Japan-Korea HPC Winter School
- Parallel numerical algorithms -

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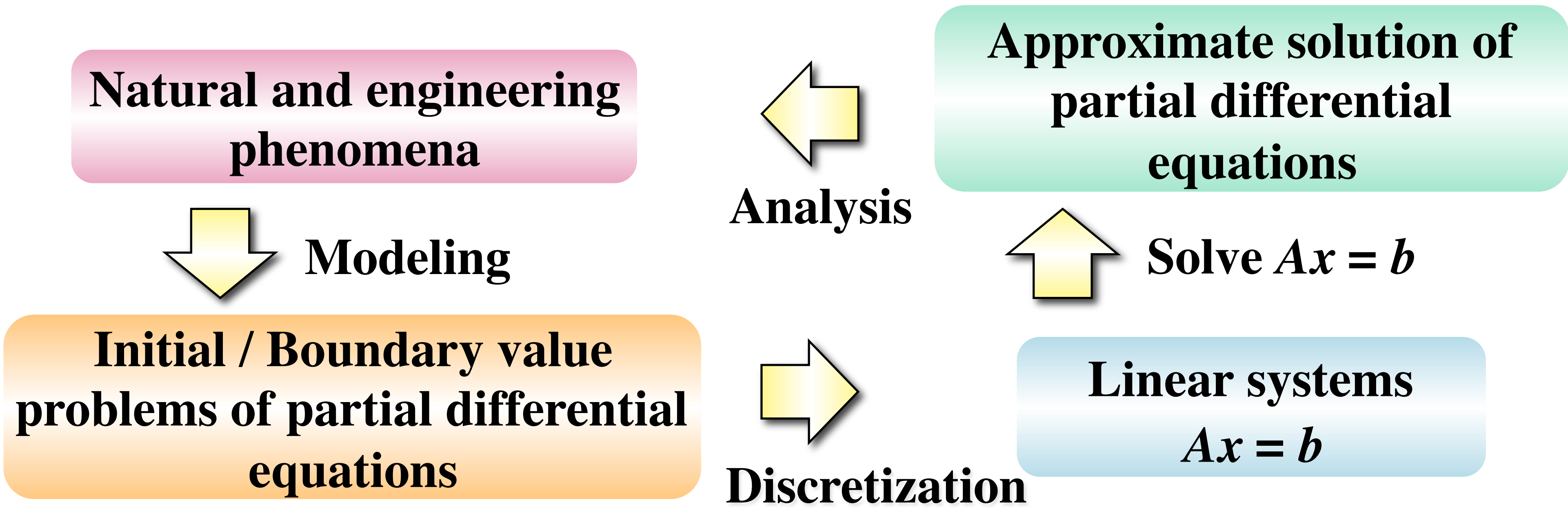
Methods for solving linear systems

$$A\boldsymbol{x} = \boldsymbol{b}$$

Analysis of natural and engineering phenomena



Linear systems appear in many scientific applications.

However, the solution of linear systems is the most time-consuming part.

Linear systems

Linear systems : $\boldsymbol{Ax = b}$

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix}, \quad \boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \quad \boldsymbol{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

Linear systems appear in many scientific applications.

However, the solution of linear systems is the most time-consuming part.

Direct methods and iterative methods

Direct methods

Gaussian elimination, LU factorization, etc.

1) We can always obtain solution in a finite number of operations.

2) Number of nonzero elements increases in transformation of coefficient matrix A.

⇒ **We cannot utilize coefficient matrix sparsity.**

Direct methods

- **Gaussian elimination method**

$$A\boldsymbol{x} = \boldsymbol{b} \qquad\qquad U\boldsymbol{x} = \boldsymbol{b}'$$

$$\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix} \Rightarrow \begin{bmatrix} u_{11} & u_{12} & \dots & u_{1n} \\ & u_{22} & \dots & u_{2n} \\ & & \ddots & \vdots \\ 0 & & & u_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b'_1 \\ b'_2 \\ \vdots \\ b'_n \end{bmatrix}$$

- **LU decomposition method**

$$LU\boldsymbol{x} = \boldsymbol{b}$$

$$\begin{bmatrix} 1 & & & 0 \\ l_{21} & 1 & & \\ \vdots & \vdots & \ddots & \\ l_{n1} & l_{n2} & \dots & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & \dots & u_{1n} \\ & u_{22} & \dots & u_{2n} \\ & & \ddots & \vdots \\ 0 & & & u_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

The coefficient matrix A is only transformed.

