Lobachevsky State University of Nizhni Novgorod

Faculty of Computational mathematics and cybernetics

Iterative Methods for Solving Linear Systems

Krylov Subspace Iterative Methods

Supported by Intel

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Contents

Problem Statement

- Let us consider a system of n linear equations like

$$\begin{aligned} a_{11}x_1 &+ a_{12}x_2 &&+ \ldots + a_{1n}x_n &&= b_1 \\ a_{21}x_1 &+ a_{22}x_2 &&+ \ldots + a_{2n}x_n &&= b_2 \\ &\ldots \\ a_{n1}x_1 &+ a_{n2}x_2 &&+ \ldots + a_{nn}x_n &&= b_n \end{aligned}$$

- As a matrix, the system may be represented as follows

$$Ax=b$$

- $A=(a_{ij})$ is a $n \times n$ real matrix; b and x are vectors consisting of n elements; let the exact system solution be x^*.
- *An iterative method* generates a sequence of vectors $x^{(s)} \in R^m$, $s=0,1,2,\ldots$, where $x^{(s)}$ is an approximate system solution.

Properties of Iterative Methods

- Iterative method is convergent if

$$\forall\ x^{(0)} \in R^m \quad \lim_{s \to \infty} \left\| x^{(s)} - x^* \right\| = 0$$

- Iterative method stop criteria: accuracy and number of iterations
  - Stop, if $\|x^{(s)} - x^{(s-1)}\| \le \varepsilon_1$. In this case, $\varepsilon_2 = \|x^{(s)} - x^{(s-1)}\|$ is the attainable method accuracy.
  - Stop, if $\|r^{(s)}\| \le \varepsilon_1$. In this case, $\varepsilon_2 = \|r^{(s)}\|$ is the attainable method accuracy.
  - Stop, if $s = N$. $x^{(N)}$ is understood as an obtained solution. The maximum number of iterations N is predefined.
- From this on, let us suppose that A is a real square matrix.

Idea of Projective Methods

1. The problem of linear system solution projection to any subspace K orthogonally to $L=AK$ is equivalent to minimization of the functional $\Phi(x) = \|r(x)\|^2$ of the space K.
2. If $A=A^T$, $A>0$, the problem of linear system solution projection to any subspace K orthogonally to K is equivalent to minimization of the functional $\Phi(x) = \|x - x^*\|_A^2$ of the space K.

Here, $\|x\|_A = \sqrt{(Ax, x)}$

Which subspace K to select?

Krylov Subspace

- The Krylov subspace of dimension m generated by the vector v and matrix A is the linear space

$$K_m = K_m(A, v) = span\left\{v, Av, A^2v, ..., A^{m-1}v\right\}$$

- For the methods $v = r_0 / \| r_0 \|$ is usually selected, where $r_0 = b - Ax_0$ is the residual of the first approximation x_0.
- Having constructed the Krylov subspace, we can adapt the initial system to it; the solution of the new system will consist in approximation to the initial system solution.
- The system must be easy to project and, as a result, to solve.
- The problem is to construct the subspace basis $K_m(A, v)$

Arnoldi Orthogonalization

- The objective is to find the orthogonal basis K_m, i. e. vectors $\{v_1, v_2, \ldots, v_m\}$
- Parameters: first vector v_1 ($\|v_1\|=1$) and dimension m.

Algorithm

for $j = 1, ..., m$ do

$w = Av_j$ //next vector

for $i = 1, \ldots, j$ do

$h_{ij} = (w, v_i)$

$w = w - h_{ij} v_i$

end i

$h_{j+1,j} = \|w\|$; $v_{j+1} = w / h_{j+1,j}$

end j

Arnoldi Orthogonalization

- As a result of the Arnoldi algorithm, we obtain:

  $V_m=[v_1,v_2,\ldots, v_m]$ is the orthonormal basis of the subspace K_m.

  $\overline{V}_m = [v_1, v_2, ..., , v_m, v_{m+1}]$ – matrix expanded by the last computed vector v_{m+1}.

