WaveHoltz: A time domain method for time independent harmonic problems

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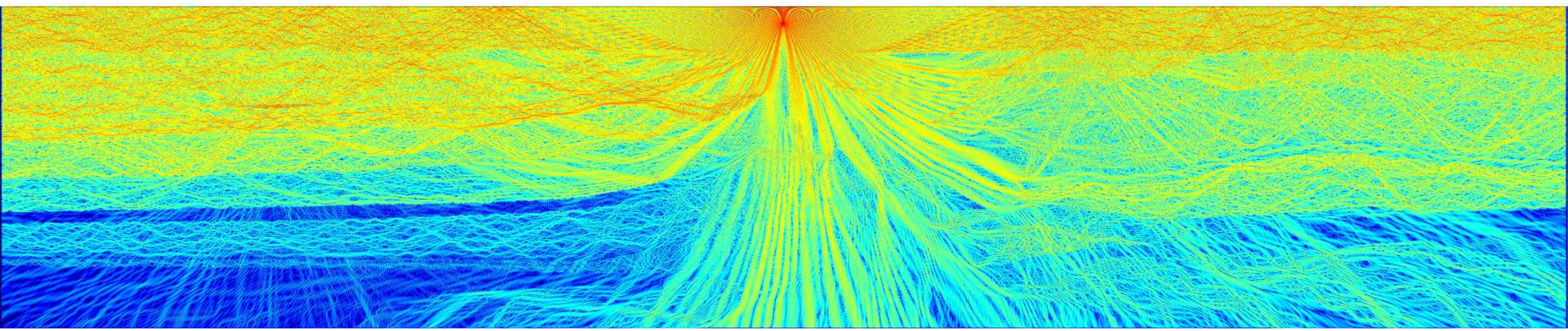

Outline

- What is Helmholtz equation?
- The WaveHoltz method and
- Some examples
-

Please ask questions throughout!

In collaboration with: Amit Rotem, Olof Runborg, Fortino Garcia, Will Pazner, Bill Henshaw, Jeff Banks & Don. Schwendeman. Supported in part by NSF 2208164 & 2210286 & STINT initiation grant.

What is Helmholtz equation?

- The wave equation at a single frequency

$$\nabla \cdot (c^2(x)\nabla u) + \omega^2 u = f(x)$$

- For computational mathematicians this equation becomes

$$(A + \omega^2 I)\mathbf{u} = \mathbf{f}$$

- As $A < 0$ and $w^2 > 0$ the problem is indefinite - challenging for iterative methods

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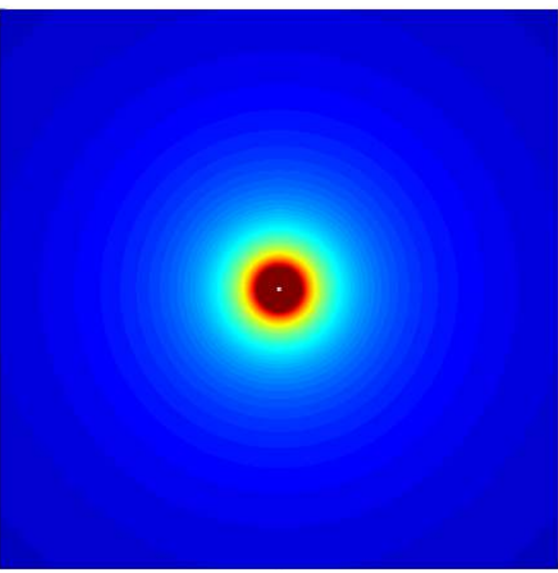
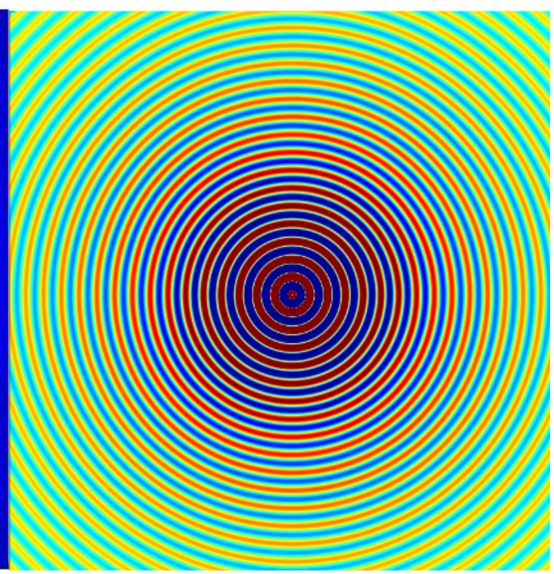
Why is it hard to solve the Helmholtz equation?

$$\Delta u(x) + \omega^2 u(x) = \delta(x) \Rightarrow u(x) = \frac{e^{i\omega R}}{R}$$

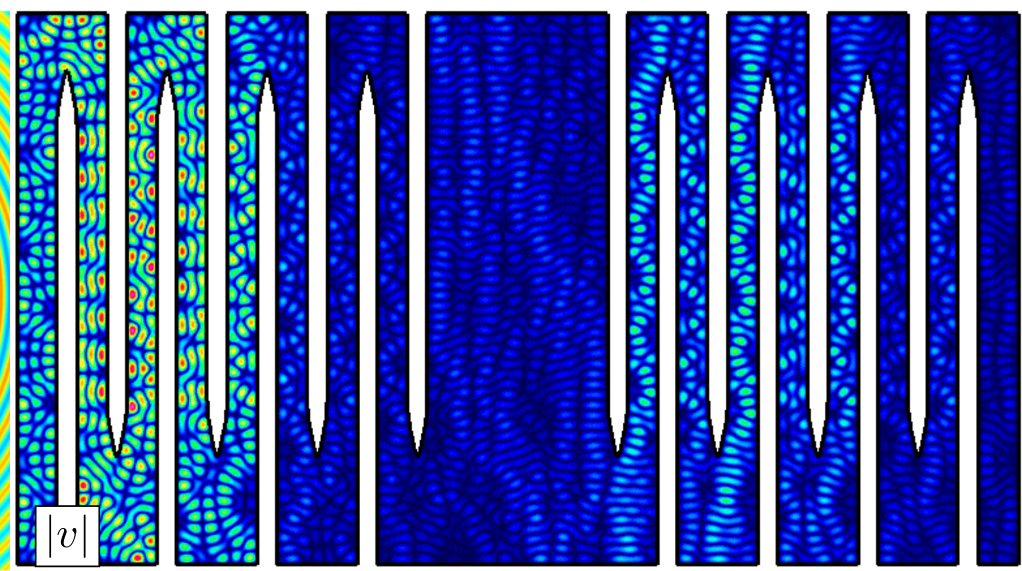
$\omega = 0$



$\omega = 200$



Closed problems are harder!!!



The Helmholtz equation

$$\nabla \cdot (c^2(x)\nabla u) + \omega^2 u = f(x), \qquad x \in \Omega,$$

With boundary conditions

$$i\alpha\omega u + \beta(c^2(x)\vec{n} \cdot \nabla u) = 0, \quad \alpha^2 + \beta^2 = 1,$$

Then for reasonable problems

$$f \in L^2(\Omega) \quad c \in L^\infty(\Omega) \quad 0 < c_{\min} \leq c(x) \leq c_{\max} < \infty$$

there is a unique weak solution $u \in H^1(\Omega)$ away from resonances

The wave equation leading to the Helmholtz eq.

