GenEO for frequency-domain wave problems

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Talk outline

1. Background and introduction
2. GenEO (for SPD)
3. GenEO for Helmholtz
   - Numerical results – “ideal” case
   - Numerical results – hard real-world problems
4. Conclusions

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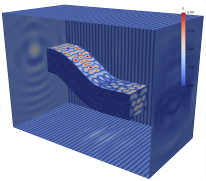
Background

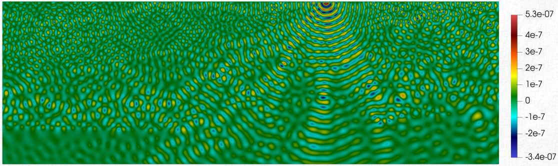
We are interested in solving the Helmholtz equation

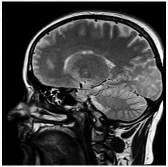
$$-\nabla^2 u - k^2 u = f \quad \text{in } \Omega$$

Applications:

- Electromagnetics
- Geophysics
- Medical imaging
- ...







Background

We are interested in solving the Helmholtz equation

$$-\nabla^2 u - k^2 u = f \ \text{ in } \Omega$$

Challenges:

- Solutions are typically highly oscillatory when k is large
- For large k, accuracy requires increasingly large systems to be solved (e.g. pollution effect – $h \sim k^{-3/2}$ for P1 elements)
- Applications commonly include impedance boundary conditions, resulting in non-self-adjoint problems
- Standard solvers fail!

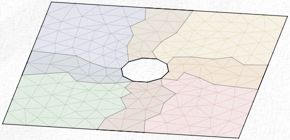
Domain decomposition

Why domain decomposition?

- Good compromise between direct and iterative methods
- Flexible approach, adaptable to compute resources available

Split into subdomains Ω_i and solve sub-problems locally in parallel

Piece together solutions on each Ω_i using transmission conditions



Often used to precondition Krylov methods (accelerates convergence)

Overlapping Schwarz methods

Assuming an appropriate discretisation (e.g. FD or FE methods) we need to solve large linear systems

$$Au = f$$

The restricted additive Schwarz (RAS) preconditioner is

$$M_{RAS}^{-1} = \sum_{i=1}^{N} R_i^T D_i A_i^{-1} R_i, \qquad A_i = R_i A R_i^T$$

For each subdomain Ω_i, A_i is the local Dirichlet matrix

(R_i – restriction, R_i^T – extension, D_i – partition of unity)

Overlapping Schwarz methods

Assuming an appropriate discretisation (e.g. FD or FE methods) we need to solve large linear systems

$$Au = f$$

The optimised restricted additive Schwarz (ORAS) preconditioner is

$$M_{ORAS}^{-1} = \sum_{i=1}^{N} R_i^T D_i B_i^{-1} R_i$$

For each subdomain Ω_i, B_i is the local impedance matrix

(R_i – restriction, R_i^T – extension, D_i – partition of unity)

Overlapping Schwarz methods

Unfortunately such one-level methods typically aren't scalable (though recent work has found they can be in certain ways!)

A second level is incorporated by way of a coarse space

Recent renewed interest for Helmholtz:

- Coarse grid [Graham, Spence and Vainikko '17]
- DtN coarse space [Conen, Dolean, Krause and Nataf '14]
- H-GenEO coarse space [Bootland, Dolean, Jolivet and Tournier '21] [Bootland, Dolean '22]

Latter two are spectral coarse spaces – solve local eigenvalue problems

GenEO

How does the GenEO idea work?

Assume we have a symmetric positive definite operator given by A

GenEO

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Assume we have a symmetric positive definite operator given by A

Provides auxiliary problems in each subdomain that, when glued together, give a rigorous condition number estimate

Local generalised eigenvalue problems provide a *global* coarse space

Bounds are independent of heterogeneity within the PDE coefficients

Can be seen through the Fictitious Space Lemma (FSL)

The fictitious space lemma[1] - conditions

Consider Hilbert spaces H and H_D and symmetric positive bilinear forms

- $a\colon H \times H \to \mathbb{R}$ with $A\colon H \to H$ such that

$$(Au, v) = a(u, v) \qquad \forall u, v \in H$$

- $b\colon H_D \times H_D \to \mathbb{R}$ with $B\colon H_D \to H_D$ such that

$$(Bu_D, v_D)_D = b(u_D, v_D) \qquad \forall u_D, v_D \in H_D$$

Suppose we have a linear surjective operator $\mathcal{R}\colon H_D \to H$ such that