  H_m – orthogonalization coefficient matrix.

$$H_m = \begin{bmatrix} h_{11} & h_{12} & h_{13} & h_{14} & \cdots & h_{1m} \\ h_{21} & h_{22} & h_{23} & h_{24} & \cdots & h_{2m} \\ 0 & h_{32} & h_{33} & h_{34} & \cdots & h_{3m} \\ \vdots & & \ddots & \ddots & & \vdots \\ 0 & \cdots & 0 & h_{m-1,m-2} & h_{m-1,m-1} & h_{m-1,m} \\ 0 & \cdots & 0 & 0 & h_{m,m-1} & h_{m,m} \end{bmatrix}$$

H_m – Hessenberg (upper) matrix

Arnoldi Orthogonalization

$\overline{H}_m$ – orthogonalization coefficient matrix expanded by a zero string with the coefficient $h_{m+1,m}$.

$$\overline{H}_m = \begin{bmatrix} h_{11} & h_{12} & h_{13} & h_{14} & \cdots & h_{1m} \\ h_{21} & h_{22} & h_{23} & h_{24} & \cdots & h_{2m} \\ 0 & h_{32} & h_{33} & h_{34} & \cdots & h_{3m} \\ \vdots & & \ddots & \ddots & & \vdots \\ 0 & \cdots & 0 & h_{m-1,m-2} & h_{m-1,m-1} & h_{m-1,m} \\ 0 & \cdots & 0 & 0 & h_{m,m-1} & h_{m,m} \\ 0 & \cdots & & & 0 & h_{m+1,m} \end{bmatrix}$$

Generalized Minimal Residual Method

1. Select as e_1 (first normal basic vector)
   $v_1 = r_0 / \beta \quad (\beta = \| r_0 \| \ , \ r_0 = b - Ax_0)$.
2. Execute m steps of the Arnoldi algoritm (to obtain V_m, H_m)

for $j = 1, ..., m$ do

$w = Av_j$ //next vector

for $i = 1, \ldots, j$ do

$h_{ij} = (w, v_i)$

$w = w - h_{ij} v_i$

end i

$h_{j+1,j} = \|w\|; \ v_{j+1} = w / h_{j+1,j}$

end j

3. Compute $x_m = x_0 + V_m y_m$, where $y_m = \arg \min_y \left\| \beta e_1 - \overline{H}_m y \right\|$

GMRes – Implementation

- How to solve $y_m = \arg\min_y \left\| \beta e_1 - \overline{H}_m y \right\|$?
- Equivalent formulation $\overline{H}_m y = \beta e_1$
  redefined linear system, matrix size $(m+1)\times m$.
  May be solved as a least squares problem.
- $\overline{H}_m$ is a Hessenberg matrix; simplify it to a triangle using givens rotations.
- At the same time, r_i can be computed without computing x_i explicitly

GMRes – Implementation

- Define the rotation matrix Ω_i
  rotation coefficients c_i, s_i
  are selected so that
  $\eta_{i+1,i}$ is zeroed.
  At the same time, $c_i^2 + s_i^2 = 1$
- Multiply the system
  $$\overline{H}_m y = \beta e_1$$
  by the matrix Ω_i on the left.

$$\Omega_i = \begin{bmatrix} 1 & & & & & & & \\ & \ddots & & & & & & \\ & & 1 & & & & & \\ & & & c_i & s_i & & & \\ & & & -s_i & c_i & & & \\ & & & & & 1 & & \\ & & & & & & \ddots & \\ & & & & & & & 1 \end{bmatrix}$$

GMRes – Implementation

- Example:

$$\overline{H}_4 = \begin{bmatrix} h_{11} & h_{12} & h_{13} & h_{14} \\ h_{21} & h_{22} & h_{23} & h_{24} \\ & h_{32} & h_{33} & h_{34} \\ & & h_{43} & h_{44} \\ & & & h_{54} \end{bmatrix} \qquad \overline{g}_0 = \beta e_1 = \begin{bmatrix} \beta \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

- Multiply by Ω_1, where

$$s_1 = \frac{h_{21}}{\sqrt{h_{11}^2 + h_{21}^2}} \qquad c_1 = \frac{h_{11}}{\sqrt{h_{11}^2 + h_{21}^2}}$$

$$\Omega_1 = \begin{bmatrix} c_1 & s_1 & & & \\ -s_1 & c_1 & & & \\ & & 1 & & \\ & & & 1 & \\ & & & & 1 \end{bmatrix}$$

GMRes – Implementation

- Thus, we obtain

$$\overline{H}_4^{(1)} = \begin{bmatrix} h_{11}^{(1)} & h_{12}^{(1)} & h_{13}^{(1)} & h_{14}^{(1)} \\ & h_{22}^{(1)} & h_{23}^{(1)} & h_{24}^{(1)} \\ & h_{32} & h_{33} & h_{34} \\ & & h_{43} & h_{44} \\ & & & h_{54} \end{bmatrix} \qquad \overline{g}_1 = \begin{bmatrix} c_1\beta \\ -s_1\beta \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