If u solves Helmholtz then the $T = \dfrac{2\pi}{\omega}$ - periodic function

$$w(t,x) := u(x)\exp(i\omega t)$$

solves the wave equation

$$w_{tt} = \nabla \cdot (c^2(x)\nabla w) - f(x)e^{i\omega t}, \quad x \in \Omega, \quad 0 \leq t \leq T,$$
$$w(0,x) = v_0(x), \quad w_t(0,x) = v_1(x),$$

where the initial data provide the connection to Helmholtz

$$\boxed{v_0 = u \quad v_1 = i\omega u}$$

In WaveHoltz we find these initial conditions

The WaveHoltz iteration

Recall: $w(x,t)$ solves wave with initial data $v_0(x)$ and $v_1(x)$

We filter the wave eq. solution for one period

$$\Pi \left[\begin{array}{c} v_0 \\ v_1 \end{array} \right] = \frac{2}{T} \int_0^T \left(\cos(\omega t) - \frac{1}{4} \right) \left[\begin{array}{c} w(t,x) \\ w_t(t,x) \end{array} \right] dt, \quad T = \frac{2\pi}{\omega},$$

This defines our WaveHoltz iteration

$$\boxed{\left[\begin{array}{c} v \\ v' \end{array} \right]^{(n+1)} = \Pi \left[\begin{array}{c} v \\ v' \end{array} \right]^{(n)}, \qquad \left[\begin{array}{c} v \\ v' \end{array} \right]^{(0)} \equiv 0.}$$

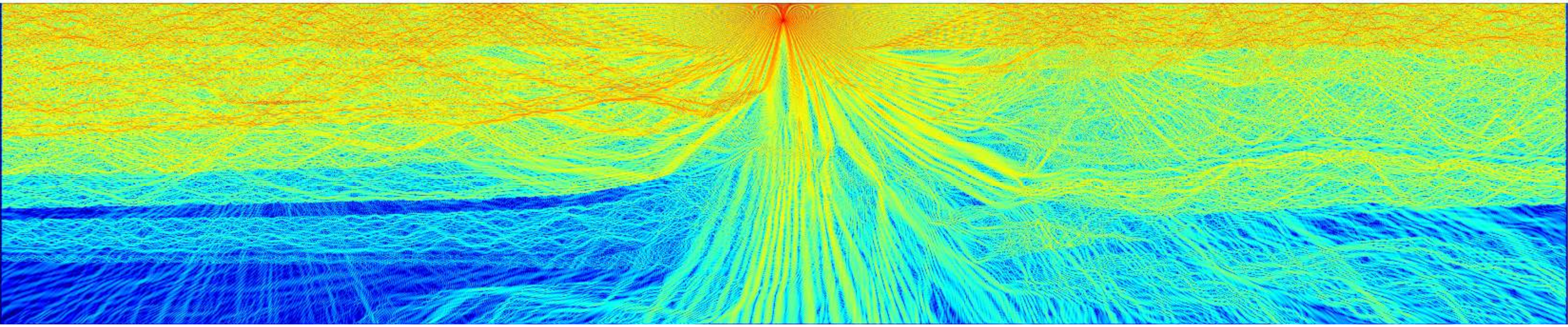
The (unique) fixpoint is the Helmholtz solution! $\left[\begin{array}{c} u \\ i\omega u \end{array} \right] = \Pi \left[\begin{array}{c} u \\ i\omega u \end{array} \right]$

Questions?!

$$\Pi \begin{bmatrix} v_0 \\ v_1 \end{bmatrix} = \frac{2}{T} \int_0^T \left(\cos(\omega t) - \frac{1}{4} \right) \begin{bmatrix} w(t,x) \\ w_t(t,x) \end{bmatrix} dt$$

- Where did the time averaging come from, and what about the strange 1/4?
- Does this actually converge?
- Isn't a fixed point iteration slow?
- Why don't I just solve Helmholtz right away?
- Does it work in practice and for high frequencies?

Marmousi2 on 13601 x 2810 grid, w = 800 rad/s. Biggest 3D problem so far is 8B DOF



Analysis

- Bounded interior problem with homogenous Dirichlet or Neumann boundary conditions.
- Then u is real and one initial condition will be enough and $e^{i\omega t} \Rightarrow \cos(\omega t)$

$$w_{tt} = \nabla \cdot (c(x)^2 \nabla w) - f(x)\cos(\omega t), \quad x \in \Omega, \quad 0 \le t \le T,$$
$$w(0,x) = v(x), \quad w_t(0,x) \equiv 0,$$

$$\Pi v = \frac{2}{T}\int_0^T \left(\cos(\omega t) - \frac{1}{4}\right) w(t,x)dt, \qquad \boxed{v^{n+1} = \Pi v^n, \qquad v^0 \equiv 0,}$$

Convergence of WaveHoltz to Helmholtz

The minimal “wave equation” and the corresponding “Helmholtz” eq. is:

$$W_{tt} = -\lambda^2 W - f\cos(\omega t) \qquad -\omega^2 u = -\lambda^2 u - f$$

Here we can just solve the Helmholtz equation: $u = \dfrac{f}{\omega^2 - \lambda^2}$

For general initial condition $\boxed{W(0) = v,}$ $W_t(0) = 0$ it can be checked that the solution is:

$$\begin{aligned} W(t) &= u[\cos(\omega t) - \cos(\lambda t)] + v\cos(\lambda t) \\ &= \frac{f}{\omega^2 - \lambda^2}[\cos(\omega t) - \cos(\lambda t)] + v\cos(\lambda t) \end{aligned}$$

Convergence of WaveHoltz to Helmholtz

Plugging in this solution in the iteration we see: $W(t) = u[\cos(\omega t) - \cos(\lambda t)] + v\cos(\lambda t)$

$$\begin{aligned}\Pi v &= \frac{2}{T}\int_0^T \left(\cos(\omega t) - \frac{1}{4}\right) W(t) dt \\ &= u[1-\beta(\lambda)] + v\beta(\lambda) \\ &= \beta(\lambda)[v-u] + u\end{aligned}$$

The error is reduced by $\beta(\lambda) \equiv \frac{2}{T}\int_0^T \left(\cos(\omega t) - \frac{1}{4}\right)\cos(\lambda t) dt$

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Convergence of WaveHoltz to Helmholtz

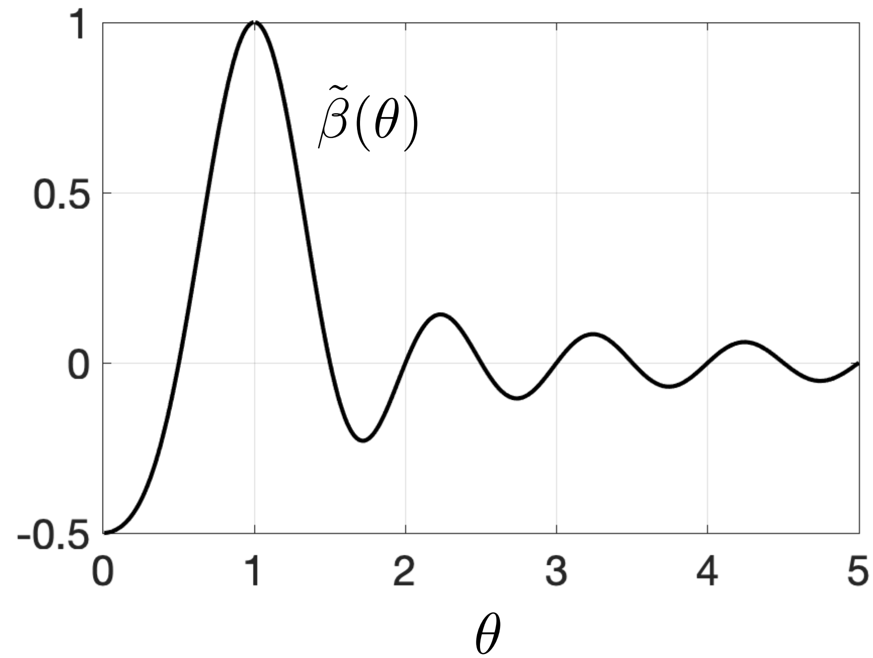
The error is reduced by

$$\beta(\lambda) \equiv \frac{2}{T}\int_0^T \left(\cos(\omega t) - \frac{1}{4}\right)\cos(\lambda t)dt$$