Direct methods: Gaussian Elimination

Step 1.

Transform the matrix A of the linear system $A\boldsymbol{x} = \boldsymbol{b}$ to an upper triangular matrix U.

- Computational complexity : n^3 / 3.

$$\underbrace{\begin{bmatrix} u_{11} & u_{12} & \dots & u_{1n} \\ 0 & u_{22} & \dots & u_{2n} \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & u_{nn} \end{bmatrix}}_{U} \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}}_{\boldsymbol{x}} = \underbrace{\begin{bmatrix} b'_1 \\ b'_2 \\ \vdots \\ b'_n \end{bmatrix}}_{\boldsymbol{b}'}$$

Step 2.

Solve the linear system $U\boldsymbol{x} = \boldsymbol{b}'$ by backward substitution with the following recursion formula.

$$x_i = (b'_i - u_{i,i+1}x_{i+1} - \dots - u_{i,n}x_n)/u_{i,i}, \quad i = n, n-1, \dots, 1$$

- Computational complexity : n^2 / 2.

Direct methods: LU decomposition

Step 1.

Perform the LU decomposition of the coefficient matrix A.

$$A = LU$$

L : Lower triangular matrix, U : Upper triangular matrix.

- Computational complexity : $n^3 / 3$.

$$\underbrace{\begin{bmatrix} 1 & & & \mathbf{0} \\ l_{2,1} & 1 & & \\ \vdots & \vdots & \ddots & \\ l_{n,1} & l_{n,2} & \ldots & 1 \end{bmatrix}}_{L} \underbrace{\begin{bmatrix} u_{1,1} & u_{1,2} & \ldots & u_{1,n} \\ & u_{2,2} & \ldots & u_{2,n} \\ & & \ddots & \vdots \\ \mathbf{0} & & & u_{n,n} \end{bmatrix}}_{U} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

Direct methods: LU decomposition

Step 2. Find $\boldsymbol{x}$ using forward / backward substitution.

1) Solve $L\boldsymbol{y} = \boldsymbol{b}$ for $\boldsymbol{y}$ by forward substitution. Here, $\boldsymbol{y} = U\boldsymbol{x}$.

$$\begin{bmatrix} 1 & & & 0 \\ l_{2,1} & 1 & & \\ \vdots & \vdots & \ddots & \\ l_{n,1} & l_{n,2} & \dots & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

2) Solve $U\boldsymbol{x} = \boldsymbol{y}$ for $\boldsymbol{x}$ by backward substitution.

$$\begin{bmatrix} u_{1,1} & u_{1,2} & \dots & u_{1,n} \\ & u_{2,2} & \dots & u_{2,n} \\ & & \ddots & \vdots \\ 0 & & & u_{n,n} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

- Computational complexity : n^2.