- Similarly, multiply by $\Omega_2, \Omega_3, \ldots$, to obtain

$$\overline{H}_4^{(4)} = \begin{bmatrix} h_{11}^{(4)} & h_{12}^{(4)} & h_{13}^{(4)} & h_{14}^{(4)} \\ & h_{22}^{(4)} & h_{23}^{(4)} & h_{24}^{(4)} \\ & & h_{33}^{(4)} & h_{34}^{(4)} \\ & & & h_{44}^{(4)} \\ & & & 0 \end{bmatrix} \qquad \overline{g}_4 = \begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_3 \\ \gamma_4 \\ \gamma_5 \end{bmatrix}$$

GMRes – implementation

- Set $Q_m = \Omega_m \cdot \Omega_{m-1} \cdot \ldots \cdot \Omega_1$, then

$$\overline{R}_m = \overline{H}_m^{(m)} = Q_m \overline{H}_m$$

$$\overline{g}_m = Q_m (\beta e_1) = (\gamma_1, \ldots, \gamma_m, \gamma_{m+1})^T$$

- As Q_m is a unitary matrix,

$$\min_y \left\| \beta e_1 - \overline{H}_m y \right\| = \min_y \left\| \overline{g}_m - \overline{R}_m y \right\|$$

- Delete the last line of the system and solve the triangular system

for y. $R_m y_m = g_m$

GMRes – Implementation

- We can prove that:
  - The rank AV_m is equal to the rank R_m.
  - The vector $y_m = \arg\min_y \left\| \beta e_1 - \overline{H}_m y \right\|$ can be obtained by solving the system $R_m y_m = g_m$, i. e. $y_m = (R_m)^{-1} g_m$
  - The residual at the step m satisfies the following relations

$$r_m = b - Ax_m = \overline{V}_m [\beta e_1 - \overline{H}_m y_m] = \overline{V}_m Q_m^T (\gamma_{m+1} e_{m+1})$$

  - As a result, $\left\| r_m \right\| = \left| \gamma_{m+1} \right|$
- The indicated value may be used as a method stop criterion $\left\| r_m \right\| < \varepsilon$ and ensure such a verification at each step of the algorithm.

GMRes(m) Restart

- As *m* increases, the memory requirements and complexity of the next method iteration grow dramatically.
- The solution consists in restarting the method every *m* iterations

1. Compute $v_1 = r_0 / \beta$ $(\beta = \| r_0 \|, r_0 = b - Ax_0)$.
2. Arnoldi algorithm: compute V_m, H_m, $\overline{V}_m$, $\overline{H}_m$
3. $y_m = \arg \min_y \left\| \beta e_1 - \overline{H}_m y \right\|$
4. $x_m = x_0 + V_m y_m$
5. If $\left\| r_m \right\| < \varepsilon$ then STOP
   else $x_0 = x_m$, go to step 1.

Preconditioned Method

1. Select as $e_1 = v_1$, where $v_1 = r_0 / \beta$
   ($\beta = \| r_0 \|$, $r_0 = M^{-1}(b - Ax_0)$).
2. Execute m steps of the Arnoldi algoritms (to obtain V_m, H_m)

