CgWaveHoltz: A Composite Grid Helmholtz Solver using the WaveHoltz Algorithm

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Abstract

Here are notes on CgWaveHoltz Helmholtz solver that is based on solving the Helmholtz equation using the wave equation solver CgWave.

Keywords: Maxwell

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1. Introduction

Here are some notes on the CgWaveHoltz solver based on WaveHoltz scheme [?] of Appelö et.al. The WaveHoltz algorithm solves the time-harmonic wave equation (Helmholtz equation) using a time-dependent wave equation solver. CgWaveHoltz uses the CgWave wave equation solver.

Things to do:

- 1. Compatibility boundary conditions for direct Helmholtz solver.
- 2. Sixth and eight-order accurate direct Helmholtz solver.

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2. WaveHoltz algorithm

The Helmholtz solution $u(\mathbf{x},t)$ satisfies,

$$-\omega^2 u = c^2 \Delta u + f(\mathbf{x}), \quad \text{for } \mathbf{x} \in \Omega,$$
 (1a)

$$Bu = g(\mathbf{x})$$
 for $\mathbf{x} \in \partial \Omega$, (1b)

Here Bw = q denotes some appropriate boundary conditions.

Let $w(\mathbf{x},t)$ be a solution to the wave equation in second-order form with a time-harmonic forcing,

$$\partial_t^2 w = c^2 \Delta w + f(\mathbf{x}) e^{i\omega t}, \qquad \text{for } \mathbf{x} \in \Omega, \, t > 0,$$
 (2a)

$$Bw = g(\mathbf{x}) e^{i\omega t} \qquad \text{for } \mathbf{x} \in \partial\Omega, \, t > 0, \tag{2b}$$

$$w(x,0) = v_0(\mathbf{x}), \quad \partial_t w(\mathbf{x},0) = v_1(\mathbf{x}), \quad \text{for } \mathbf{x} \in \partial\Omega.$$
 (2c)

and initial conditions for u and u_t given by $v_0(\mathbf{x})$ and $v_1(\mathbf{x})$.

The WaveHoltz algorithm [?] defines an affine operator Π that acts on the initial conditions $\mathbf{v} = [v_0, v_1]^T$ by solving the wave equation (2) with initial conditions \mathbf{v} over a time period $T = 2\pi/\omega$ and then forming the time integral

$$\Pi \mathbf{v} = \frac{2}{T} \int_0^T \left(\cos(\omega t) - \frac{1}{4} \right) \begin{bmatrix} w(\mathbf{x}, t) \\ w_t(\mathbf{x}, t) \end{bmatrix} dt.$$
 (3)

Note that w implicitly depends on v and f, $w = w(\mathbf{x}, t; v, f)$. Note that Π is an affine operator of the form

$$\Pi v = Lv + b = (I - A)v + b,\tag{4}$$

where L and A are a linear operators. The solution to the Helmholtz problem (1) is found as the solution to the fixed point iteration

$$\mathbf{v}^n = \Pi \mathbf{v}^{n-1},\tag{5}$$

where $\mathbf{v}^0 = 0$ (or some other initial guess).

3. Using Krylov methods to accelerate the WaveHoltz algorithm

The fixed point iteration (5) can be accelerated with a Krylov method such as GMRES. A Krylov method solves a linear system

$$Ax = b. (6)$$

At the most basic level Krylov methods only require a function to evaluate b and a function to compute A times a vector. For the fixed point iteration (5), b is defined as the application of Π to the vector $\mathbf{v}^0 = \mathbf{0}$ (zero initial conditions),

$$b \stackrel{\text{def}}{=} \Pi \mathbf{0}, \tag{7}$$

while the application of A to an iterate \mathbf{v}^n is defined as

$$A\mathbf{v}^n = \mathbf{v}^n - \Pi\mathbf{v}^n + b. \tag{8}$$

Formula (8) looks a bit funny at first glance but this is the correct definition.

