

Iterative Method for Linear Equation

$$Ax = b$$

Outline

- ▶ Some History
- ▶ Basic Iteration Method
- ▶ Multigrid Method
- ▶ Algebraic Multigrid Method
- ▶ KSP Method
- ▶ Preconditioner
- ▶ PETSc and HYPRE
- ▶ Reference

Some History

- ▶ Prehistory: Gauss to 1940: no computer
- ▶ First period(Stationary iterative method): SOR was proposed by David Young: $x^{k+1} = Tx^k + c$ (hard to estimate, too slow)
- ▶ Second period(Krylov subspace method): CG was discovered by Lanczos, Stiefel and Hestenes (only for symmetric, definite), MINRES, SYMMLQ for indefinite. GMRES, Bi-CGSTAB for nonsymmetric.
- ▶ Multigrid method: was given by Brandt and Hackbusch targeted at solving 2nd order elliptic equation

Basic iteration methods

► Basic iteration methods for $Ax = b$

1. Matrix split: $A = D - L - U$

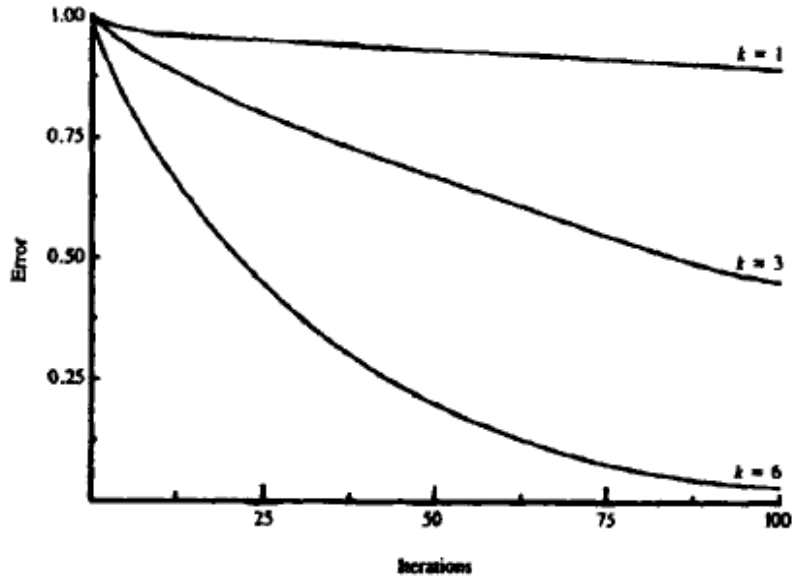
$$(D - L - U)x = b$$

2. Fixed point iteration:

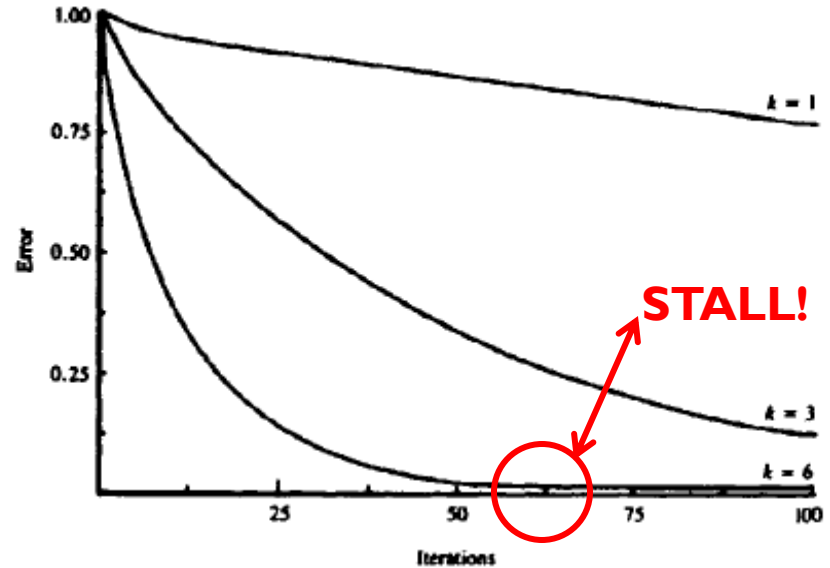
$$x_{n+1} = D^{-1}(L + U)x_n + D^{-1}b \quad (\text{Jacobi})$$