for $j = 1, ..., m$ do

$w = M^{-1} A v_j$ //next vector

for $i = 1, \ldots, j$ do

$h_{ij} = (w, v_i)$

$w = w - h_{ij} v_i$

end i

$h_{j+1,j} = \|w\|$; $v_{j+1} = w / h_{j+1,j}$

end j

3. Compute $x_m = x_0 + V_m y_m$, where $y_m = \arg \min_y \left\| \beta e_1 - \overline{H}_m y \right\|$

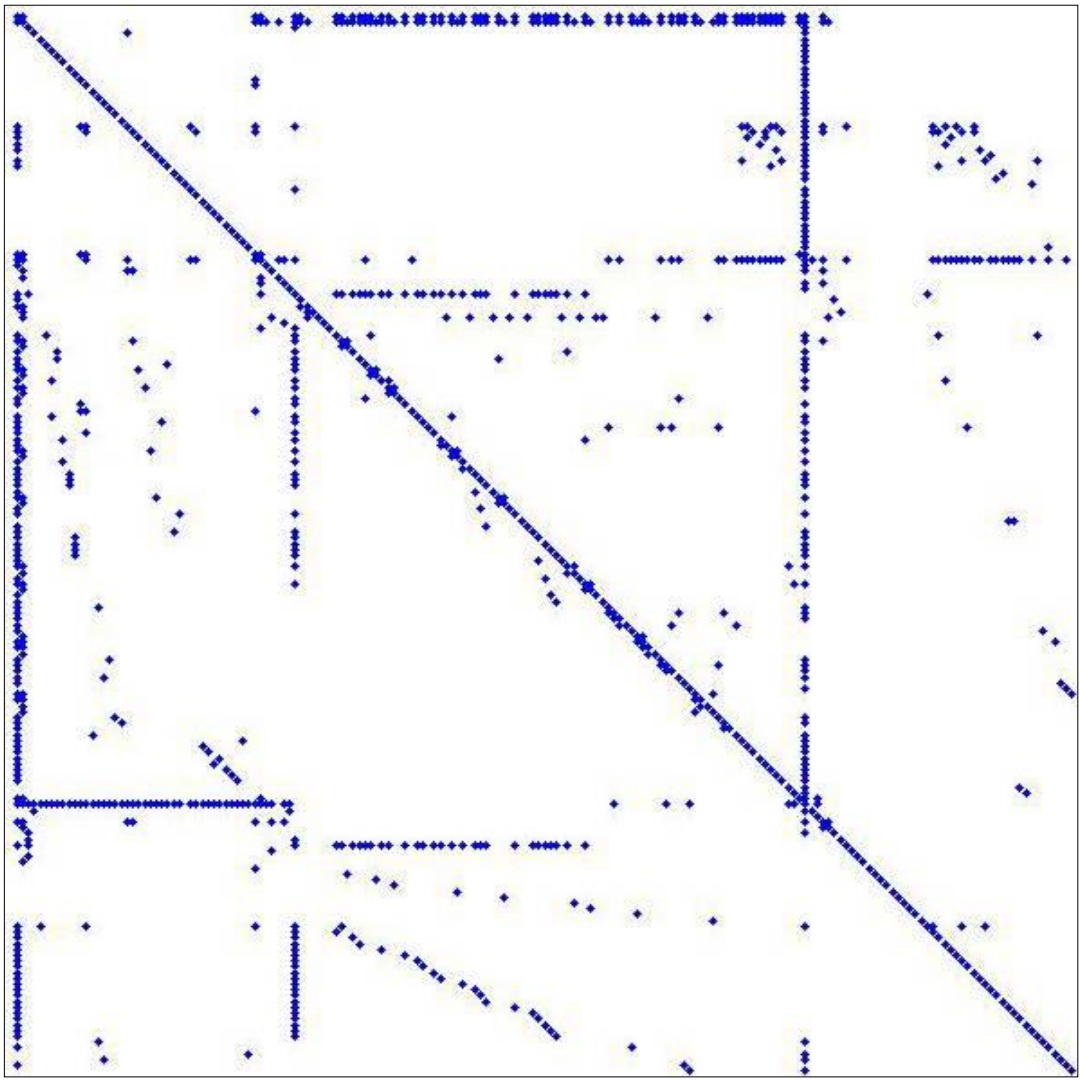
Experimental Results (Sparse)

- The University of Florida Sparse Matrix Collection
  http://www.cise.ufl.edu/research/sparse/matrices/
- Parameters of the matrices involved

Name	n	nz	μ_A
fs_183_1	183	998	$2{,}2 \cdot 10^{13}$
fs_541_1	541	4282	4467
sherman2	1080	23094	$9{,}6 \cdot 10^{11}$
watt_1	1856	11360	$4{,}4 \cdot 10^{9}$
cage10	11397	150645	11

Experimental Results (Sparse)

- Matrix pattern
  fs_183_1
- Exact solution
  $x^* = \{x_i = 1, 1 \le i \le n\}$
- Right side
  $b = Ax^*$
- System
  $Ax=b$



Experimental Results (Sparse)

- Method accuracy $\varepsilon = 10^{-8}$
- ILU(0)-preconditioner

Matrix name	n	s	
		GMRes	PGMRes
fs_183_1	183	78	16
fs_541_1	541	13	2
sherman2	1080	100	18
watt_1	1856	40	48
cage10	11397	24	7

- The use of preconditioner reduces the number of iterations (for most problems)

Lancsoz Biorthogonalization

- The vector systems $\{v_1,\ldots,v_m\}$ and $\{w_1,\ldots,w_m\}$ are biorthogonal if $(v_i,w_j)=0$ when $i\neq j$.
- The systems are biorthonormal if $(v_i,w_j)=\delta_{i\varphi}$.
- Let us set $V=[v_1,\ldots,v_m]$, $W=[w_1,\ldots,w_m]$, so the biorthonormality condition is equivalent to

$$W^T V = E.$$

- Let X be the basis of K and Y the basis of L, so, similar to the orthogonalization procedure, the biorthogonalization algorithm may be proposed to construct V and W, i. e.
the biorthonormal bases of K and L.