- Continuity: $\exists c_R > 0$ s.t. $\quad a(\mathcal{R}u_D, \mathcal{R}u_D) \leq c_R\, b(u_D, u_D) \quad \forall u_D \in H_D$
- Stable decomposition: $\exists c_T > 0$ s.t. $\forall u \in H\ \exists u_D \in H_D$ with $\mathcal{R}u_D = u$ and

$$c_T\, b(u_D, u_D) \leq a(\mathcal{R}u_D, \mathcal{R}u_D) = a(u, u)$$

[1] [Nepomnyaschikh, 1991]

The fictitious space lemma[1] - conclusions

Denote the adjoint operator $\mathcal{R}^*: H \to H_D$ such that

$$(\mathcal{R}u_D, u) = (u_D, \mathcal{R}^* u)_D \qquad \forall u_D \in H_D,\ u \in H$$

Under these assumptions we have the following spectral estimate:

$$c_T\, a(u,u) \le a\left(\mathcal{R}B^{-1}\mathcal{R}^* Au, u\right) \le c_R\, a(u,u) \qquad \forall u \in H$$

Thus the eigenvalues of the preconditioned operator

$$\mathcal{P}^{-1}A := \mathcal{R}B^{-1}\mathcal{R}^* A$$

are bounded from below by c_T and from above by c_R so we have the condition number estimate

$$\kappa_2(\mathcal{P}^{-1}A) \le c_T^{-1} c_R$$

[1] [Nepomnyaschikh, 1991]

Back to GenEO

For additive Schwarz methods a stable decomposition is required:

Only have (with $\mathcal{R}u_D = \sum_{i=0}^{N} R_i^T u_{D_i} = u$)

$$b(u_D, u_D) \leq 2a(u,u) + (2k_0+1)\sum_{i=1}^{N} a(R_i^T u_{D_i}, R_i^T u_{D_i})$$

However, if we have a $\tau > 0$ such that

$$\sum_{i=1}^{N} a(R_i^T u_{D_i}, R_i^T u_{D_i}) \leq \tau \sum_{i=1}^{N} \tilde{a}_{\Omega_i}(R_i u, R_i u) \leq \tau k_1 a(u,u)$$

where $\tilde{a}_{\Omega_i}$ stems from the (natural) Neumann problem on Ω_i, then

$$c_T^{-1} = 2 + (2k_0+1)k_1\tau$$

Back to GenEO

Thus, we want to ensure

$$a(R_i^T u_{D_i}, R_i^T u_{D_i}) \leq \tau\, \tilde{a}_{\Omega_i}(R_i u, R_i u)$$

To this end, define the (GenEO) generalised eigenvalue problem

Find $(u_i, \lambda) \in \mathbb{R}^{\#\mathcal{N}_i} \setminus \{0\} \times \mathbb{R}$ such that

$$D_i R_i A R_i^T D_i u_i = \lambda \widetilde{A}_i u_i$$

Collecting $(R_i^T D_i u_i)$ for all $\lambda > \tau$ and over all subdomains Ω_i gives the appropriate coarse space

Applying the FSL yields

$$\kappa(M_{AS,GenEO}^{-1} A) \leq (2 + (2k_0 + 1)k_1 \tau)2k_0$$

Back to GenEO

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GenEO

Conceptually, the GenEO eigenproblem links the bad term with a good term

Puts the problematic vectors in the coarse space

This is done locally in parallel

The number of problematic vectors can depend on complexity of heterogeneity but not on the contrast

Overall provides robust solvers for positive definite elliptic problems

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What about frequency-domain wave problems?

H-GenEO

Back to Helmholtz: $A \sim -\nabla^2 u - k^2 u$

Heuristically proposed H-GenEO:

$$\text{Find } (u_i, \lambda) \in \mathbb{C}^{\#\mathcal{N}_i} \setminus \{0\} \times \mathbb{C} \text{ such that}$$
$$\widetilde{A}_i u_i = \lambda D_i L_i D_i u_i$$

where $L \sim -\nabla^2$, and take eigenvectors with $Re(\lambda) < \eta_{\text{max}}$