We use the Krylov solvers from PETSc [1] to solve the fixed point iteration (5). PETSc has a "matrix-free" option that allows one to provide function to compute a matrix-vector product. PETSc has many Krylov solvers suh as CG, GMRES, bi-CG-stab, etc.

4. Numerical Results

Here we present some numerical results.

4.1. Exact trigonometric Helmholtz solution

An exact solution to the Helmholtz equation on a square domain $[0,1]^2$ is given by the trigonometric function

$$u_e(\mathbf{x}, t) \stackrel{\text{def}}{=} \sin(k_x x) \sin(k_u y) \cos(\omega t),$$

where the forcing function is

$$f(\mathbf{x},t) = \left(-\omega^2 + c^2(k_x^2 + k_y^2)\right)u_e(\mathbf{x},t)$$

This solution is also used on other domains in which case we allow for in-homogeneous BCs.

FD22s Errors and convergence of WaveHoltz solutions on a square.

grid	N	u	r
square8	1	5.5e-2	
square16	2	1.3e-2	4.04
square32	4	3.4e-3	4.01
square64	8	8.4e-4	3.99
rate		2.00	

Table 1: CgWaveHoltz, boxHelmholtz, max norm, solver=krylov, order=2, t=0.5, cfl=0.9, ad4=1, omega=2, tol=1e-05 Sat May 22 06:17:07 2021

FD44s Errors and convergence of WaveHoltz solutions on a square.

grid	N	u	r
square8	1	3.4e-3	
square16	2	3.4e-4	10.12
square32	4	1.5e-5	22.97
square64	8	5.1e-7	28.96
square128	16	3.8e-8	13.34
square256	32	2.7e-9	14.03
square512	64	1.9e-10	14.52
rate		4.10	

Table 2: CgWaveHoltz, boxHelmholtz, max norm, solver=krylov, order=4, t=0.5, cfl=0.9, ad4=1, omega=2, tol=1e-8 Sat May 22 06:36:05 2021

****** OLD STUFF ******

Maximum residual = 1.058e-03

Here are some initial results for $k_x=2\pi,\ k_y=2\pi$ and $\omega=2.$ Notes on output:

- line with "TIME INTEGRAL v" gives the true solution error.
- lines with "Maximum residual = 9.319e-05" gives the residual in the Helmholtz equation.
- lines with "it=3: max(|v-v0ld|)=8.47e-06 (tol=0.0001)" give the residual in the WaveHoltz iteration $||v^{n+1} \mathbf{v}^n||_{\infty}$

Square: fixed-point iteration. SECOND-ORDER - looks OK

```
RESIDUAL IS SMOOTH
../bin/cgwh -grid=square64.order2 -cmd=boxHelmholtz.cmd -omega=2 -tol=1e-4
../bin/cgwh -grid=square32.order2 -cmd=boxHelmholtz.cmd -omega=2 -tol=1e-3
G64
cgWave: t=5.030e-01 (65 steps) maxErr= 4.55e-04
cgWave: t=1.006e+00 (130 steps) maxErr= 3.53e-04
cgWave: t=1.509e+00 (195 steps) maxErr= 8.45e-04
cgWave: t=2.012e+00 (260 steps) maxErr= 5.42e-04
cgWave: t=2.515e+00 (325 steps) maxErr= 2.72e-04
cgWave: t=3.018e+00 (390 steps) maxErr= 8.21e-04
cgWave: t=3.142e+00 TIME INTEGRAL v: maxErr= 8.45e-04
cgWave: t=3.142e+00 (406 steps) maxErr= 8.54e-04
it=3: max(|v-v01d|)=8.47e-06 (tol=0.0001)
Maximum residual = 9.319e-05
G32
advWave: sosupParameter= 0.10E+01
cgWave: t=4.952e-01 (32 steps) maxErr= 2.00e-03
cgWave: t=9.905e-01 (64 steps) maxErr= 9.78e-04
cgWave: t=1.486e+00 (96 steps) maxErr= 3.71e-03
cgWave: t=1.981e+00 (128 steps) maxErr= 2.45e-03
cgWave: t=2.476e+00 (160 steps) maxErr= 1.27e-03
cgWave: t=2.971e+00 (192 steps) maxErr= 3.05e-03
cgWave: t=3.142e+00 TIME INTEGRAL v: maxErr= 3.38e-03
cgWave: t=3.142e+00 (203 steps) maxErr= 3.81e-03
it=2: max(|v-v01d|)=4.51e-04 (tol=0.001)
```