Lancsoz Bi-orthogonalization– Algorithm

- Let $\delta_1=\beta_1=0$, $v_0=w_0=0$,
- Select vectors v_1, w_1 so that $(v_1, w_1) = 1$

for $j=1,\ldots,m$ do

$$\alpha_j = (Av_j, w_j)$$

$$\overline{v}_{j+1} = Av_j - \alpha_j v_j - \delta_j v_{j-1} \qquad \overline{w}_{j+1} = A^T w_j - \alpha_j w_j - \delta_j w_{j-1}$$

$$\delta_{j+1} = \sqrt{|(\overline{v}_{j+1}, \overline{w}_{j+1})|} \quad \text{If} \quad \delta_{j+1} = 0 \quad \text{then STOP}$$

$$\beta_{j+1} = (\overline{v}_{j+1}, \overline{w}_{j+1}) / \delta_{j+1}$$

$$w_{j+1} = \overline{w}_{j+1} / \beta_{j+1} \qquad v_{j+1} = \overline{v}_{j+1} / \delta_{j+1}$$

end j

Lancsoz Bi-orthogonalization – Properties

- Bi-orthogonalization coefficients $\alpha_i, \beta_i, \delta_i$ form the tridiagonal matrix T_m
- Similar to the Arnoldi method:

$$AV_m = V_m T_m + \delta_{m+1} v_{m+1} e_m^T$$

$$AW_m = W_m T_m^T + \beta_{m+1} w_{m+1} e_m^T$$

$$W_m^T A V_m = T_m$$

$$T_m = \begin{bmatrix} \alpha_1 & \beta_2 & & & \\ \delta_2 & \alpha_2 & \beta_3 & & \\ & \ddots & & & \\ & & \delta_{m-1} & \alpha_{m-1} & \beta_m \\ & & & \delta_m & \alpha_m \end{bmatrix}$$

- Iterative process:

$$x_m = x_0 + V_m T_m^{-1} (\beta e_1)$$

- Directions will be bi-conjugate - use biorthogonalization instead of explicit computation of x_m.

Bi-conjugate Gradient Method

Algorithm

- $r_0 = b - Ax_0$, select $\bar{r}_0$ so that $(r_0, \bar{r}_0) \neq 0$ (e.g. $\bar{r}_0 = r_0$)
- Let $p_0 = r_0 \quad \bar{p}_0 = \bar{r}_0$

for j=0,1,…, n do

$$\alpha_j = (r_j, \bar{r}_j) / (Ap_j, \bar{p}_j) \;,\; x_{j+1} = x_j + \alpha_j p_j$$

$$r_{j+1} = r_j - \alpha_j A p_j \;,\; \bar{r}_{j+1} = \bar{r}_j - \alpha_j A^T \bar{p}_j$$

$$\beta_j = (r_{j+1}, \bar{r}_{j+1}) / (r_j, \bar{r}_j)$$

if β_j=0 or $\| r_{j+1} \| < \varepsilon$ then STOP

$$p_{j+1} = r_{j+1} + \beta_j p_j \;,\; \bar{p}_{j+1} = \bar{r}_{j+1} + \beta_j \bar{p}_j$$

end j

Preconditioned Method

Algorithm with the preconditioner *M*

- $r_0 = b - Ax_0$, select $\bar{r}_0$ so that $(r_0, \bar{r}_0) \neq 0$ (e.g. $\bar{r}_0 = r_0$)
- Solve $Mz_0 = r_0$, $M^T \bar{z}_0 = \bar{r}_0$. Let $p_0 = z_0$ $\bar{p}_0 = \bar{z}_0$

  for j=0,1,…, n do

  $$\alpha_j = (z_j, \bar{r}_j) / (Ap_j, \bar{p}_j) \ , \ x_{j+1} = x_j + \alpha_j p_j$$

  $$r_{j+1} = r_j - \alpha_j Ap_j \ , \ \bar{r}_{j+1} = \bar{r}_j - \alpha_j A^T \bar{p}_j$$

  $$Mz_{j+1} = r_{j+1} \quad M^T \bar{z}_{j+1} = \bar{r}_{j+1}$$

  $$\beta_j = (z_{j+1}, \bar{r}_{j+1}) / (z_j, \bar{r}_j)$$

  if β_j=0 or $\| r_{j+1} \| < \varepsilon$ then STOP

  $$p_{j+1} = r_{j+1} + \beta_j p_j \ , \ \bar{p}_{j+1} = \bar{r}_{j+1} + \beta_j \bar{p}_j$$

  end j

Experimental Results (Sparse)