Direct methods and iterative methods

Iterative methods

Krylov subspace methods

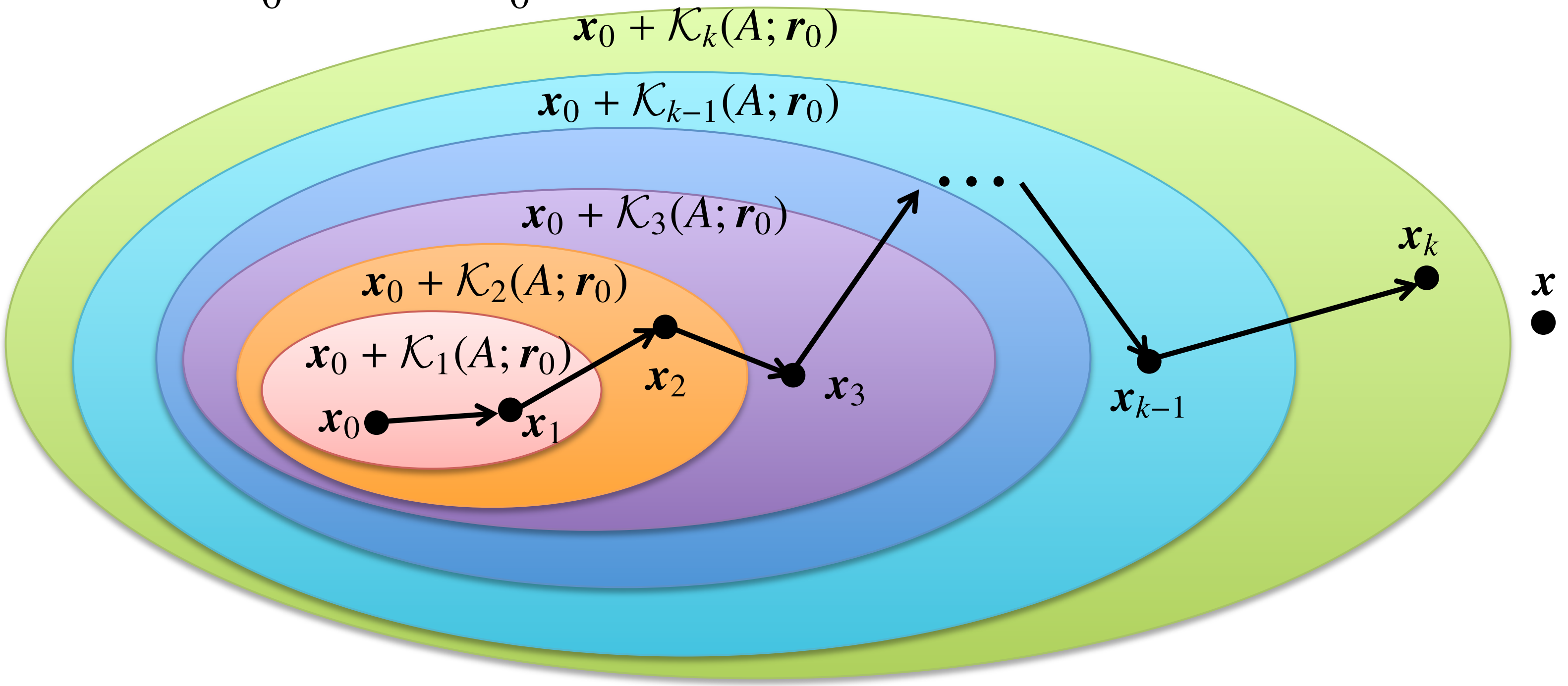
1) Required operations are
   - Multiplication of a coefficient matrix and a vector : $A\boldsymbol{u}$
   - Inner product of vectors : $(\boldsymbol{u}, \boldsymbol{v}) = \boldsymbol{u}^{\mathrm{T}}\boldsymbol{v}$
   - Constant times a vector plus a vector (AXPY) : $a\boldsymbol{u} + \boldsymbol{v}$

   ⇒ We can utilize coefficient matrix sparsity.

2) Some problems may require many number of iterations

Krylov subspace methods

- $\boldsymbol{x}_0$ is an initial guess. The vector $\boldsymbol{x}_k$ is k-th approximate solution of the linear system $A\boldsymbol{x} = \boldsymbol{b}$. $\boldsymbol{x}_k$ is updated by the iteration process.
- $\mathcal{K}_j(A; \boldsymbol{r}_0)$ is called a Krylov subspace. This subspace is spanned by the vectors $\boldsymbol{r}_0, A\boldsymbol{r}_0, \ldots, A^{j-1}\boldsymbol{r}_0$.
- The vector $\boldsymbol{r}_0 = \boldsymbol{b} - A\boldsymbol{x}_0$ is called an initial residual vector.



Sketch of Krylov subspace methods.

Methods for symmetric matrix

1. Coefficient matrix is a symmetric matrix ($A = A^{\mathrm{T}}$)

- **C**onjugate **G**radient (**CG**) method
- **C**onjugate **R**esidual (**CR**) method
- **Min**imal **Res**idual (**MINRES**) method

Using the symmetric property of the coefficient matrix A, algorithms with short recurrence formula (low computational complexity) can be obtained.