Introducing $\theta \equiv \dfrac{\lambda}{\omega}$

We get the explicit expression:

$$\tilde{\beta}(\theta) = \begin{cases} -0.5, & \theta = 0, \\ 1, & \theta = 1, \\ \frac{\sin(2\pi\theta)}{2\pi}\left(\frac{1}{\theta+1} + \frac{1}{\theta-1} - \frac{1}{2\theta}\right), & \text{otherwise.} \end{cases}$$



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Convergence of WaveHoltz to Helmholtz

Let the eigenpairs of $-\nabla \cdot (c^2(x)\nabla)$ be (ϕ_j, λ_j^2)

Expand everything in this ON-eigenbasis to find:

$$\Pi v = \mathcal{S}[v-u] + u, \quad \mathcal{S}q(x) \equiv \sum_{j=0}^{\infty} \beta(\lambda_j)\hat{q}_j\phi_j(x)$$

$$v^{n+1} = \mathcal{S}[v^n - u] + u \Rightarrow v^{n+1} - u = \mathcal{S}[v^n - u]$$

The linear operator $\mathcal{S}$ has eigenpairs $(\phi_j, \beta(\lambda_j))$ and is contractive.

Convergence of WaveHoltz to Helmholtz

Defining the relative distance to resonance as: $\delta = \inf_j \frac{|\lambda_j - \omega|}{\omega} > 0$

and let $\rho \equiv \max_j |\beta(\lambda_j)| = 1 - c\delta^2$

We have $\|v^{n+1} - u\|^2_{L^2(\Omega)} = \|\mathcal{S}[v^n - u]\|^2_{L^2(\Omega)} = \sum_{j=0}^{\infty} \beta(\lambda_j)^2 |\hat{v}^n_j - \hat{u}_j| \leq \rho^2 \|v^n - u\|^2_{L^2(\Omega)}$

H1 is similar and we thus have

Theorem (Convergence)

The WaveHoltz iteration converges in $H^1(\Omega)$ *to the solution of the Helmholtz equation, for the Dirichlet and Neumann problems away from resonances. The convergence rate is* $1 - O(\delta^2)$.

Rate of convergence - acceleration by conjugate gradients

The rate of convergence $\rho \equiv \max_j |\beta(\lambda_j)| = 1 - c\delta^2$ means that for fixed TOL #iterations is $\mathcal{O}(\delta^{-2})$

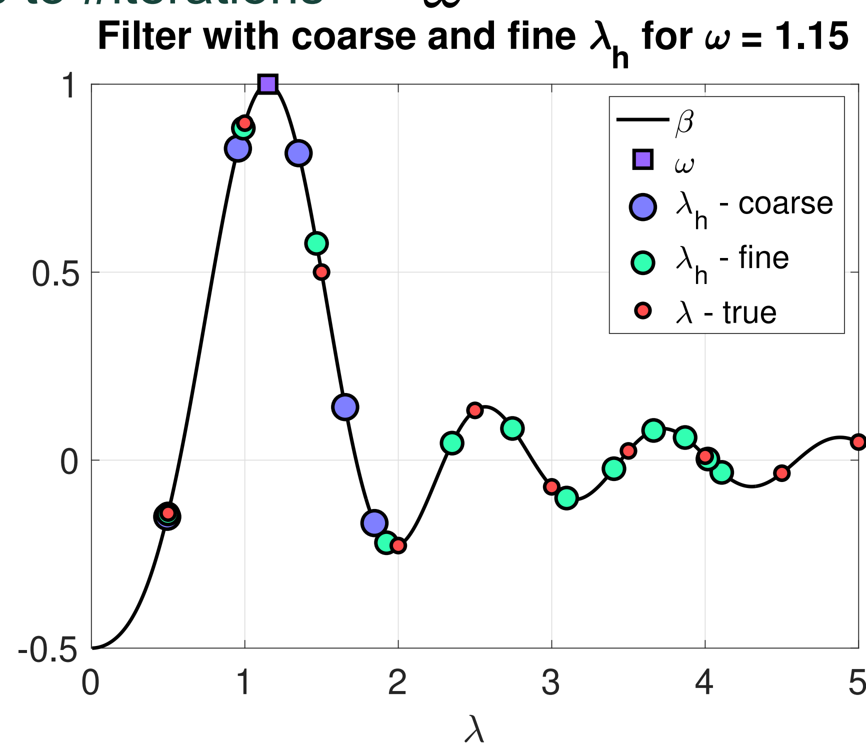
From Weyl's law we have $\lambda_j \sim j^{\frac{1}{d}}$ and this leads to #iterations $\sim \omega^{2d}$

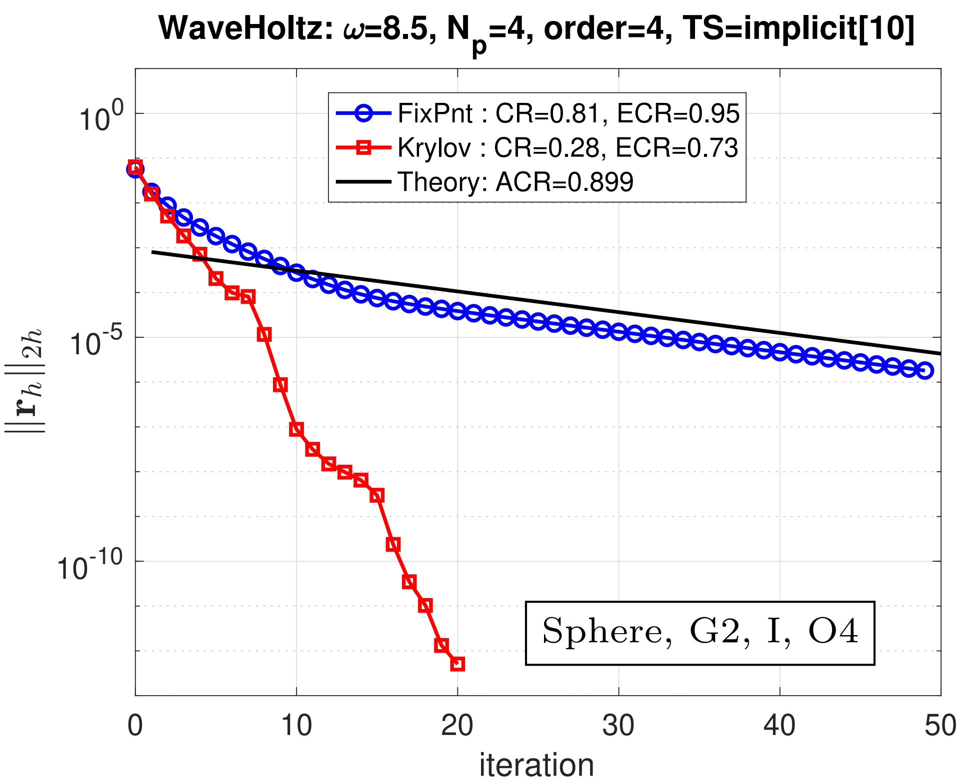
Write as a linear system - accelerate with CG