Links the problematic Helmholtz term to a Laplace term

2D test problem - wave guide

Use P1 elements with $h \sim k^{-3/2}$ and minimal overlap

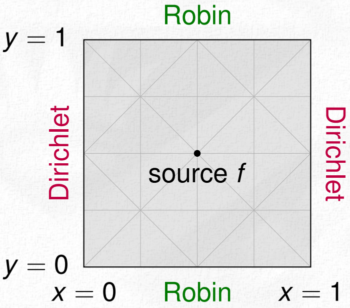


Figure: Schematic of the 2D wave guide model problem with example mesh

Homogeneous results - comparison

Table: Preconditioned GMRES iteration counts and size of coarse space (in parentheses) when using ORAS on a 5×5 square decomposition

k	h^{-1}	one-level	DtN	Δ-GenEO	H-GenEO
18.5	100	73	19 (147)	53 (135)	21 (164)
29.3	200	97	26 (218)	100 (271)	18 (370)
46.5	400	125	35 (303)	148 (560)	17 (779)
73.8	800	156	42 (502)	220 (1120)	15 (1712)

Homogeneous results - eigenvalue threshold

Table: Preconditioned GMRES iteration counts and size of coarse space (in parentheses) when using ORAS on a 5×5 square decomposition

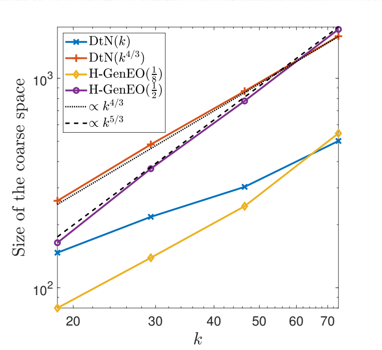
		DtN			H-GenEO		
k	h^{-1}	$\eta_{\max} = k$	$\eta_{\max} = k^{4/3}$	$\eta_{\max} = k^{3/2}$	$\eta_{\max} = \frac{1}{8}$	$\eta_{\max} = \frac{1}{4}$	$\eta_{\max} = \frac{1}{2}$
18.5	100	19 (147)	13 (260)	11 (403)	46 (80)	31 (105)	21 (164)
29.3	200	26 (218)	14 (483)	13 (759)	53 (139)	33 (189)	18 (370)
46.5	400	35 (303)	14 (868)	12 (1479)	56 (245)	35 (378)	17 (779)
73.8	800	42 (502)	16 (1588)	15 (2925)	40 (546)	25 (800)	15 (1712)

Homogeneous results - eigenvalue threshold

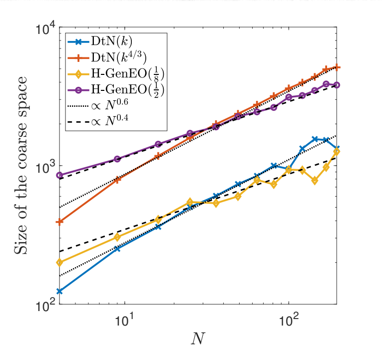
Table: Preconditioned GMRES iteration counts (above) and average number of eigenvectors per subdomain (below) for $k = 73.8$ and $h^{-1} = 800$

N	16	25	36	49	64	81	100	121	144	169	196
DtN(k)	40	42	51	76	49	94	90	36	37	96	154
DtN($k^{4/3}$)	19	16	16	16	15	16	15	15	16	17	17
H-GenEO($\frac{1}{8}$)	36	40	71	70	65	127	81	116	247	194	138
H-GenEO($\frac{1}{2}$)	15	15	16	16	16	18	16	18	18	18	19
DtN(k)	22.6	20.1	16.8	15.0	13.2	12.3	9.5	11.0	10.8	9.0	6.8
DtN($k^{4/3}$)	73.4	63.5	55.4	48.3	43.0	39.2	36.1	32.9	30.3	29.3	26.1
H-GenEO($\frac{1}{8}$)	25.5	21.8	14.9	12.2	12.3	9.0	9.4	7.7	5.4	5.8	6.4
H-GenEO($\frac{1}{2}$)	89.3	68.5	52.9	46.1	38.2	32.5	31.2	26.5	24.2	23.0	19.5

Homogeneous results - size of coarse space



(a) Varying the wave number k for $N = 25$



(b) Varying the number of subdomains N for $k = 73.8$

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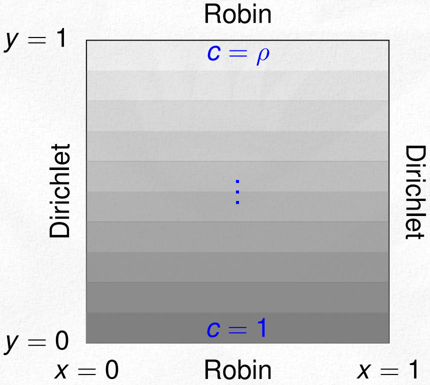
Heterogeneous layers problem