Algorithm of the CG method

$\boldsymbol{x}_0$ is an initial guess,

Compute $\boldsymbol{r}_0 = \boldsymbol{b} - A\boldsymbol{x}_0$,

Set $\boldsymbol{p}_0 = \boldsymbol{r}_0$,

For $k = 0, 1, \ldots,$ **until** $\|\boldsymbol{r}_k\|_2 \le \varepsilon_{\mathrm{TOL}} \|\boldsymbol{b}\|_2$ **do** :

$$\boldsymbol{q}_k = A\boldsymbol{p}_k,$$ ← **Matrix-vector multiplication**

$$\alpha_k = \frac{(\boldsymbol{r}_k, \boldsymbol{r}_k)}{(\boldsymbol{p}_k, \boldsymbol{q}_k)},$$ ← **Inner product**

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \alpha_k \boldsymbol{p}_k,$$

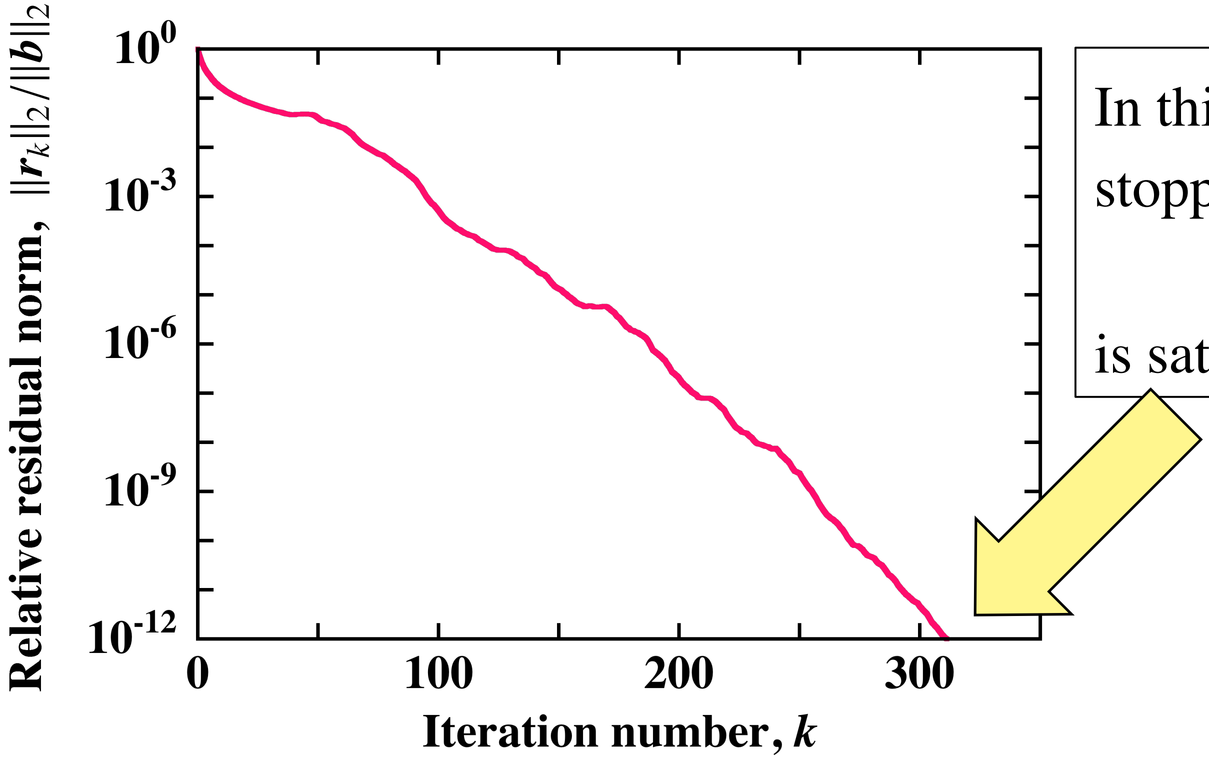
$$\boldsymbol{r}_{k+1} = \boldsymbol{r}_k - \alpha_k \boldsymbol{q}_k,$$ ← **AXPY**

$$\beta_k = \frac{(\boldsymbol{r}_{k+1}, \boldsymbol{r}_{k+1})}{(\boldsymbol{r}_k, \boldsymbol{r}_k)},$$ ← **Inner product**

$$\boldsymbol{p}_{k+1} = \boldsymbol{r}_{k+1} + \beta_k \boldsymbol{p}_k,$$ ← **AXPY**

End For

Relative residual history of the CG method



In this figure, the iteration is stopped when the condition

$$\|\boldsymbol{r}_k\|_2/\|\boldsymbol{b}\|_2 \le 10^{-12}$$

is satisfied.