$$x_{n+1} = (D - L)^{-1}Ux_n + (D - L)^{-1}b \quad (\text{Gauss Seidel})$$

Weakness of basic iteration method



Error of Jacobi iteration




Error of Gauss-Seidel iteration

The reasons

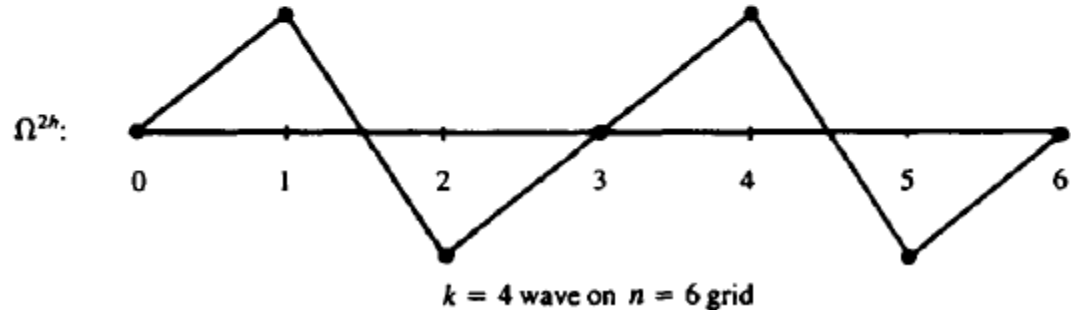
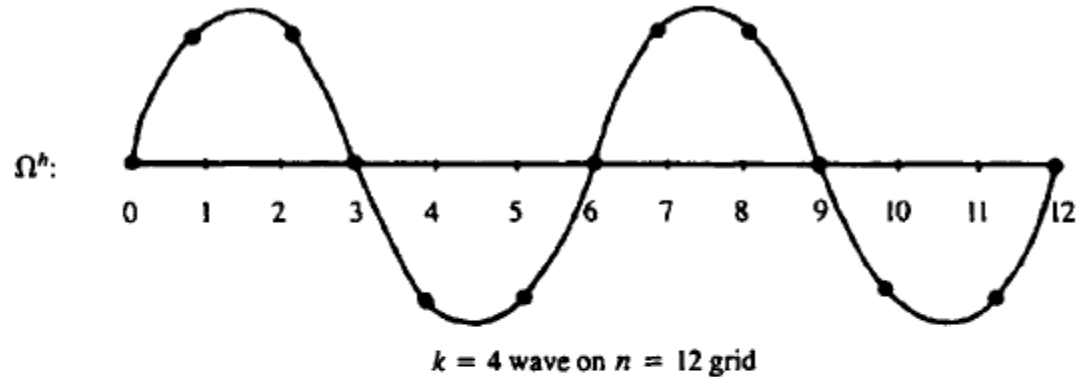
- ▶ *“The slow elimination of the low-frequency components degrades the performance of these methods” [2]*

$$e^{(0)} = \sum_{k=1}^{n-1} c_k w_k$$

- ▶ w_k is the Fourier modes 
- ▶ c_k give the “amount” of each mode in the error

Multigrid method

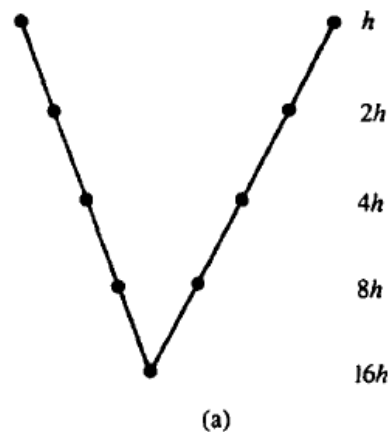
- ▶ The **coarse grid** "sees" a wave that is **more oscillatory** on the coarse grid than on the **fine grid**