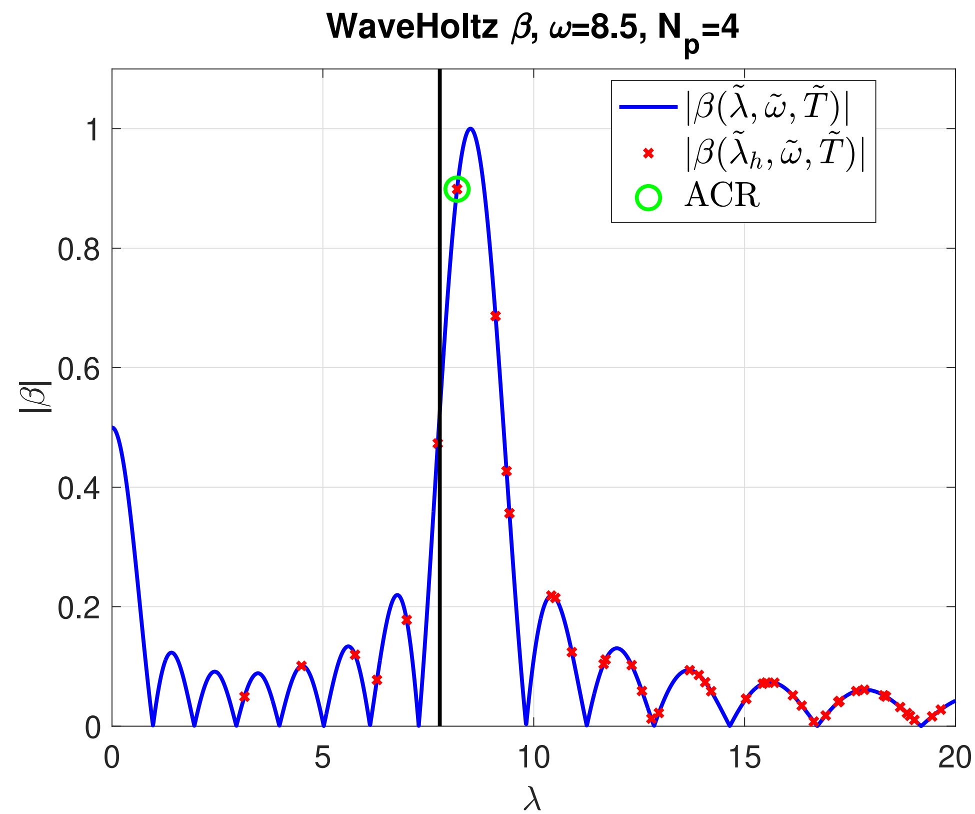
$$v = \Pi v \Leftrightarrow \underbrace{(I - \mathcal{S})}_{\mathcal{A}} v = \Pi 0$$

Eigenvalues of $\mathcal{A}$ are $0 < 1 - \beta(\lambda) \leq \frac{3}{2}$

The eigenpairs of $-\nabla \cdot (c^2(x)\nabla)$ are (ϕ_j, λ_j^2)

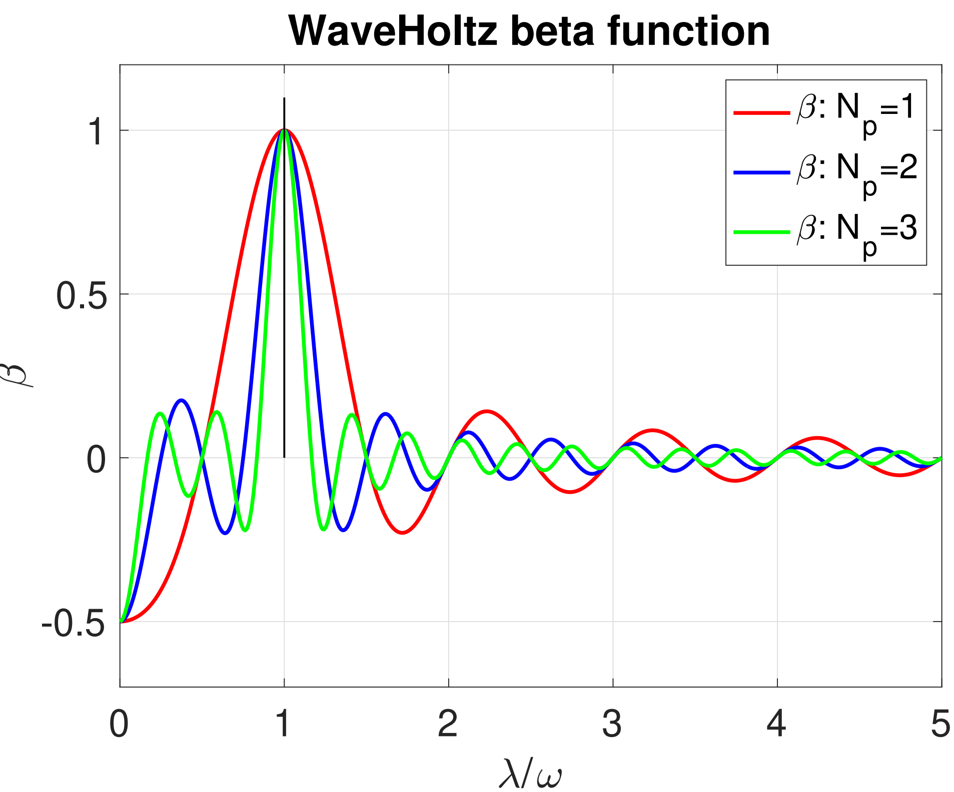



WaveHoltz: ω=8.5, N_p=4, order=4, TS=implicit[10]
FixPnt : CR=0.81, ECR=0.95
Krylov : CR=0.28, ECR=0.73
Theory: ACR=0.899
Sphere, G2, I, O4
$\|\mathbf{r}_h\|_{2h}$
iteration
10^{0}
10^{-5}
10^{-10}
0
10
20
30
40
50


WaveHoltz β, ω=8.5, N_p=4
$|\beta(\tilde{\lambda}, \tilde{\omega}, \tilde{T})|$
$|\beta(\tilde{\lambda}_h, \tilde{\omega}, \tilde{T})|$
ACR
$|\beta|$
λ
0
0.2
0.4
0.6
0.8
1
0
5
10
15
20