The relative residual norm $\|\boldsymbol{r}_k\|_2/\|\boldsymbol{b}\|_2$ is monitored during the iterations.
If the condition $\|\boldsymbol{r}_k\|_2/\|\boldsymbol{b}\|_2 \le \varepsilon_{\mathrm{TOL}}$ is satisfied, the iteration is stopped.
Then, the approximate solution $\boldsymbol{x}_k$ is employed as the solution.

Methods for non-symmetric matrix

2. Coefficient matrix is a non-symmetric matrix ($A \neq A^{\mathrm{T}}$)

Methods derived from residual bi-orthobonality condition

- **Bi**-Conjugate **G**radient (**BiCG**) method
- Conjugate **G**radient **S**quared (**CGS**) method
- **BiCG Stab**ilization (**BiCGSTAB**) method

→ Computational complexity is low, but the residual norm does not decrease monotonically.

Methods derived from residual norm minimization condition

- **G**eneralized **C**onjugate **R**esidual (**GCR**) method
- **G**eneralized **M**inimal **Res**idual (**GMRES**) method

→ Residual norm decreases monotonically, but long-term recurrence relations are required.

Algorithm of the BiCG method

$\boldsymbol{x}_0$ is an initial guess,
Compute $\boldsymbol{r}_0 = \boldsymbol{b} - A\boldsymbol{x}_0$,
Choose $\boldsymbol{r}_0^*$ such that $(\boldsymbol{r}_0^*, \boldsymbol{r}_0) \neq 0$,
Set $\boldsymbol{p}_0 = \boldsymbol{r}_0$ and $\boldsymbol{p}_0^* = \boldsymbol{r}_0^*$,
For $k = 0, 1, \ldots,$ **until** $\|\boldsymbol{r}_k\|_2 \leq \varepsilon_{\mathrm{TOL}}\|\boldsymbol{b}\|_2$ **do**:

$$\boldsymbol{q}_k = A\boldsymbol{p}_k, \quad \boldsymbol{q}_k^* = A^{\mathrm{T}}\boldsymbol{p}_k^*,$$

$$\alpha_k = \frac{(\boldsymbol{r}_k^*, \boldsymbol{r}_k)}{(\boldsymbol{p}_k^*, \boldsymbol{q}_k)},$$

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \alpha_k \boldsymbol{p}_k,$$

$$\boldsymbol{r}_{k+1} = \boldsymbol{r}_k - \alpha_k \boldsymbol{q}_k, \quad \boldsymbol{r}_{k+1}^* = \boldsymbol{r}_k^* - \alpha_k \boldsymbol{q}_k^*,$$

$$\beta_k = \frac{(\boldsymbol{r}_{k+1}^*, \boldsymbol{r}_{k+1})}{(\boldsymbol{r}_k^*, \boldsymbol{r}_k)},$$

$$\boldsymbol{p}_{k+1} = \boldsymbol{r}_{k+1} + \beta_k \boldsymbol{p}_k, \quad \boldsymbol{p}_{k+1}^* = \boldsymbol{r}_{k+1}^* + \beta_k \boldsymbol{p}_k^*,$$

End For

Matrix-vector multiplication

Inner product

AXPY

Algorithm of the GCR method

$\boldsymbol{x}_0$ is an initial guess,

Compute $\boldsymbol{r}_0 = \boldsymbol{b} - A\boldsymbol{x}_0$,

Set $\boldsymbol{p}_0 = \boldsymbol{r}_0$ and $\boldsymbol{q}_0 = \boldsymbol{s}_0 = A\boldsymbol{r}_0$,

