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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   - Three-dimensional problems

5. **Perspectives and conclusions**
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:

\[-\Delta u - \frac{\omega^2}{\nu^2} u = g \text{ in } \Omega\]

- with radiation boundary conditions \([k = \frac{\omega}{\nu}: \text{wavenumber}]:\)

\[\frac{\partial u}{\partial n} - ik u = 0 \text{ or } \frac{\partial u}{\partial n} - ik u - \frac{i}{2k} \frac{\partial^2 u}{\partial^2 \tau} = 0 \text{ on } \delta\Omega\]

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

**Notations**

\(\omega = 2\pi f\) is the angular frequency, \(\nu\) the velocity of the wave, \(u\) the pressure of the wave, \(g\) represents the source term
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**Finite difference frequency domain approach**

**Finite difference methods**
- $\Omega$ 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!
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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.
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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
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 \( \left( \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right) \).
Constant wavenumber: parallel experiments on CERFACS IBM JS21, direct coarse solver

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- Direct coarse grid approximation, linear interpolation and adjoint as restriction.
- **Smooother**: 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

<table>
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- **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

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

Three-dimensional problems

Constant wavenumber: history of convergence (32 processors)

Communication and concurrency

Multigrid for geophysics applications
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.