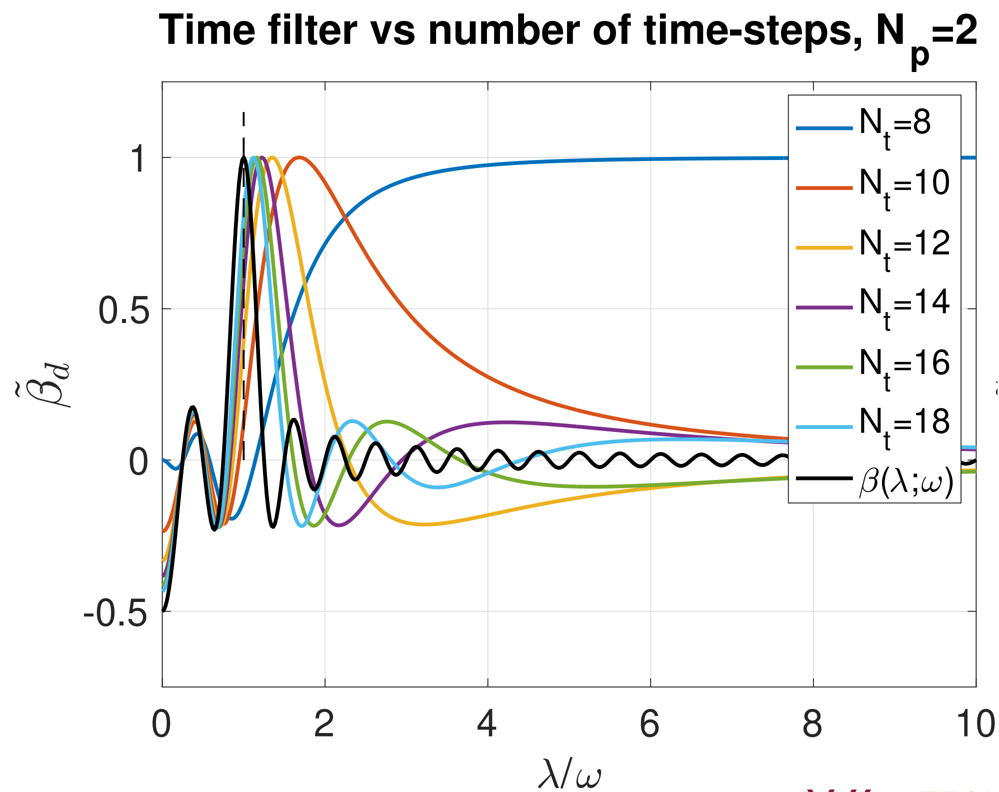
Increase number of periods

$$\frac{2}{N_pT}\int_0^{N_pT}(\cos(\omega t)-\frac{1}{4})\cos(\lambda t)dt$$



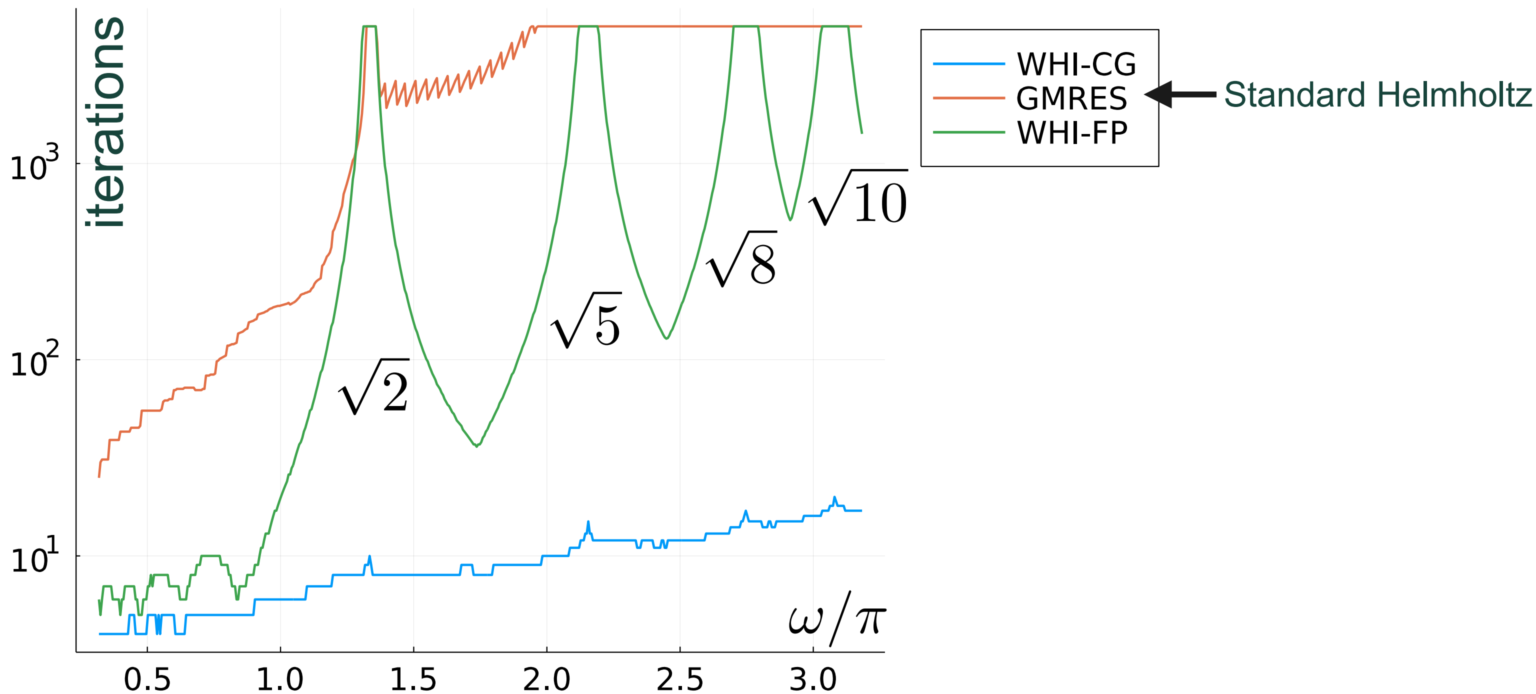
Replace with polynomial

$$\frac{2}{T}\sum_{n=0}^{N_t}\left(\cos(\omega_e t^n)-\frac{\alpha_d}{2}\right)\,\hat{W}_m^n\,\sigma_n\,\Delta t,$$



Numerical examples

WaveHoltz + CG is insensitive to distance to resonance



Unit square with fixed PPW, resonances at $\omega_{\mathrm{R}}/\pi = \sqrt{m^2 + n^2}$

Textbook 2nd order FD method.

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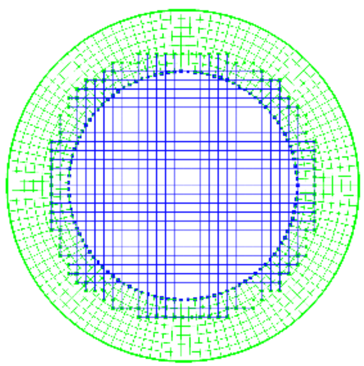
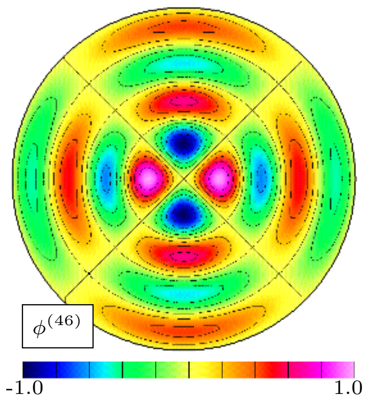
Optimal $\mathcal{O}(N)$ algorithm via (A)MG for linear systems and eigs

EigenWave - set forcing = 0 and use Krylov-Schur (slepc)





EigenWave scaling: disk, order 4						
Δs	grid-points	eigen-pairs	wave-solves	multigrid cycles	CPU seconds	CPU ratio
1/40	6.8e+03	18	86	6.0	7.8e+00	
1/80	2.8e+04	20	86	6.8	2.6e+01	3.35
1/160	1.1e+05	21	88	8.7	1.1e+02	4.15
1/320	4.2e+05	19	90	8.2	4.2e+02	3.87
1/640	1.7e+06	21	88	9.0	1.3e+03	3.16
1/1280	6.7e+06	18	92	9.8	6.1e+03	4.61

Inverting the same nice system every timestep using MG

$$\left(I - \frac{\Delta t^2}{2} L_{p,h}\right)\left(W_{\mathbf{j}}^{n+1} + W_{\mathbf{j}}^{n-1}\right) = g.$$

		WaveHoltz			GMRES+ILU(5)	
grid	N	its	ECR	CPU (s)	its	CPU (s)
square	256^2	14	0.58	4.3	5.3e2	1.7e0
square	512^2	14	0.58	16	2.8e3	5.0e1
square	1024^2	14	0.58	63	2.6e4	2.0e3
square	2048^2	14	0.58	258	1.3e5	5.8e4