Square: fixed-point iteration. FOURTH-ORDER – not bad, errors may be skewed by poor BC's

```
Maximum residual = 7.956e-04
```

CIC grid: fixed-point iteration. SECOND-ORDER - looks OK

```
cgWave: t=5.045e-01 (44 steps) maxErr= 2.23e-03 (max(|u|)= 5.35e-01)
cgWave: t=1.009e+00 (88 steps) maxErr= 2.95e-03 (max(|u|)= 4.35e-01)
cgWave: t=1.513e+00 (132 steps) maxErr= 4.82e-03 (max(|u|)= 9.98e-01)
cgWave: t=2.018e+00 (176 steps) maxErr= 1.64e-03 (max(|u|)= 6.28e-01)
cgWave: t=2.522e+00 (220 steps) maxErr= 3.43e-03 (max(|u|)= 3.30e-01)
cgWave: t=3.027e+00 (264 steps) maxErr= 4.38e-03 (max(|u|)= 9.78e-01)
cgWave: t=3.142e+00 TIME INTEGRAL v: maxErr= 4.58e-03
cgWave: t=3.142e+00 (274 steps) maxErr= 3.90e-03 (max(|u|)= 1.00e+00)
it=3: max(|v-v01d|)=4.52e-04 (tol=0.001)
Maximum residual = 4.049e-03
G2 - ORDER=2
cgWave: t=5.094e-01 (24 steps) maxErr= 9.28e-03 (max(|u|)= 5.33e-01)
cgWave: t=1.019e+00 (48 steps) maxErr= 7.21e-03 (max(|u|)= 4.57e-01)
cgWave: t=1.528e+00 (72 steps) maxErr= 1.72e-02 (max(|u|)= 1.01e+00)
cgWave: t=2.038e+00 (96 steps) maxErr= 1.14e-02 (max(|u|)= 6.05e-01)
cgWave: t=2.547e+00 (120 steps) maxErr= 6.96e-03 (max(|u|)= 3.80e-01)
cgWave: t=3.057e+00 (144 steps) maxErr= 1.74e-02 (max(|u|)= 1.00e+00)
cgWave: t=3.142e+00 TIME INTEGRAL v: maxErr= 1.74e-02
cgWave: t=3.142e+00 (148 steps) maxErr= 1.80e-02 (max(|u|)= 1.02e+00)
it=5: max(|v-v01d|)=9.19e-04 (tol=0.001)
Maximum residual = 8.508e-03
```

