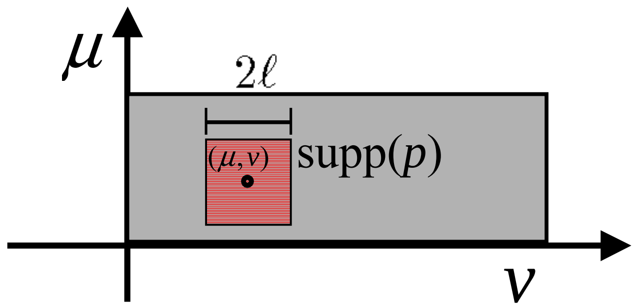
Costly $\Rightarrow$ Accelerate with equivalent sources

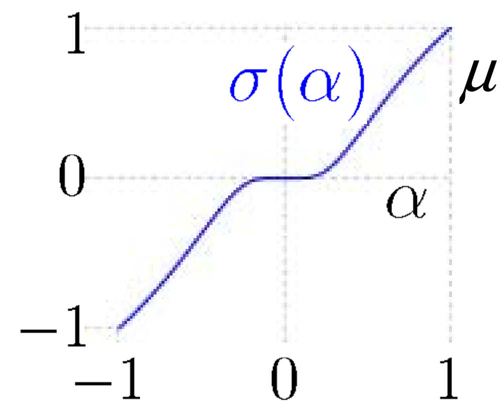
Adjacent Interactions

$$\iint_{\mathrm{supp}(p)} g(x(u,v)-x(\mu',v'))\, p(\mu',v')\, w(\mu',v')\, d\mu' dv' =$$

Regularize singularity at (μ,v):

$$\mu' = \mu + \ell\sigma(\alpha)$$
$$v' = v + \ell\sigma(\beta)$$





$$= \iint_{\mathrm{supp}(p)} g(x(u,v)-x(\mu',v'))\, p(\mu',v')\, w(\mu',v')\, \ell^2 d\sigma(\alpha)\, d\sigma(\beta)$$

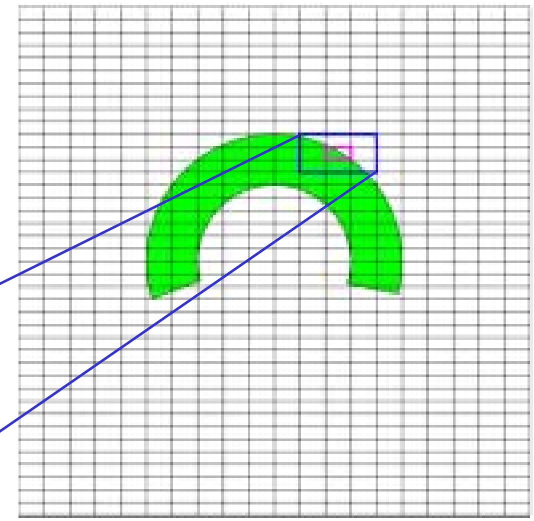
$\Rightarrow$ Trapezoidal Rule $\Rightarrow$ Superalgebraic convergence!

Non-adjacent Interactions

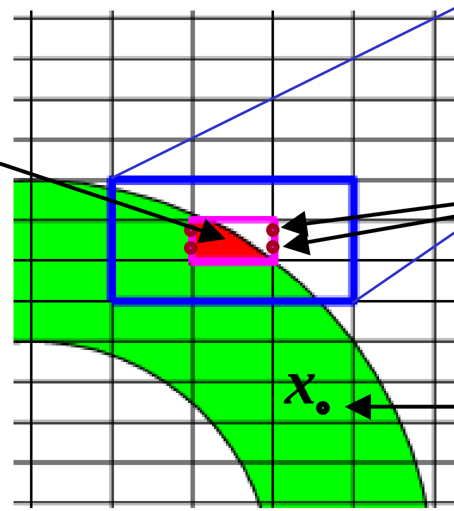
$$\iint_{(\mu',v')} g(x-x(\mu',v'))\big(1-p(\mu',v')\big)w(\mu',v')\,d\mu'\,dv \approx$$

$$\sum_{j,k} g(x-x(\mu',v'))\big(1-p(\mu'_j,v'_k)\big)w(\mu'_j,v'_k)$$

Expensive!



Accelerator:



⇒ Compute interactions with FFTs