Increasing layers problem – the heterogeneous contrast is $\rho > 1$



$$k = \frac{\omega}{c(\mathbf{x})}$$

Heterogeneous layers problem

Table: Preconditioned GMRES iteration counts – increasing layers problem

			Number of subdomains N											
			DtN($k^{4/3}$)						**H-GenEO**($\frac{1}{2}$)					
ω	h^{-1}	ρ	16	36	64	100	144	196	16	36	64	100	144	196
		10	29	37	41	52	55	58	15	16	19	18	18	19
29.3	200	100	44	44	51	58	52	52	15	15	17	18	17	17
		1000	44	44	50	58	52	52	15	15	17	18	17	17
		10	32	38	41	66	65	73	15	16	16	19	18	18
46.5	400	100	60	67	75	84	73	72	14	15	16	18	17	17
		1000	63	69	74	84	73	71	14	15	16	18	17	17
		10	35	43	42	40	58	69	15	17	16	17	18	17
73.8	800	100	87	95	108	112	117	110	14	15	15	16	17	16
		1000	89	93	107	111	114	109	14	15	15	16	17	16

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Heterogeneous layers problem - METIS

Table: Preconditioned GMRES iteration counts – alternating layers problem with $\rho = 10/100/1000$ when using H-GenEO($\frac{1}{2}$). A non-uniform decomposition into N subdomains is used, given by METIS.

ω	h^{-1}	Number of subdomains N with sub-columns for $\rho = 10/100/1000$: 40			80			120			160			200		
18.5	100	19	19	19	21	21	21	27	27	27	31	31	31	33	33	33
29.3	200	17	17	17	19	19	19	20	20	20	21	21	21	23	23	23
46.5	400	18	18	18	22	23	23	25	26	26	27	28	28	28	29	29
73.8	800	17	17	17	18	18	18	18	19	19	19	20	20	23	23	23
117.2	1600	15	16	16	16	16	16	16	16	16	16	16	16	16	16	16

Weak scaling test

Alternating layers problem – the heterogeneous contrast is $\rho = 100$

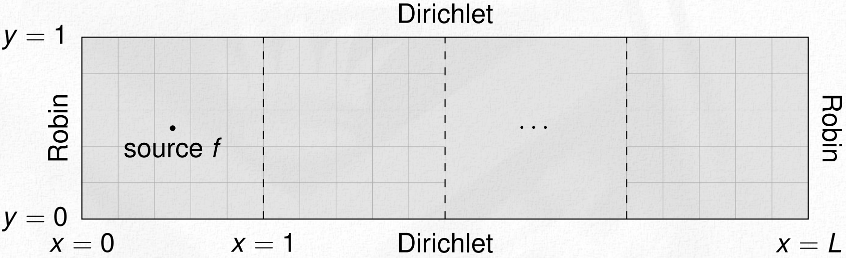

Figure: Schematic of the growing 2D wave guide model problem used in a weak scaling test on $N = 25L$ fixed size subdomains

Weak scaling test

Table: H-GenEO weak scaling results for $k = 73.8$, $h^{-1} = 800$ and $\rho = 100$, reaching up to 10,253,601 dofs when N = 400

N	50	100	150	200	250	300	350	400
Iteration count	17	18	18	19	19	20	21	21
Coarse space size	3010	6150	9290	12430	15570	18710	21850	24990
Total run time (s)	45.8	48.6	53.0	58.7	63.5	70.0	79.7	88.1
Weak scaling efficiency	–	94.2%	86.4%	78.0%	72.1%	65.4%	57.5%	52.0%
Eigensolve time (s)	37.1	37.9	37.9	38.3	37.8	37.9	37.9	37.7
Setup time (s)	5.5	7.7	12.9	16.5	19.9	23.8	27.4	30.8
Efficiency without setup	–	98.5%	100.5%	95.5%	92.4%	87.2%	77.1%	70.3%

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Overview so far

	GenEO (SPD)	H-GenEO
Theory	✓	✗
Irregular decompositions	✓	✓
Robust to heterogeneity	✓	✓
Scalable with N	✓	✓
Coarse space size independent of N	✗	✗
Robust to decreasing h	✓	✓
Coarse space size independent of h	✗✓	✗✓
Robust to increasing wave number	–	✓
Coarse space size independent of k	–	✗