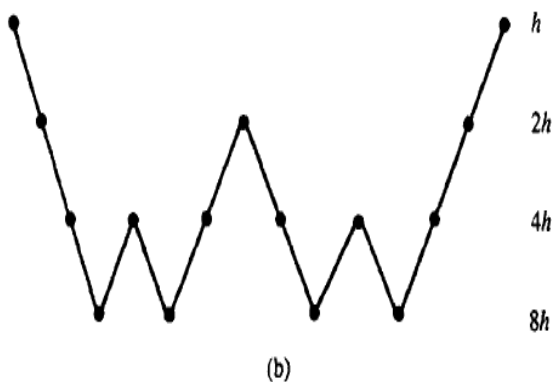
Procedure

- ▶ Iterate one step for $Ax = b$ on Ω^h , obtain x^h
- ▶ Compute residual $r^h = b - Ax^h$
- ▶ **Inject** r^h to Ω^{2h} , obtain r^{2h}
- ▶ Iterate one step for $Ae = r$ on Ω^{2h} , obtain e^{2h}
- ▶ **Interpolate** e^{2h} to Ω^h , obtain e^h
- ▶ $x^h \leftarrow x^h + e^h$

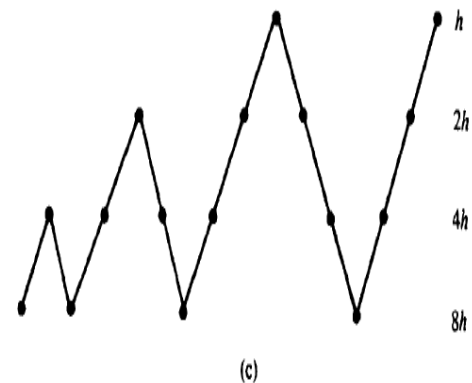
Procedure



Cheap
V-cycle



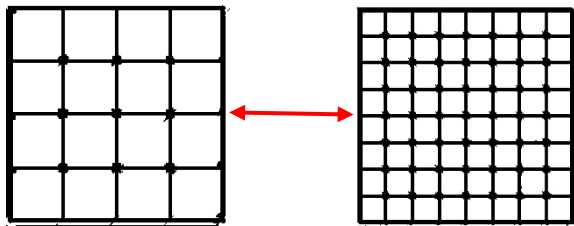
Expensive
W-cycle



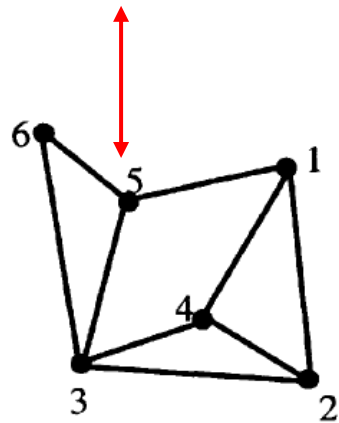
Combination
F-cycle

Algebraic multigrid method (AMG)

- ▶ What if we don't have grid?
- ▶ How to define the coarse grid?
- ▶ How to define interpolation? ($\mathbf{C} \rightarrow \mathbf{F}$)
- ▶ How to define injection? ($\mathbf{F} \rightarrow \mathbf{C}$)
- ▶ **AMG** solves the above problems.



$$A = \begin{bmatrix} X & X & & X & X & \\ X & X & X & X & & \\ & X & X & X & X & X \\ X & X & X & X & & \\ X & & X & & X & X \\ & & X & & X & X \end{bmatrix}$$



Krylov Subspace method

- ▶ We are looking for “good” combinations of $A^j r_0$

$$x_k - x_0 = \sum_{j=0}^{k-1} c_j A^j r_0$$

- ▶ $\kappa_k(A, r_0) = \text{Span}\{r_0, Ar_0, \dots, A^{k-1}r_0\}$ is Krylov Subspace
- ▶ Two ways to define “good”:
 1. $\min \|Ax_k - b\|_2$ (GMRES)
 2. $Ax_k - b \perp \kappa_k(A, r_0)$ (FOM, Bi-CG)

