Solution of 3D-Helmholtz equation in the frequency domain, using Krylov methods preconditioned by multigrid.

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Gene Golub Day

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Outline

1 Motivations
   - Depth migration in geophysics

2 Wave propagation modelling
   - Continuous problem
   - Discrete problem

3 Solution method components: Iterative method and multigrid
   - Classical GMRES / Restarted GMRES
   - Multigrid

4 Solution strategy
   - State of the art
   - Our approach

5 Numerical experiments
   - Three-dimensional problems

6 Perspectives and conclusions
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6. 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
Heterogeneous velocity field $540 \times 600$ from TOTAL
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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6. Perspectives and conclusions

Multigrid for geophysics applications
Helmholtz problem

Continuous problem

- Helmholtz equation in the frequency domain \[ k = \frac{\omega}{v} \] : wavenumber:

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

- 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
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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 $0.625 \times \frac{3}{4}$ e.g. $k = 480$ induces $h = \frac{1}{1024}$
- This leads to a large complex sparse linear system!
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   - Classical GMRES / Restarted GMRES
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Multigrid for geophysics applications
Classical GMRES

- The solution $x_m$ of $Ax = b$ is sought in the Krylov subspace:
  
  $$x_0 + K_m(A, r_0) = x_0 + \text{Span} \{ r_0, Ar_0, A^2r_0, \ldots, A^{m-1}r_0 \} = x_0 + \text{Span} \{ V_m \},$$

  minimizing $\| r_m \|_2 = \| b - Ax_m \|_2$, $r_0$: initial residual.

- Arnoldi’s relation: $AV_m = V_{m+1}H_m$.

- Convergence reached in $n \ (\text{dim}(A))$ iterations at most.

- $O(nm^2)$ complexity.

Practicable GMRES variants

- Restart GMRES: Alternative in memory ,CPU to the classical GMRES.

- Principle: restart GMRES(m), m small, up to the convergence.

- FGMRES: Enables preconditioner to vary at each iteration.
Outline

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   - Continuous problem
   - Discrete problem

3. Solution method components: Iterative method and multigrid
   - Classical GMRES / Restarted GMRES
   - Multigrid

4. Solution strategy
   - State of the art
   - Our approach

5. Numerical experiments
   - Three-dimensional problems

6. Perspectives and conclusions
Multigrid

- Multigrid: multiscale solver designed for elliptic operators.
- Main advantages: Scalable in memory, $O(n)$ complexity for elliptic operators if $n$ denotes the number of unknowns
- **Smoothing** reduces high frequency components of the error
- **Coarse grid approximation** handles the low frequency components

Relaxation methods

![Diagram of V-cycle and W-cycle](image)

**Figure:** Left: two-grid V-cycle, right: three-grid W-cycle
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3. Solution method components: Iterative method and multigrid
   - Classical GMRES / Restarted GMRES
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4. Solution strategy
   - State of the art
   - Our approach

5. Numerical experiments
   - Three-dimensional problems

6. Perspectives and conclusions
State of the art

- **Sparse multifrontal direct methods:**
  - Very robust but too greedy in memory for large-scale problems, limit size: $409 \times 109 \times 102$ (192 procs) [Operto et al., 2004].

- **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, 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 [Riyanti et al. 2007], limit size: $517 \times 293 \times 326$.
    - Standard smoothers are effective thanks to the shift.
    - $h$-ellipticity is preserved on all the grid hierarchy.
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   - Classical GMRES / Restarted GMRES
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6. Perspectives and conclusions

State of the art
Our approach

Multigrid for geophysics applications
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
Outline

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   - State of the art
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5. Numerical experiments
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6. Perspectives and conclusions

Three-dimensional problems
Three-dimensional for a 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 \((\frac{1}{2}, \frac{1}{2}, \frac{1}{2})\).
Overview

Numerical methods

- **FGMRES(5)** [Saad, 1993] as a Krylov subspace method for solving $Ax = b$.

  - Stopping criterion: $\frac{\|r^{(it)}\|_2^2}{\|r^{(0)}\|_2^2} \leq 10^{-6}$

  - Zero initial guess: $r^{(0)} = b$

Two grid properties

- Matrix-free implementation.

- Smoother: Two iterations of GMRES preconditioned by a symmetric Gauss-Seidel iteration.

- Direct coarse grid approximation.

- Linear interpolation and adjoint as restriction.
BLUE GENE/L machine at CERFACS

Configuration

- 1024 bi-processor nodes.
- Processors: Power PC440 700 Mhz.
- Memory: 512 Mbytes per processor.
- Used with 1GB memory per processor.
Motivations
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Solution strategy
Numerical experiments
Perspectives and conclusions

Three-dimensional problems

Direct method on the coarse grid

Experiments on 128 processors

- Distributed MUMPS implementation [Amestoy et al, 2000].

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<td>6</td>
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Table: Iterations of FGMRES(5) versus grid sizes and wavenumbers

- Problem gets harder with increasing wavenumbers on a fixed grid [Elman, 2001].
- Slight increase of the iterations when $kh = constant$ (diagonal).
Iterative method on the coarse grid

<table>
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<th>Time/it (s)</th>
<th>It</th>
<th>Time (s)</th>
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Coarse grid solver GMRES(10) preconditioned by one Gauss-Seidel cycle.
History of convergence: $1024^3$ grid with $k = 480$
Heterogeneous velocity field: Seg-salt

$200 \times 100 \times 200$, $h = 40m$, $f=3.125Hz$

8 processors run on KALI

- Velocity varies from $1500m/s$ to $4482m/s$.
- Plot of one plane of the solution for $y=34$.
- 18 iterations of FGMRES(5), time 824.49 s.
Conclusions

Summary

- Two-grid preconditioner: efficient as a preconditioner in combination with GMRES based Krylov subspace methods.
- Scalability in memory and in frequency studied for a basic algorithm and some variants.
- Two-grid: Algorithm able to solve linear system of size larger than one billion.

Perspectives

- Analysis of efficiency on massively parallel architectures.
- Multiple left-hand side issues.
- Helmholtz with Robin boundary conditions for comparison with published material.
- Integrate this solution method in the reverse time migration framework.