Overview so far

So far we have seen “ideal case” problems

What about more real-world problems:

Overview so far

So far we have seen "ideal case" problems

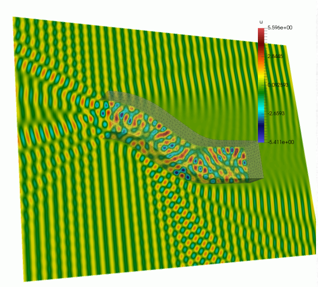
What about more real-world problems:

- Under-resolved meshes
- Higher order FEM
- Only can use a fixed number of eigenvectors

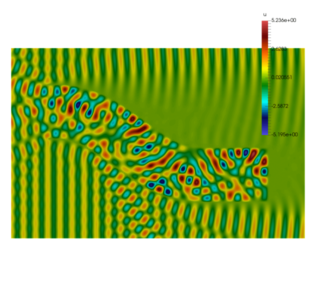
3D COBRA cavity problem

The COBRA cavity problem is a benchmark test in electromagnetics

Use P2 finite elements and 5 points per wavelength



(a) 3D view



(b) 2D cross-section

3D COBRA cavity problem

Table: Preconditioned GMRES iteration counts with ORAS. A non-uniform decomposition into N subdomains is used as given by METIS

	Number of subdomains N							
	One-level				**Coarse Grid**			
k	20	40	80	160	20	40	80	160
200	161	203	259	303	87	90	91	91
300	326	429	574	727	277	309	330	562
400	326	426	581	705	375	450	463	471
	DtN (320 evs)				**H-GenEO** (320 evs)			
k	20	40	80	160	20	40	80	160
200	10	10	50	51	145	207	281	383
300	100	60	45	29	308	422	601	817
400	271	233	147	44	401	527	730	994

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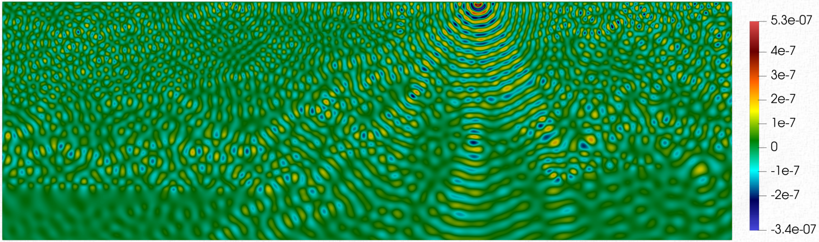
2D geophysics problem

The Marmousi problem is a benchmark test in geophysics

Use P2 finite elements and 10 points per wavelength

Vary frequency f with $k = \frac{2\pi f}{c}$ with c the heterogeneous wave speed through the subsurface media



2D geophysics problem

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	Number of subdomains N							
	One-level				**Coarse Grid**			
f	20	40	80	160	20	40	80	160
1	49	72	143	—	18	19	21	—
5	94	137	191	268	29	34	34	36
10	136	185	272	371	41	43	46	45
20	152	213	299	419	47	48	49	49
	DtN (160 evs)				**H-GenEO** (160 evs)			
f	20	40	80	160	20	40	80	160
1	7	5	6	—	8	8	13	—
5	11	12	17	24	9	10	10	12
10	23	25	25	24	16	14	13	13
20	46	47	56	59	40	34	25	19

Concluding comments

Benefits:

- Robustness to heterogeneity
- Scalability
- Robustness to irregular decompositions
- Robustness to increasing wave number
- Precomputed eigenvectors leveraged if multiple RHSs

Drawbacks:

- Can fail for “hard” problems
- Scalability requires growing coarse space
- Robustness to k requires growing coarse space
- Number of eigenvectors required may not be known

Concluding comments

Challenges:

- How to solve the coarse problem more efficiently?
- What factors determine whether H-GenEO is a good choice?
  - Underlying mesh resolution
  - Order of FE approximation
  - Eigenvalue threshold/number of eigenvectors
  - Other?
- Theory?
  - Some initial exploration for Δ-GenEO on indefinite and non-self-adjoint problems (homogeneous Dirichlet BCs) [Bootland, Dolean, Graham, Ma and Scheichl '22]
- Other eigenproblems?
- Other applications?

References

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