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watt_1	1856	11360	$4{,}4 \cdot 10^{9}$
cage10	11397	150645	11

Experimental Results (Sparse)

- Method accuracy $\varepsilon = 10^{-4}$
- ILU(0)-preconditioner

Matrix name	n	s	
		GMRes	PGMRes
fs_183_1	183	183	10
fs_541_1	541	6	1
sherman2	1080	1080	20
watt_1	1856	839	36
cage10	11397	10	3

- More iterations than in GMRes
- Less memory requirements

Lancsoz Symmetric Method

- The matrix A is symmetric. Then, for the Arnoldi method, $H_m = V_m^T A V_m$ must be symmetric
- H_m: Hessenberg+symmetric=tridiagonal
  of the vector v in the course of orthogonalization satisfies the following

$$\beta_{j+1} v_{j+1} = A v_j - \alpha_j v_j - \beta_j v_{j-1} .$$

- Orthogonalization process is simplified

$$H_m = \begin{bmatrix} \alpha_1 & \beta_2 & & & \\ \beta_2 & \alpha_2 & \beta_3 & & \\ & & \ddots & & \\ & & \beta_{m-1} & \alpha_{m-1} & \beta_m \\ & & & \beta_m & \alpha_m \end{bmatrix}$$

Lancsoz Symmetric Method - Algorithm

- Let $\beta_1=0$, $v_0=0$,
- Select the vector v_1, $\|v_1\| = 1$

for $j=1,\ldots,m$ do

$$w_j = Av_j - \beta_j v_{j-1}$$

$$\alpha_j = (v_j, w_j)$$

$$w_j = w_j - \alpha_j v_j$$

$$\beta_{j+1} = \|w_j\| \quad \text{If} \quad \beta_{j+1} = 0 \quad \text{then STOP}$$

$$v_{j+1} = w_j / \beta_{j+1}$$

end j

Conjugate gradient method (CG)

Algorithm

- Preliminary step $r_0 = p_0 = b - Ax_0$
- Main steps

for i=0,…, n do

$$\alpha_i = \frac{(r_i, r_i)}{(Ap_i, p_i)} \qquad x_{i+1} = x_i + \alpha_i p_i$$

$$r_{i+1} = r_i - \alpha_i A p_i$$

$$\beta_i = \frac{(r_{i+1}, r_{i+1})}{(r_i, r_i)} \qquad p_{i+1} = r_{i+1} + \beta_i p_i$$

end j

Preconditioned Method (PCG)

Algorithm

- Preliminary step $r_0 = b - Ax_0 \quad z_0 = M^{-1} r_0 \qquad p_0 = z_0$
- Main steps

for i=0,…, n do

$$\alpha_i = \frac{(r_i, z_i)}{(Ap_i, p_i)} \qquad x_{i+1} = x_i + \alpha_i p_i$$

$$r_{i+1} = r_i - \alpha_i A p_i \qquad z_{i+1} = M^{-1} r_{i+1}$$

$$\beta_i = \frac{(r_{i+1}, z_{i+1})}{(r_i, z_i)} \qquad p_{i+1} = z_{i+1} + \beta_i p_i$$

end j

Experimental Results (Sparse)

- The University of Florida Sparse Matrix Collection
  http://www.cise.ufl.edu/research/sparse/matrices/
- Parameters of the matrices involved

Name	n	nz	μ_A
bcsstk01	48	400	882 336
bcsstk05	153	2 423	14 281.1
bcsstk10	1086	22 070	524 225
bcsstk13	2003	83 883	1.06e+10
parabolic_fem	525 825	3 674 625	2.11e+10
tmt_sym	726 713	5 080 961	---

Experimental Results (Sparse)