CIC grid: Krylov iteration. FOURTH-ORDER - v error looks OK, check residual compared to order=2, residual is large near boundaries

```
../bin/cgwh boxHelmholtz.cmd -g=cice4.order4.ng3.hdf -omega=2 -solver=krylov -tol=1e-5 -imode=1
../bin/cgwh boxHelmholtz.cmd -g=cice2.order4.ng3.hdf -omega=2 -solver=krylov -tol=1e-5 -imode=1
G4 : ORDER=4
advWave: ADVANCE dim=2 order=4
                                              grid=curvilinear... t= 0.11E-01
cgWave: t=4.966e-01 (46 steps) maxErr= 1.12e-05, ||u||= 5.46e-01
cgWave: t=9.932e-01 (92 steps) maxErr= 8.34e-06, ||u||= 4.04e-01
cgWave: t=1.490e+00 (138 steps) maxErr= 2.00e-05, ||u||= 9.87e-01
cgWave: t=1.986e+00 (184 steps) maxErr= 1.39e-05, ||u||= 6.74e-01
cgWave: t=2.483e+00 (230 steps) maxErr= 5.05e-06, ||u||= 2.51e-01
cgWave: t=2.980e+00 (276 steps) maxErr= 1.97e-05, ||u||= 9.48e-01
cgWave: t=3.142e+00 TIME INTEGRAL v: maxErr= 2.05e-05
cgWave: t=3.142e+00 (291 steps) maxErr= 2.07e-05, ||u||= 1.00e+00
it=-1: max(|v-v0ld|)=1.30e-06, tol=1e-05
 ******* DONE KYRLOV ITERATIONS -- numberOfIterations=8 **********
Maximum residual = 6.903e-03
G2 order=4
```

CIC grid: Krylov iteration. SECOND-ORDER - looks OK, residual is smooth

Maximum residual = 4.955e-04

4.2. Gaussian forcing

We consider solving the Helmholtz problem with a source term consisting of a sum of generalized Gaussians,

$$f(x, y, z, t) = \sum_{m} a_m \cos(\omega_m(t - t_{0,m})) e^{-\beta_m[(x - x_{0,m})^2 + (y - y_{0,m})^2 + (z - z_{0,m})^2]^{p_m}}.$$
 (9)

4.2.1. Gaussian source in a square

Figure 1 shows results from CgWaveHoltz for a square. Source term: $\omega = 17.17$, a = 100, $(x_0, y_0) = (.7, .7)$, $\beta = 50$, p = 1.

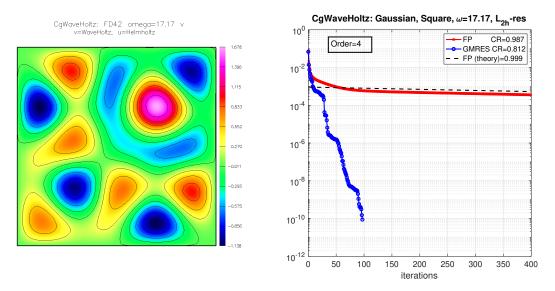


Figure 1: Gaussian source, $\omega=17.17,$ square 64, order 4

Figure 2 shows results from CgWaveHoltz for a square. Source term: $\omega = 15$, a = 100, $(x_0, y_0) = (.7, .7)$, $\beta = 50$, p = 1. The FPI convergence rate matches the theory.

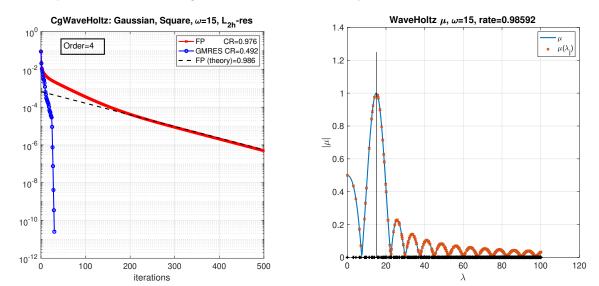


Figure 2: Gaussian source, $\omega = 15$, square 128, order 4. Right: β function with distribution of eigenvalues λ_i

########### DONE KYRLOV ITERATIONS -- KSP residual=2.54e-11 (tol=1.00e-10) numberOfIterations=31 ########## CgWaveHoltz::residual: c=1, omega= 1.50000e+01, omegas= 1.49974e+01 (from symbol of D+D-), dt=4.273544e-03, adjustOmega=1 CgWaveHoltz::residual: max-res=4.010e-04 (using omega), max-res=5.004e-02 (using omega from discrete symbol)

CgWaveHoltz: omega=1.500e+01, max-res=4.010e-04, CR=0.492 CR-perPeriod=0.492, cpu= 1.58e+00(s)

CgWaveHoltz::Results saved to file gaussianWHSquare12804Omega15Krylov.m

4.2.2. Gaussian source in an annulus

Figure 3 shows results from CgWaveHoltz for an Annulus. Eigenvalues for this problem were computed in cg/ad/codes/annulusEigenvalues.maple.