Preconditioner

- ▶ KSP has high performance, but still can **stall**
- ▶ Use AMG as a preconditioner (how?)

$$\text{ILU: } A \approx LU$$

$$L^{-1}AU^{-1}u = L^{-1}b, \quad x = U^{-1}u$$

ILU is accomplished by AMG. [1]

- ▶ This combination gives a “black box” solver
- ▶ Unstructured mesh or mesh free application
- ▶ General purpose, purely algebraic methods

PETSc and HYPRE

- ▶ The **Portable, Extensible Toolkit for Scientific Computation (PETSc)**, pronounced PET-see; the S is silent): Linear solver, nonlinear solver, parallel, preconditioner
- ▶ The **High Performance Preconditioner (HYPRE)**: Parallel multigrid method for both structured and unstructured grid problems.

PETSc in FronTier++

- ▶ Located on:
`FronTier++/solver/solver.cpp`
- ▶ Simplify the procedure
- ▶ Only need to set up matrix
- ▶ Solving is automatic

```
#if defined __HYPRE__
void PETSc::Solve_HYPRE(void)
{
    PC pc;
    start_clock("Assemble matrix and vector");
    ierr = MatAssemblyBegin(A,MAT_FINAL_ASSEMBLY);
    ierr = MatAssemblyEnd(A,MAT_FINAL_ASSEMBLY);

    ierr = VecAssemblyBegin(x);
    ierr = VecAssemblyEnd(x);

    ierr = VecAssemblyBegin(b);
    ierr = VecAssemblyEnd(b);
    stop_clock("Assemble matrix and vector");

    KSPSetType(ksp,KSPBCGS);
    KSPSetOperators(ksp,A,A,DIFFERENT_NONZERO_PATTERN);
    KSPGetPC(ksp,&pc);
    PCSetType(pc,PCHYPRE);
    PCHYPRESetType(pc,"boomeramg");
    KSPSetFromOptions(ksp);
    KSPSetUp(ksp);

    start_clock("KSPSolve");
    KSPSolve(ksp,b,x);
    stop_clock("KSPSolve");
}
#endif // defined __HYPRE__
```

A simple example of PETSc

Create matrix A, vector b, solution x:

```
for (i = 1; i < 5; i++)
```

```
{  
    col[0] = i-1; col[1] = i; col[2] = i+1;  
    value[3] = {1, -2, 1};  
    MatSetValues(A,1,&i,3,col,value,INSERT_VALUE);  
}
```

$$\begin{vmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{vmatrix}$$

The first row and last row need to be set separately

A simple example of PETSc

- ▶ Create linear solver

PC pc;

KSPSetType(ksp,KSPGMRES); /*determine KSP solver*/

KSPSetOperators(ksp,A,A,DIFFERENT_NONZERO_PATTERN);

KSPGetPC(ksp,&pc);

PCSetType(pc,PCHYPRE); /*determine preconditioner*/

PCHYPRESetType(pc,"boomeramg");

KSPSetFromOptions(ksp);

KSPSetup(ksp);

A simple example of PETSc

- ▶ Solve equation and obtain solution

```
double *values;
```

```
KSPSolve(ksp,b,x);
```

```
/*Solve equation*/
```

```
VecGetArray(x,&values);
```

```
/*Get solution*/
```

Summary

- ▶ Basic iteration may stall
- ▶ Multigrid can accelerate, but need structure grid.
- ▶ AMG is purely algebraic, no structure information needed
- ▶ A combination of AMG and KSP gives a good solver
- ▶ PETSc and HYPRE do this for us
- ▶ Enjoy!

Reference

- [1] M. Benzi, Preconditioning techniques for Large Linear System:A Survey, Journal of Computational Physics, 182: 418-477, 2002.
- [2] W. Briggs, V. Henson, S. McCormick, A Multigrid Tutorial, Society for Industrial and Applied Mathematics, 2000.