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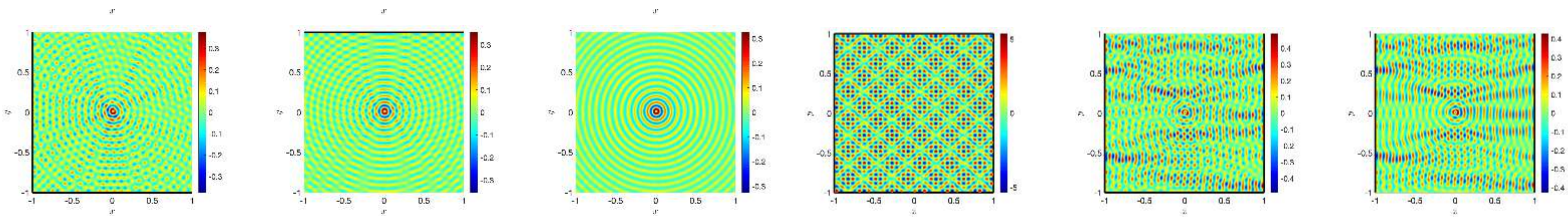
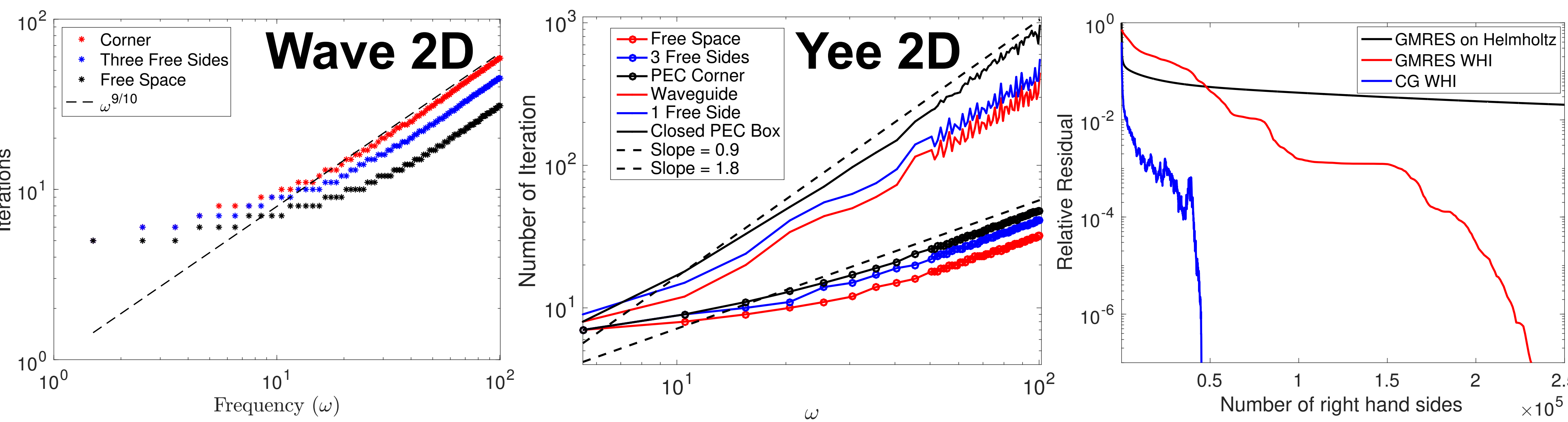
Two dimensions - point source - iteration vs. frequency



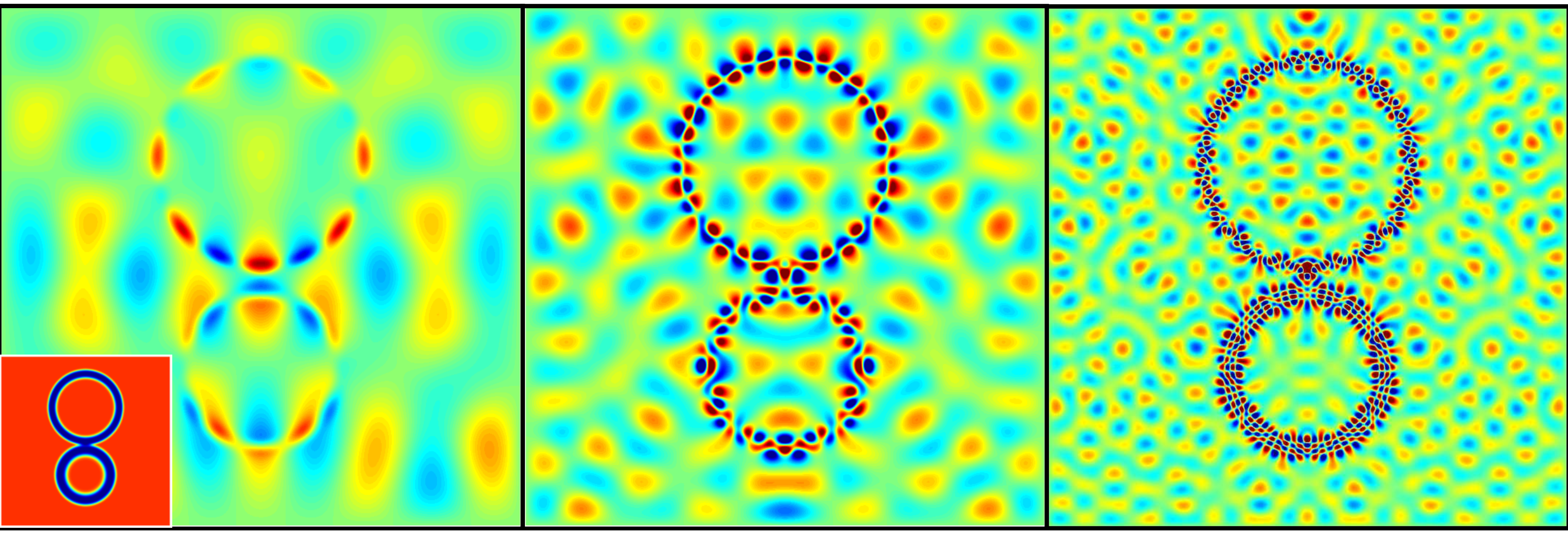
Finite difference WHI-CG (bounded domain) WHI-GMRES (unbounded), fixed PPW, TOL = 1e-5



Free lunch

$$w_{tt} = c(x)^2 \Delta w - f(x)(\cos(\omega t) + \cos(2\omega t) + \cos(4\omega t)),$$

$$\Pi v = \frac{2}{T}\int_0^T \left(\cos(\omega t) + \cos(2\omega t) + \cos(4\omega t) - \frac{1}{4}\right) w(t,x)dt$$



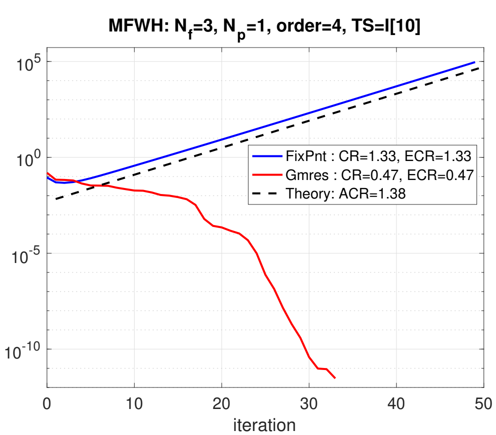
Free lunch

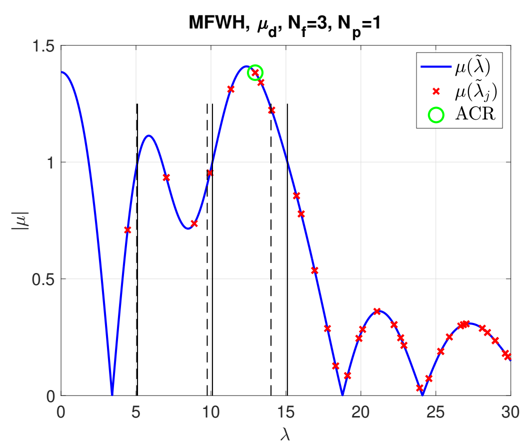
$$\mathcal{L}u^{(m)} + \omega_m^2\, u^{(m)} = f^{(m)}(\mathbf{x}), \qquad \mathcal{B}u^{(m)} = g^{(m)}(\mathbf{x}),$$