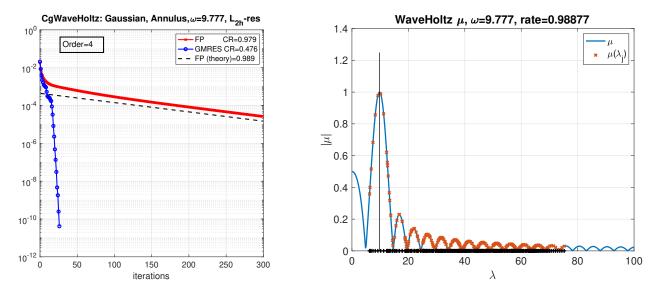


Figure 3: Gaussian source, $\omega = 9.777$, annulus8, order 4. Right: β function with distribution of eigenvalues λ_j

Figure 4 shows results from CgWaveHoltz for an Annulus for $\omega = 18.4$. It takes quite a iterations for the CR of the FPI to approach the theory; likely due to there being a few eigenvalues near the worst case. GMRES is also quite slow.

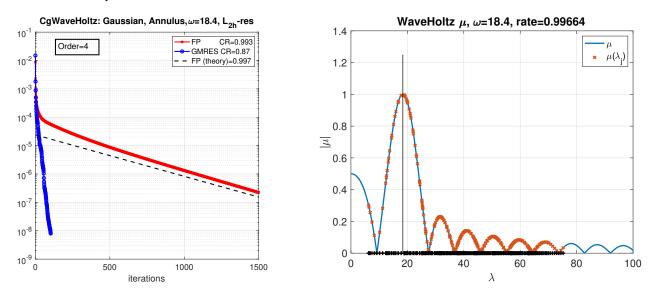


Figure 4: Gaussian source, $\omega = 18.4$, annulus8, order 4. Right: β function with distribution of eigenvalues λ_j

4.2.3. Gaussian source in a disk

Figure 5 shows results from CgWaveHoltz for an disk. Eigenvalues for this problem were computed in cg/ad/codes/diskEigenvalues.maple.

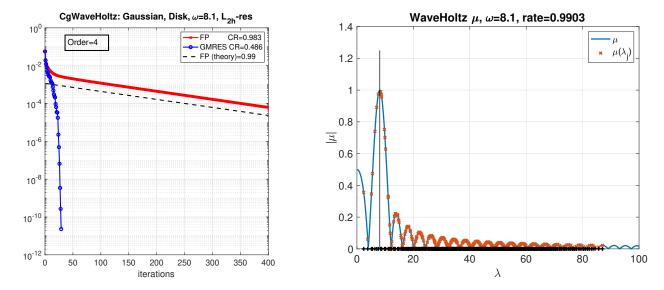


Figure 5: Gaussian source, $\omega = 8.1$, disk8, order 4. Right: β function with distribution of eigenvalues λ_j

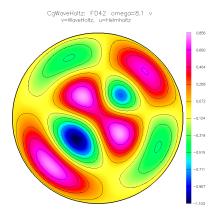


Figure 6: Gaussian source, $\omega = 8.1$, disk8, order 4.

Solution is close to the direct solver.

CgWaveHoltz::Results saved to file gaussianWHDiskO4Omega8p1Krylov.m

CgWaveHoltz: max-diff=3.25e-03 (between WaveHoltz and Direct Helmholtz solution)

4.2.4. Gaussian source in a box

Figure 7 shows results from CgWaveHoltz for a 3D box.