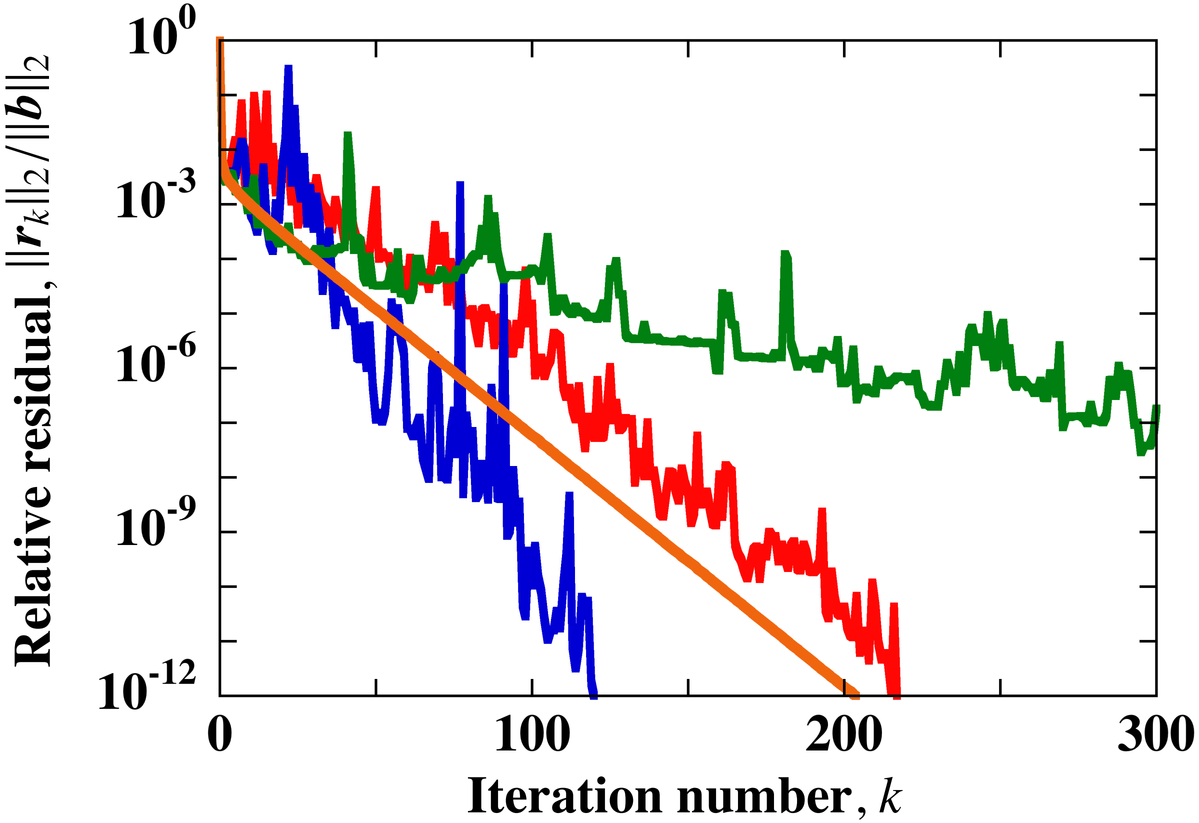
For $k = 0, 1, \ldots,$ **until** $\|\boldsymbol{r}_k\|_2 \le \varepsilon_{\mathrm{TOL}}\|\boldsymbol{b}\|_2$ **do** :

$$\begin{aligned}
\alpha_k &= \frac{(\boldsymbol{q}_k, \boldsymbol{r}_k)}{(\boldsymbol{q}_k, \boldsymbol{q}_k)}, \\
\boldsymbol{x}_{k+1} &= \boldsymbol{x}_k + \alpha_k \boldsymbol{p}_k, \\
\boldsymbol{r}_{k+1} &= \boldsymbol{r}_k - \alpha_k \boldsymbol{q}_k, \\
\boldsymbol{s}_{k+1} &= A\boldsymbol{r}_{k+1}, \\
\beta_{k,i} &= -\frac{(\boldsymbol{q}_i, \boldsymbol{s}_{k+1})}{(\boldsymbol{q}_i, \boldsymbol{q}_i)}, \quad (i = 0, 1, \ldots, k) \\
\boldsymbol{p}_{k+1} &= \boldsymbol{r}_{k+1} + \sum_{i=0}^{k} \beta_{k,i}\boldsymbol{p}_i, \\
\boldsymbol{q}_{k+1} &= \boldsymbol{s}_{k+1} + \sum_{i=0}^{k} \beta_{k,i}\boldsymbol{q}_i,
\end{aligned}$$

End For

- The number of matrix-vector multiplications per iteration is 1.
- This method requires large computational complexity and memory requirement.
- Computational complexity and memory requirement can be reduced by restart technique.

