Solution of the three-dimensional Helmholtz equation using Krylov methods preconditioned by multigrid.

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Outline

1. Motivations
    - Depth migration in geophysics
2. Wave propagation modelling
    - Continuous problem
    - Discrete problem
3. Solution strategy
    - State of the art
    - Our approach
4. Numerical experiments
    - Three-dimensional problems
5. Perspectives and conclusions

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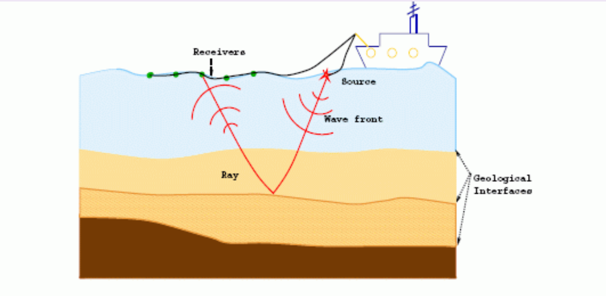
Depth migration in geophysics

- Search for the location and the amplitude of reflecting layers that is of crucial interest in oil exploration
- Acquisition principle of a marine survey



- **Goal of the long-term project**: deduce an interpretative map of the subsoil only from large-scale massively parallel computer simulations

Main features and challenges

Modelling

- Wave propagation problems modelled by the Helmholtz equation with absorbing boundary conditions
- Simulations should be made for multiple Dirac sources and for multiple frequencies
- Large computational domain [truncation of an infinite domain in the x- and y- directions]

Numerical methods

- Robust Helmholtz solution method required especially for large wavenumbers
- Able to solve multiple right-hand side and left-hand side problems
- Must be efficient on massively parallel computers due to huge problem size

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Helmholtz problem

Continuous problem

- Helmholtz equation in the frequency domain:

$$-\Delta u - \frac{\omega^2}{v^2} u = g \quad \text{in} \quad \Omega$$

- with radiation boundary conditions [$k = \frac{\omega}{v}$: wavenumber]:

$$\frac{\partial u}{\partial n} - i\,k\,u = 0 \quad or \quad \frac{\partial u}{\partial n} - i\,k\,u - \frac{i}{2\,k}\frac{\partial^2 u}{\partial^2 \tau} = 0 \quad \text{on} \quad \delta\Omega$$

- or with Perfectly Matched Layer (PML) [Berenger, 1994]

Notations

$\omega = 2\pi f$ is the angular frequency, v the velocity of the wave, u the pressure of the wave, g represents the source term

Outline

Finite difference frequency domain approach

Finite difference methods

- Ω is always box shaped
- Second-order finite difference discretization methods on non-equidistant grids
- Seven-point discretization in three dimensions

Accuracy requirement for second order schemes

- Accuracy requirement for second order discretization: $k\,h \leq \frac{\pi}{5}$ for 10 points per wavelength
- Rule of thumb: $k\,h$ is kept constant to 0.625 e.g. $k = 640$ induces $h = \frac{1}{1028}$
- This leads to a large complex sparse linear system !

Outline

State of the art

- **Sparse multifrontal direct methods**:
  - Very robust but too greedy in memory for large-scale problems
- **Multigrid methods**:
  - **Smoothing difficulty**: standard smoothers unstable for indefinite problems
  - **Coarse grid correction difficulty**: coarse grids approximations of the discrete Helmholtz operator are poor.
  - Multigrid method on the original Helmholtz problem [Elman et al, 2001].
    - use of Krylov methods as smoother.
    - use of a large coarse grid and multigrid as a preconditioner.
  - Geometric multigrid preconditioner on a complex shifted Helmholtz operator [Erlangga, Oosterlee, Vuik, 2006].
    - Standard smoothers are effective thanks to the shift.
    - h-ellipticity is preserved on all the grid hierarchy.

Outline

Two-grid preconditioner for the original Helmholtz problem

Intention

- Our intention is to use a two-level hierarchy to avoid both smoothing and coarse grid correction difficulties.
- Use of direct or iterative methods on coarse grid level.

