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

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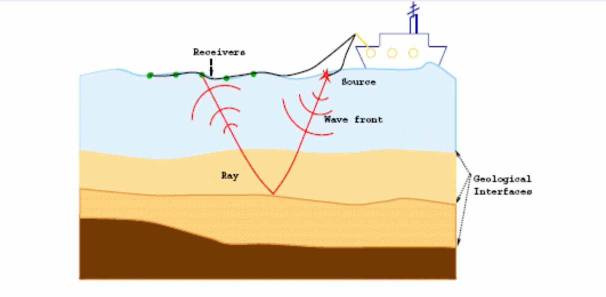
Outline

Outline

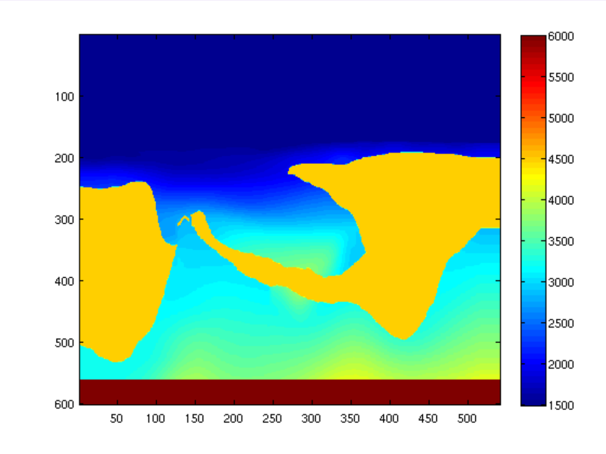
Depth migration in geophysics

- 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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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

- 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: $k\,h \leq \dfrac{\pi}{5}$ 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 $h = \dfrac{1}{1024}$
- This leads to a large complex sparse linear system !

Outline

Classical GMRES

- The solution x_m of $Ax = b$ is sought in the Krylov subspace:

$$x_0 + K_m(A, r_0) = x_0 + \mathrm{Span}\left\{r_0, Ar_0, A^2 r_0, \ldots, A^{m-1} r_0\right\} = x_0 + \mathrm{Span}\left\{V_m\right\},$$

  minimizing $||r_m||_2 = ||b - Ax_m||_2$, r_0: initial residual.
- Arnoldi's relation: $AV_m = V_{m+1}\bar{H}_m$.
- Convergence reached in n ($dim(A)$) 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.

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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

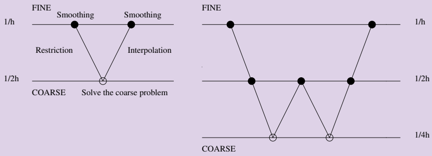


Figure: Left: two-grid V-cycle, right: three-grid W-cycle

Outline

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.

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

Outline

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

Direct method on the coarse grid

Experiments on 128 processors

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

Grid \ k	30	45	60	90
64^3	7			
96^3	6	8		
128^3	5	6	8	
192^3	5	5	6	9

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).

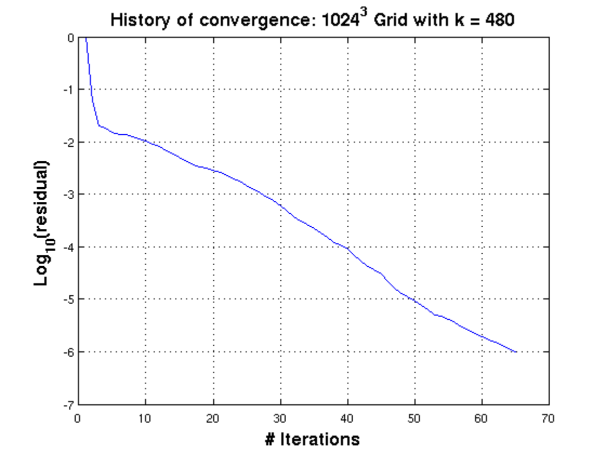
Iterative method on the coarse grid

Experiments with the same amount of memory per processor

FGMRES(5) preconditioned by a Two grid cycle								
			k					
Grid	procs		0	30	60	120	240	480
128^3	2	It	4	5	8			
		Time (s)	95.63	131.10	217.10			
		Time/it (s)	23.90	26.22	27.13			
256^3	16	It	5	6	5	10		
		Time (s)	129.72	175.67	147.17	295.99		
		Time/it (s)	25.94	29.27	29.43	29.60		
512^3	128	It	6	18	11	10	20	
		Time (s)	155.39	519.92	318.15	290.54	579.05	
		Time/it (s)	25.89	28.88	28.92	29.05	28.95	
1024^3	1024	It	9	74	60	41	33	64
		Time (s)	270.58	2240.08	1823.02	1252.53	1013.75	1942.21
		Time/it (s)	30.06	30.27	30.38	30.55	30.72	30.35

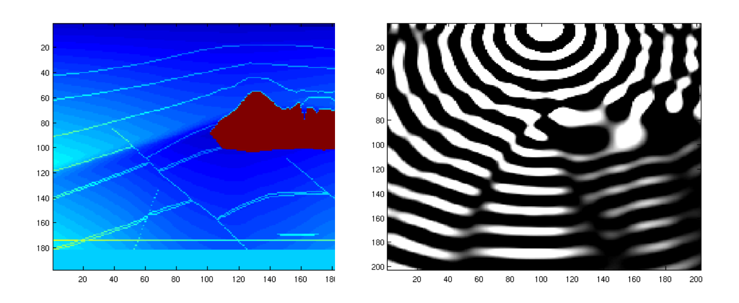
- Coarse grid solver GMRES(10) preconditioned by one Gauss-Seidel cycle.

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.