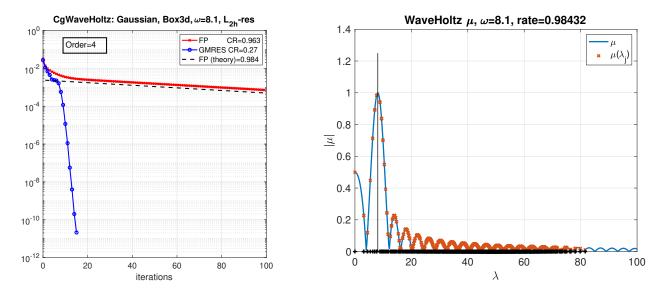


Figure 7: Gaussian source, $\omega = 8.1$, box4, order 4. Right: β function with distribution of eigenvalues λ_j

4.2.5. Gaussian source in a sphere

Figure 8 shows results from CgWaveHoltz for a 3D solid sphere.

FIX ME – EIGENVALUES FOR A SPHERE NEEDED

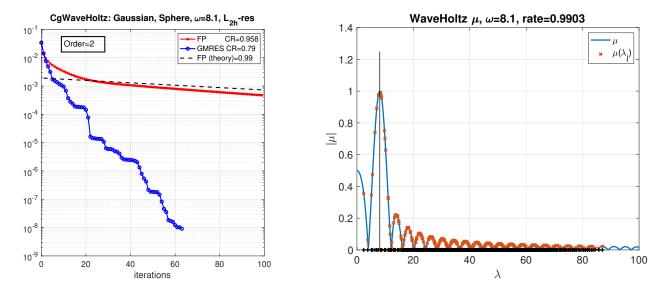


Figure 8: Gaussian source, $\omega = 8.1$, sphere4, order 2. Right: β function with distribution of eigenvalues λ_j

4.2.6. Gaussian source in a domain with three shapes

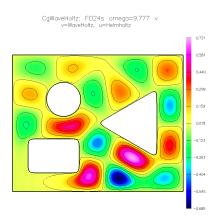


Figure 9: Gaussian pulse for shapes, $\omega = 9.777$, source at (.3, -.75)

SHAPES: omega=9.777

CgWaveHoltz::residual: max-res=3.500e-02 (using omega), max-res=3.382e-02 (using omega from discrete symbol)

CgWaveHoltz: omega=9.777e+00, max-res=3.500e-02, CR=0.872 CR-perPeriod=0.872, cpu= 9.54e+01(s)

CgWaveHoltz::Results saved to file cgWaveHoltz.m

CgWaveHoltz: max-diff=1.16e-02 (between WaveHoltz and Direct Helmholtz solution)

****** OLD STUFF *****

• The Krylov method works much better than the fixed-point iteration.

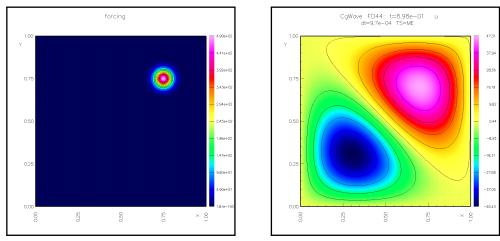


Figure 10: Gaussian forcing on a square. Left forcing. Right solution for $\omega=7$.

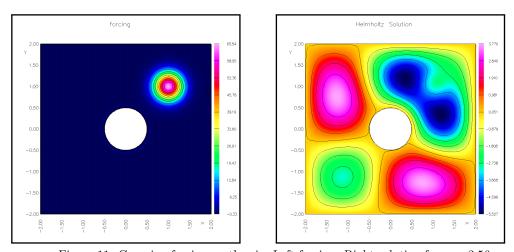


Figure 11: Gaussian forcing on the cic. Left forcing. Right solution for $\omega=2.56.$