Convergence properties of iterative methods



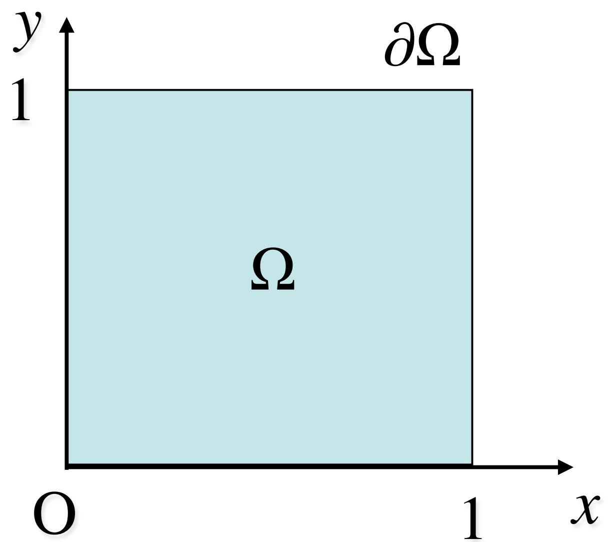
Relative residual norm histories of iterative methods.
■ : BiCG, ■ : CGS, ■ : BiCGSTAB, ■ : GCR.

Example of sparse matrix

2D Poisson problem

$$\begin{cases} \dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2} = f, & \text{in } \Omega \\ u = \bar{u}, & \text{on } \partial\Omega \end{cases}$$

$f,\ \bar{u}$ are given functions



The region Ω is divided into (M+1) equal parts in x, y directions and discretized by central difference with 5-points.

A linear system with matrix of order M^2 can be obtained.

- Total number of elements in matrix : M^4
- Number of nonzero elements : $5M^2 - 4M$

Sparse matrix storage format

Compressed **R**ow **S**torage (**CRS**) format
Search row-wise for nonzero elements

$$A = \begin{bmatrix} a_{11} & 0 & a_{13} & 0 & a_{15} \\ 0 & a_{22} & 0 & a_{24} & a_{25} \\ a_{31} & a_{32} & a_{33} & 0 & 0 \\ 0 & 0 & a_{43} & a_{44} & 0 \\ 0 & a_{52} & 0 & a_{54} & a_{55} \end{bmatrix}$$

`val` stores nonzero elements of A.

`col_ind` stores column number of nonzero elements of A.

`row_ptr` stores location of first nonzero element in each row.

`val:`	a_{11}	a_{13}	a_{15}	a_{22}	a_{24}	a_{25}	a_{31}	a_{32}	a_{33}	a_{43}	a_{44}	a_{52}	a_{54}	a_{55}
`col_ind:`	1	3	5	2	4	5	1	2	3	3	4	2	4	5

`row_ptr:`	1	4	7	10	12	15

The last entry is the number of nonzero elements + 1

Sparse matrix storage format

Compressed **C**olumn **S**torage (**CCS**) format
Search column-wise for nonzero elements

$$A = \begin{bmatrix} a_{11} & 0 & a_{13} & 0 & a_{15} \\ 0 & a_{22} & 0 & a_{24} & a_{25} \\ a_{31} & a_{32} & a_{33} & 0 & 0 \\ 0 & 0 & a_{43} & a_{44} & 0 \\ 0 & a_{52} & 0 & a_{54} & a_{55} \end{bmatrix}$$

`val` stores nonzero elements of A.

`row_ind` stores row number of nonzero elements of A.

`col_ptr` stores location of first nonzero element in each column.

`val:`

a_{11}	a_{31}	a_{22}	a_{32}	a_{52}	a_{13}	a_{33}	a_{43}	a_{24}	a_{44}	a_{54}	a_{15}	a_{25}	a_{55}

`row_ind:`

1	3	2	3	5	1	3	4	2	4	5	1	2	5

`col_ptr:`

1	3	6	9	12	15

The last entry is the number of nonzero elements + 1.