[Duff, Gratton, Pinel, Vasseur, 2007]

- Large coarse grid multigrid preconditioner method acting on the original Helmholtz problem
- Multigrid is not a convergent method but acts as a preconditioner for the original (unshifted) Helmholtz operator
- Clustered eigenspectrum of AC^{-1} around 1 and capture the isolated eigenvalues with Krylov subspace methods

Overview

Numerical methods

- FGMRES [Saad, 1993] as a Krylov subspace method for solving $Ax = b$.
- Stopping criterion: $\frac{\|r^{(it)}\|_2}{\|r^{(0)}\|_2} \leq 10^{-6}$
- Zero initial guess: $r^{(0)} = b$
- Robustness of the solution method with respect to k ?

Benchmark problems

- Three-dimensional problems
- Homogeneous velocity fields
- PML formulation
- Possibly large wavenumbers

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Constant wavenumber

Discretization

- Helmholtz equation in the frequency domain:

$$-\Delta u - k^2 u = g \quad \text{in} \quad \Omega = [0,1]^3$$

- with Perfectly Matched Layer formulation [Operto et al., 2002].
- PML width: 1/8.
- Dirac source term located at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$.

Constant wavenumber: parallel experiments on CERFACS IBM JS21, direct coarse solver

Two-grid preconditioned FGMRES(5)					
k	Grid	It	Time (s) Fac.	Mem. (Mb) Fac.	Proc
30	64^3	6	3.90	404	2
45	96^3	7	25.18	2926	4
60	128^3	8	71.85	10246	16
90	192^3	9	692.43	54940	32

- Direct coarse grid approximation, linear interpolation and adjoint as restriction.
- Smoother: GMRES(2) preconditioned by Gauss-Seidel
- Matrix-free implementation, distributed MUMPS implementation [Amestoy et al, 2000].

Constant wavenumber: parallel experiments on CERFACS IBM JS21, iterative coarse solver

Two-grid preconditioned FGMRES(5)					
k	Grid	It	Time (s)	Iteration Time (s)	Proc
30	64^3	7	2.87	0.41	32
45	96^3	8	6.34	0.79	32
60	128^3	8	15.52	1.94	32
90	192^3	10	93.92	9.39	32
120	256^3	11	360.20	32.75	32
180	384^3	15	1947.39	129.82	32
240	512^3	21	8438.04	401.81	32

- Smoother: GMRES(2) preconditioned by Gauss-Seidel
- On coarse level: 100 iterations of GMRES(5) preconditioned by a Gauss-Seidel iteration.

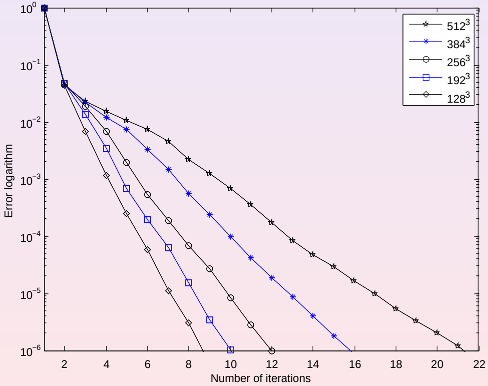
Constant wavenumber: parallel experiments on CERFACS IBM JS21, iterative coarse solver

Iteration time comparison with different numbers of processors

4 processors				32 processors			
Grid	It	Time (s)	Iteration Time (s)	Grid	It	Time (s)	Iteration Time (s)
32^3	6	0.65	0.11	64^3	7	2.87	0.41
48^3	7	2.85	0.41	96^3	8	6.34	0.79
64^3	7	9.83	1.40	128^3	8	15.52	1.94
96^3	8	65.62	8.20	192^3	10	93.92	9.39
128^3	8	241.41	30.17	256^3	11	360.20	32.75
192^3	9	1131.58	125.73	384^3	15	1947.39	129.82
256^3	11	3352.43	304.76	512^3	21	8438.04	401.81

- Equivalent results in time using the same memory by processors, except for the last row.

Constant wavenumber: history of convergence (32 processors)



Conclusions

Summary

- Robustness of the two-grid approach with respect to the wavenumber k.
- Two-grid preconditioner: efficient as a preconditioner in combination with GMRES based Krylov subspace methods.
- Preconditioner based on the original Helmholtz operator.

Perspectives

- To carry on parallel implementation, analysis of efficiency.
- Improve grid transfer operators in order to use three levels in multigrid and thus reduce the size of the coarse grid problem.
- Use of direct methods on the coarse grid and Krylov subspace informations: interesting for Multiple RHS but a lot of processors is needed to handle large problems.