Square: Krylov iteration. SECOND-ORDER - looks OK

```
Maximum residual = 3.792e-02
############ DONE KYRLOV ITERATIONS -- KSP residual=1.64e-03 (tol=1.00e-03) numberOfIterations=11 #############
CgWaveHoltz::residual: c=1, omega=7
Maximum residual = 1.449e-01
G128 FIXED-POINT ITERATION
FIXED-POINT -omega=7 has trouble, may be close to a resonance!! TRY -omega=6.869 ...converges NOTE numPeriods
cgwh waveHoltz.cmd -g=square128.order2.hdf -x0=.75 -y0=.75 -omega=6.869 -solver=fixedPoint -tol=1e-3 -tp=1 -ad4=0 -imode=1 -max
it=75: max(|v-v01d|)=9.70e-04 (tol=0.001)
Maximum residual = 4.527e-02
   Square: Krylov iteration. FOURTH-ORDER - not bad - RESIDUAL LARGE AT
BOUNDARY probably degrades convergence
cgwh waveHoltz.cmd -g=square512.order4.hdf -x0=.75 -y0=.75 -omega=7 -solver=krylov -tol=1e-6 -tp=1 -ad4=0 -imode=1
cgwh waveHoltz.cmd -g=square256.order4.hdf -x0=.75 -y0=.75 -omega=7 -solver=krylov -tol=1e-5 -tp=1 -ad4=0 -imode=1
cgwh waveHoltz.cmd -g=square128.order4.hdf -x0=.75 -y0=.75 -omega=7 -solver=krylov -tol=1e-3 -tp=1 -ad4=0 -imode=1
cgwh waveHoltz.cmd -g=square64.order4.hdf -x0=.75 -y0=.75 -omega=7 -solver=krylov -tol=1e-3 -tp=1 -ad4=0 -imode=1
G512
########## DONE KYRLOV ITERATIONS -- KSP residual=1.54e-05 (tol=1.00e-06) numberOfIterations=13 ###############
Maximum residual = 4.732e-05
########### DONE KYRLOV ITERATIONS -- KSP residual=7.44e-07 (tol=1.00e-07) numberOfIterations=14 ##############
Maximum residual = 4.734e-05
G256
########## DONE KYRLOV ITERATIONS -- KSP residual=1.67e-04 (tol=1.00e-05) numberOfIterations=12 ###############
Maximum residual = 5.578e-04
--- tol=1e-4 not enough
########## DONE KYRLOV ITERATIONS -- KSP residual=3.14e-03 (tol=1.00e-04) numberOfIterations=11 ###############
Maximum residual = 4.488e-03
G128
########## DONE KYRLOV ITERATIONS -- KSP residual=1.57e-03 (tol=1.00e-03) numberOfIterations=11 ###############
Maximum residual = 1.392e-02
########## DONE KYRLOV ITERATIONS -- KSP residual=7.93e-04 (tol=1.00e-03) numberOfIterations=11 ###############
CgWaveHoltz::residual: c=1, omega=7
Maximum residual = 1.531e-01
   CIC: Krylov iteration. SECOND-ORDER - NOT BAD, some wiggles in RESIDUAL near
interpolation points, worse for cice16.
cgwh waveHoltz.cmd -g=cice8.order2 -beta=10 -x0=1 -y0=1 -omega=2.56 -solver=krylov -tol=1e-5 -tp=1 -ad4=1 -imode=1
cgwh waveHoltz.cmd -g=cice4.order2 -beta=10 -x0=1 -y0=1 -omega=2.56 -solver=krylov -tol=1e-3 -tp=1 -ad4=1 -imode=1
########## DONE KYRLOV ITERATIONS -- KSP residual=1.31e-03 (tol=1.00e-05) numberOfIterations=14 ###############
```

omega=2.560e+00, Maximum residual = 7.921e-04

References

omega=2.560e+00, Maximum residual = 1.640e-02

[1] S. Balay, W. D. Gropp, L. C. McInnes, B. F. Smith, The portable extensible toolkit for scientific computation, Tech. Rep. http://www.mcs.anl.gov/petsc/petsc.html, Argonne National Laboratory (1999).