- Matrix pattern bcsstk13
- Exact solution

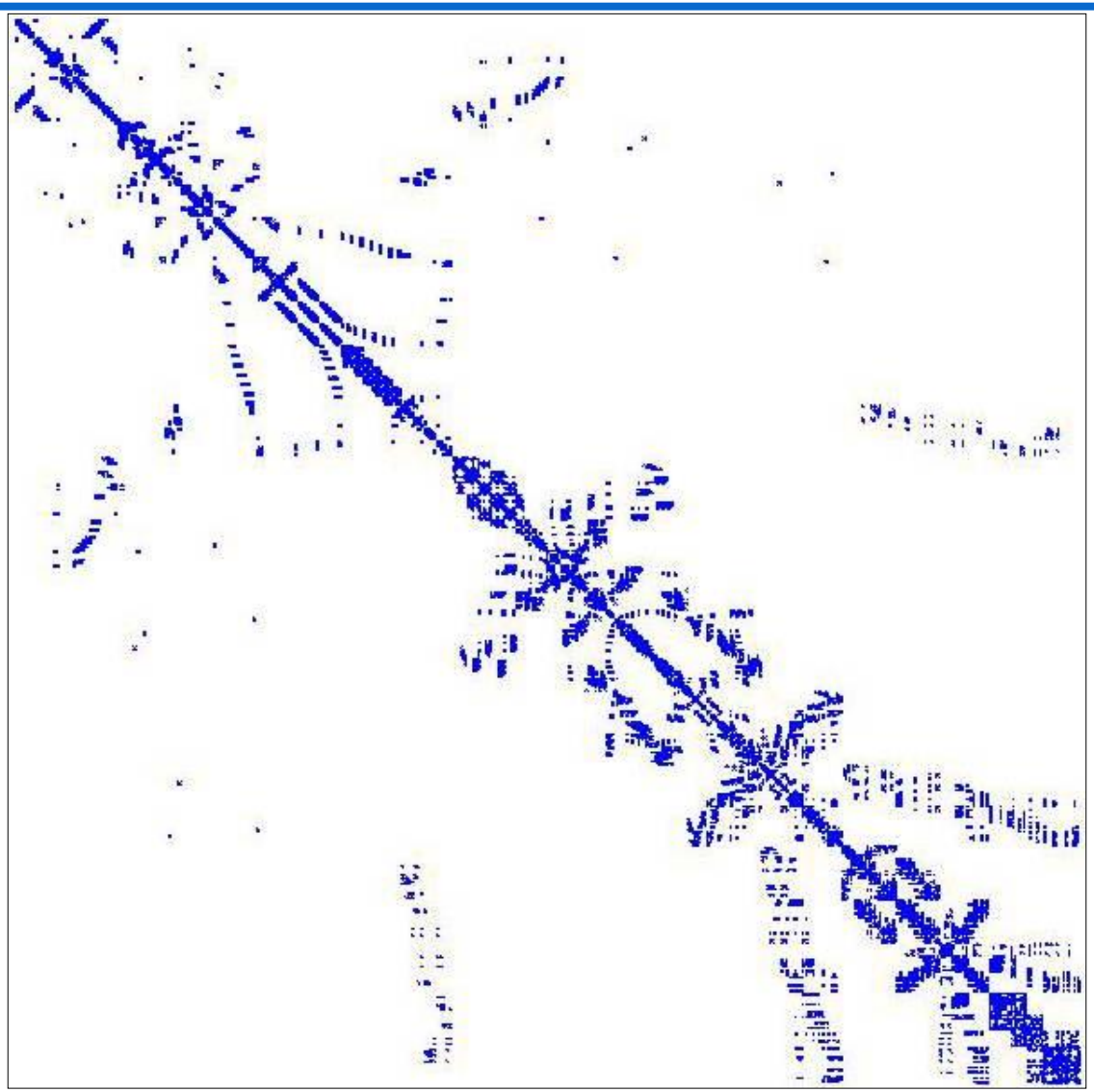
$$x^* = \{x_i = 1, 1 \le i \le n\}$$

- Right side

$$b = Ax^*$$

- System

$$Ax = b$$



Experimental Results (Sparse)

- Method accuracy $\varepsilon = 10^{-7}$
- ILU(0)-preconditioner

Matrix name	n	Accuracy	
		CG	PCG
bcsstk01	48	125	15
bcsstk05	153	272	35
bcsstk10	1086	2335	149
bcsstk13	2003	20031	10016
parabolic_fem	525 825	1690	1045
tmt_sym	726 713	5356	1210

- Convergence is ensured by more than n iterations
- The use of preconditioner reduces the number of iterations

CG – Parallel Algorithm (Dense)

- Iterations are accomplished in a sequence, so it makes sense to parallelize computations performed as part of individual iterations,
  - Basic computations according to the selected method, consist in multiplication of the matrix *A* by the vector *h*,
  - Additional computations (scalar multiplication and addition of vectors) that are less complex include various vector processing operations (scalar product, addition, subtraction, scalar multiplication).
- Known parallel algorithms of matrix multiplication by a vector are used

CG – Parallel Algorithm (Dense)