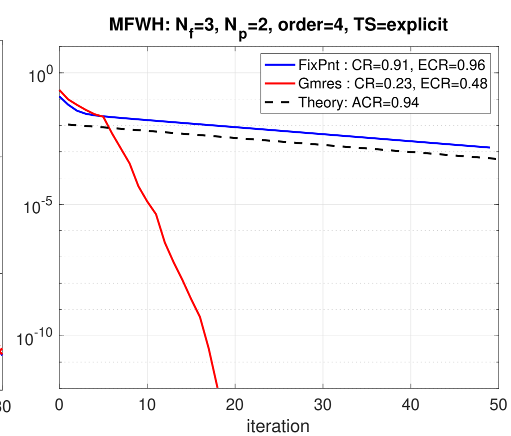
$$\begin{aligned} \partial_t^2 w &= \mathcal{L}w - F(\mathbf{x},t), && \mathbf{x}\in\Omega, \quad t\in[0,T_f], \\ \mathcal{B}w &= G(\mathbf{x},t), && \mathbf{x}\in\partial\Omega, \\ F(\mathbf{x},t) &= \sum_{m=1}^{\mathcal{N}_f} f^{(m)}(\mathbf{x})\,\cos(\omega_m t), \end{aligned}$$

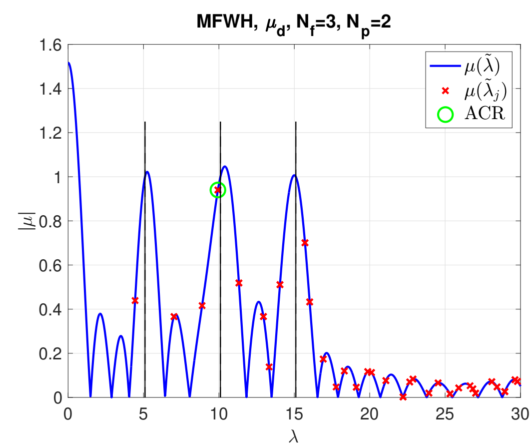
Filter each solution

$$v^{(m,k+1)} \stackrel{\text{def}}{=} \frac{2}{T_{f,m}} \int_0^{T_{f,m}} \left(\cos(\omega_m t) - \frac{\alpha_m}{2}\right) \left[w^{(k)}(\mathbf{x},t;\, v^{(:,k)}) - \sum_{j=1, j\neq m}^{\mathcal{N}_f} v^{(j,k+1)}(x)\cos(\omega_j t) \right] dt,$$



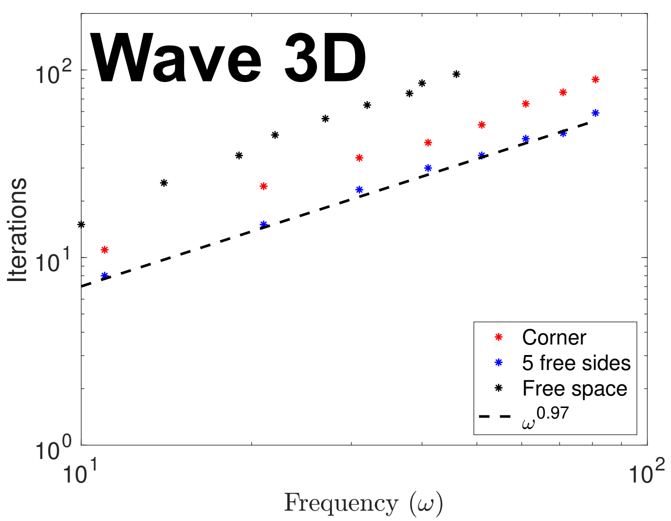


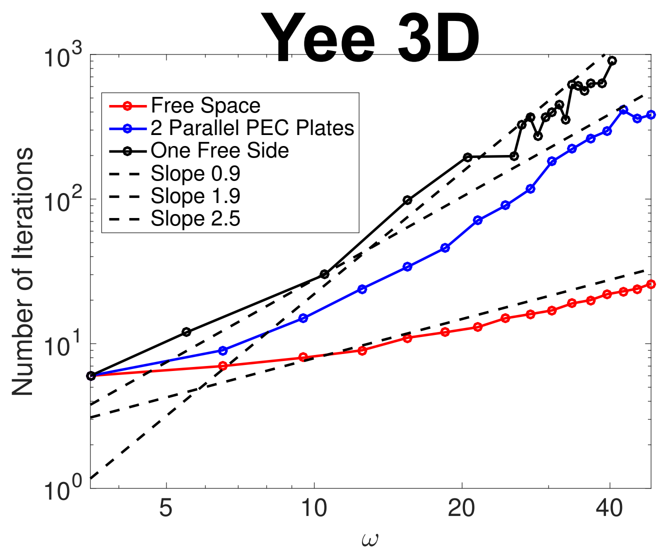


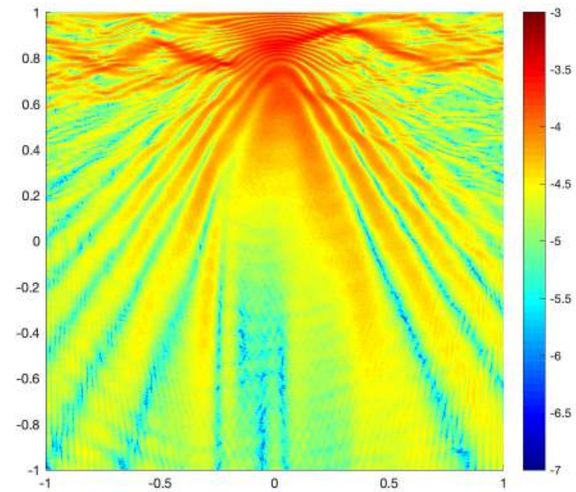


Three dimensions - iterations vs. frequency

- Simple FD code with variable coefficient
- Iterations for open problems scale as in 2D - linear in frequency
- Iterations for all Dirichlet scale roughly as expected
- Largest problem so far 8 Billion DOF







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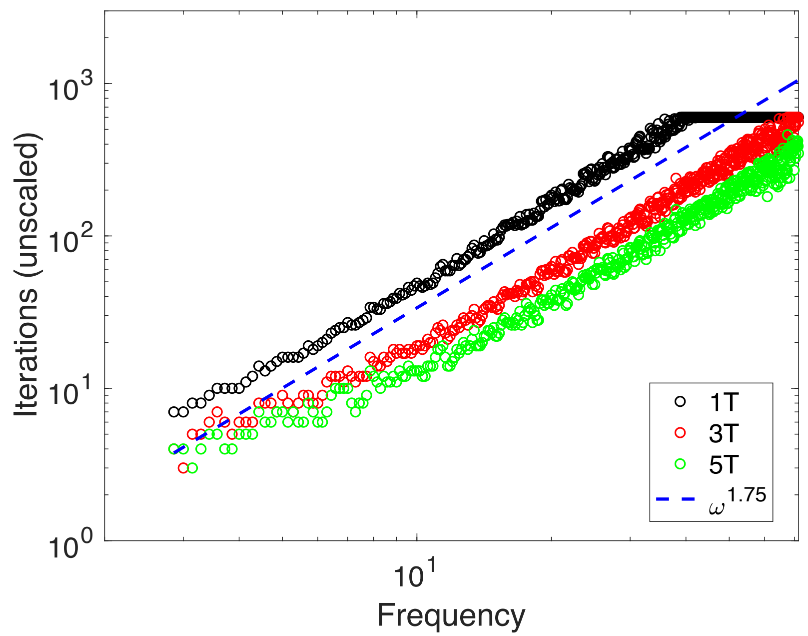
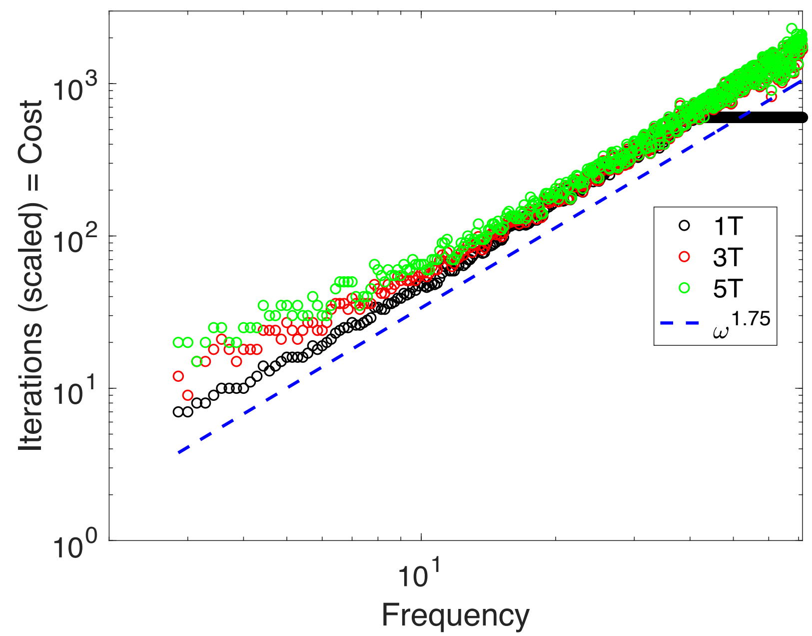
Memory lean example

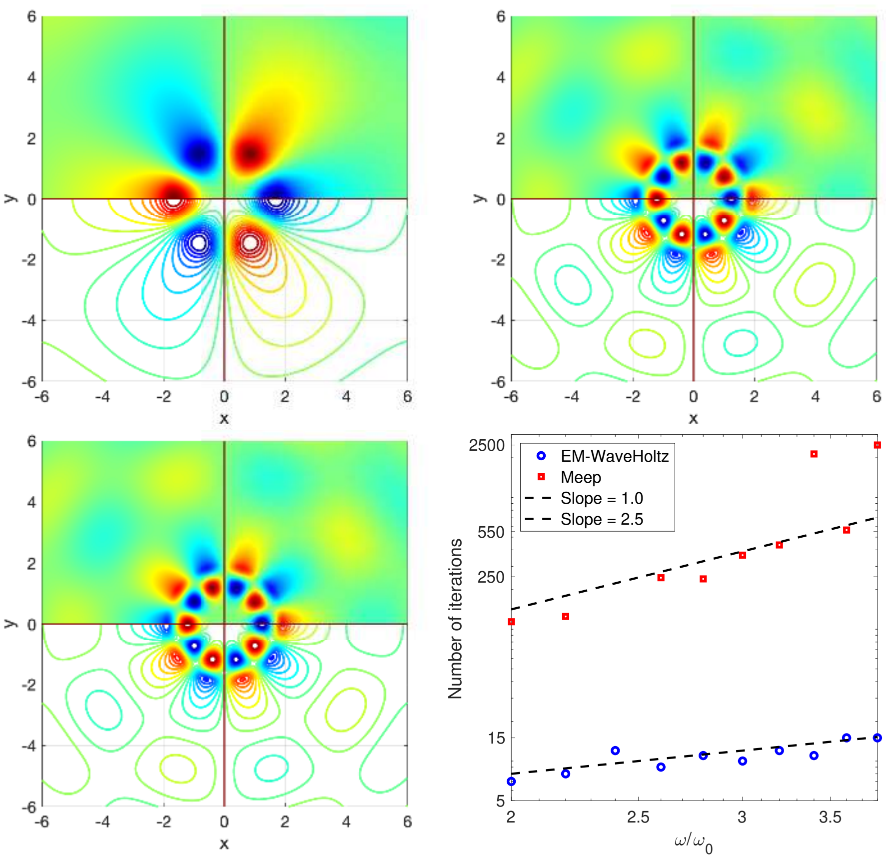
- Use a longer filter to reduce memory. Define the iteration to be over 1T, 3T or 5T (up to 5 x smaller Krylov subspace)
- 2x2 square with a point-source near the middle 6th order SBP-FD
- Fixed number of points per wavelength
- WHI - GMRES res < 1e-8.

$$\frac{2}{kT}\int_0^{kT}(\cos(\omega t)-\frac{1}{4})w(x,t)dt$$





EM-WaveHoltz



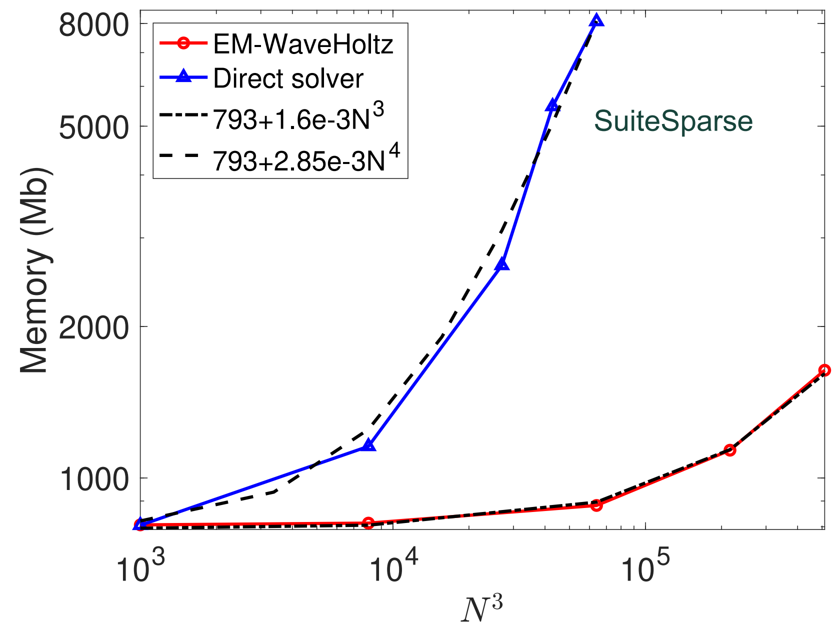


TABLE II
TOTAL NUMBER OF ITERATIONS WITH 10^{-7} RELATIVE RESIDUAL

	N	$\omega = \omega_0$	$\omega = 2.24\omega_0$	$\omega = 2.7\omega_0$
EM-WH	120	8	11	14
	240	8	11	15
	480	8	11	15
BICG-Stab(l) MEEP	120	144	256	405
	240	280	449	557
	480	586	800	1092

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Comparison of Explicit and Implicit ElWaveHoltz with Direct Discretization of ElasticHelmholtz

2D problem discretized using SIPDG

		$p = 1$	2	3	4	5	6	7	8	9
h	WH	57	102	115	126	132	138	141	144	148
$h/2$	WH	68	108	114	126	130	133	138	143	146
$h/4$	WH	79	107	114	122	130	135	137	142	146
$h/8$	WH	83	108	114	125	130	133	137	142	146
h	IWH	81	182	160	173	213	237	192	235	201
$h/2$	IWH	97	151	157	168	220	263	188	276	196
$h/4$	IWH	112	147	153	163	171	178	264	188	275
$h/8$	IWH	117	147	154	165	171	213	217	N/A	N/A
h	HH	480	25084	18298	37926	80262	144863	204694	230688	500000
$h/2$	HH	15686	32063	57338	106688	256801	347279	500000	500000	500000
$h/4$	HH	46667	79865	184331	334665	500000	500000	500000	500000	500000
$h/8$	HH	500000	304561	500000	500000	500000	500000	500000	N/A	N/A

Indicates that the condition number of WaveHoltz is independent of gridsize

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