- Complexity estimation for the parallel $Ah^{(s)}$ operation in case of horizontal band division of the matrix A is

$$2n^2/p + \delta$$

n is the vector length, *p* is the number of flows, δ – contingency

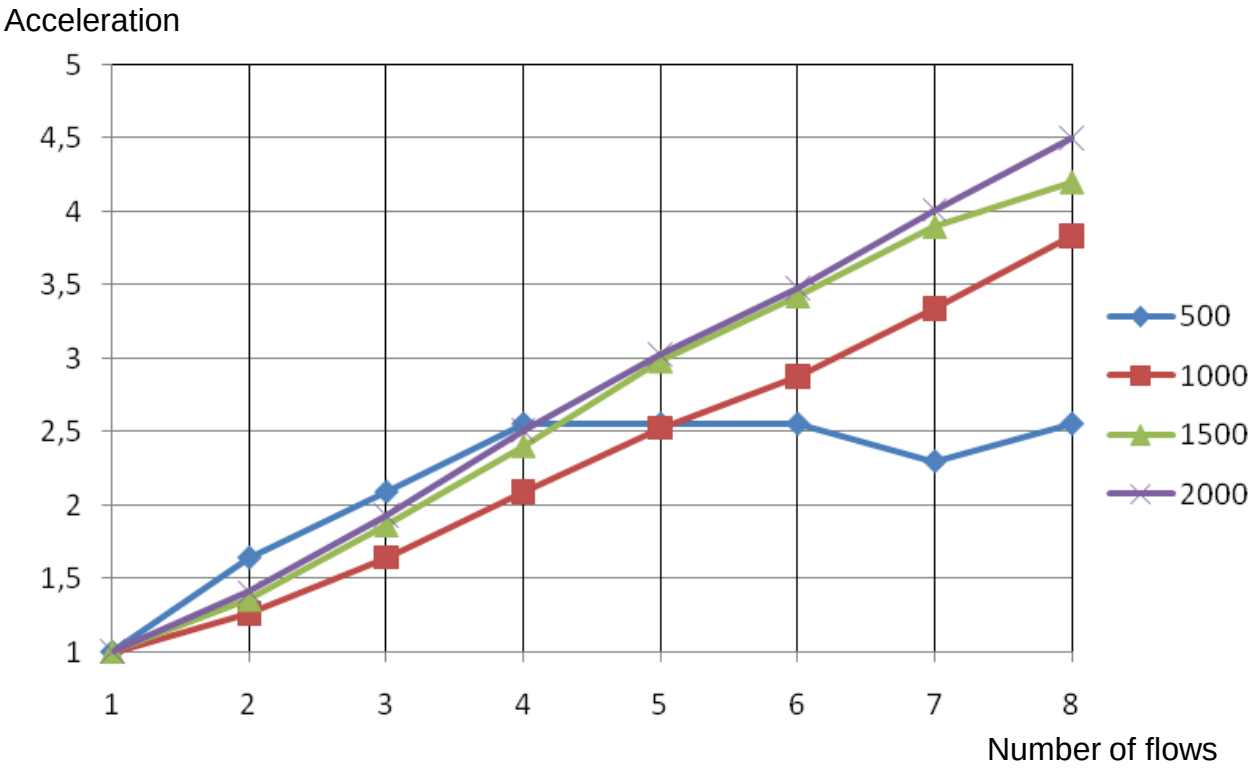
- Less complex computations are subject to single threading.
- Total complexity estimation of the parallel CG method

$$T_p = L\left(\frac{2n^2}{p} + 13n + \delta\right)$$

where *L* is the number of method iterations.

Experimental Results (Dense)

- Acceleration in relation to the single-flow version



- Effect of insufficient computation load on the flow if N=500.

Conclusion

The lecture gives a review of the following:

- Idea of projective methods
- Krylov subspace, subspace basis
  - Arnoldi orthogonalization
  - Lancsoz biorthogonalization
  - Symmetric Lancsoz algorithm
- Krylov subspace iterative methods
  - Generalized minimal residual method
  - Bi-conjugate gradient method
  - Conjugate gradient method
  - Preconditioning in the method pattern
- Experimental results

References

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3. J. Dongarra et al. Templates for the solution of linear systems: building blocks for iterative methods. SIAM, 1994.
4. Y. Saad. Iterative Methods for Sparse Linear Systems. SIAM, 2003.

Web Resources

5. The University of Florida Sparse Matrix Collection – [http://www.cise.ufl.edu/research/sparse/matrices/]
6. Intel Math Kernel Library Reference Manual.

   [http://software.intel.com/sites/products/documentation/hpc/mkl/mklman.pdf].

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- Anna Pirova and Evgeni Kozinov (education software codes)