Matrix-vector multiplication CRS format

Multiplication of matrix A and vector x for $y = Ax$

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

Fortran Code

```
do i=1,n
  y(i) = 0.0D0
  do j=row_ptr(i), row_ptr(i+1)-1
    y(i) = y(i) + val(j) * x(col_ind(j))
  end do
end do
```

Matrix-vector multiplication CCS format

Multiplication of matrix A and vector x for $y = Ax$

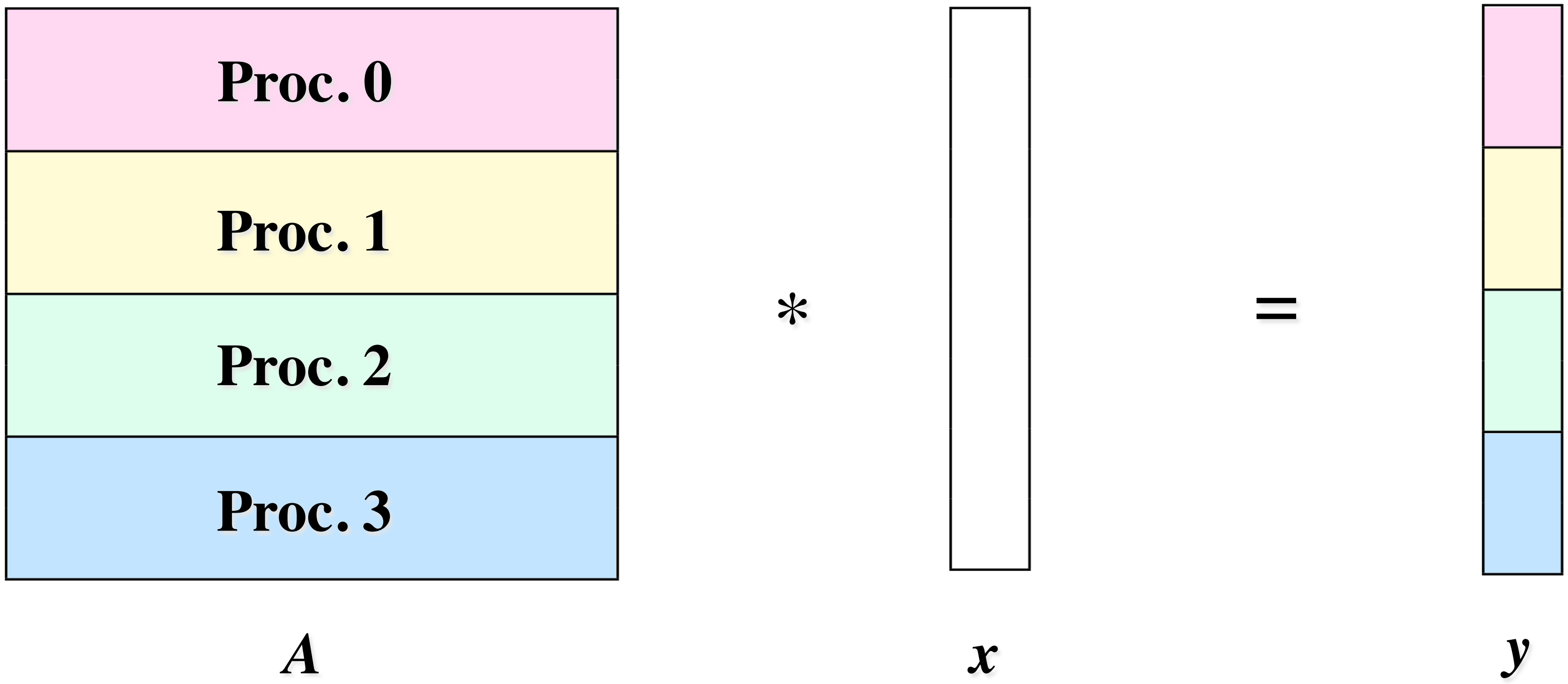
$$\boldsymbol{y} = [\boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_n] \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \sum_{i=1}^{n} \boldsymbol{a}_i x_i$$

Fortran Code

```
do i=1,n
  y(i) = 0.0D0
end do
do j=1,n
  do i=col_ptr(j), col_ptr(j+1)-1
    y(row_ind(i)) = y(row_ind(i)) + val(i) * x(j)
  end do
end do
```

Parallelization of matrix-vector multiplication

- $y = Ax$ in CRS format

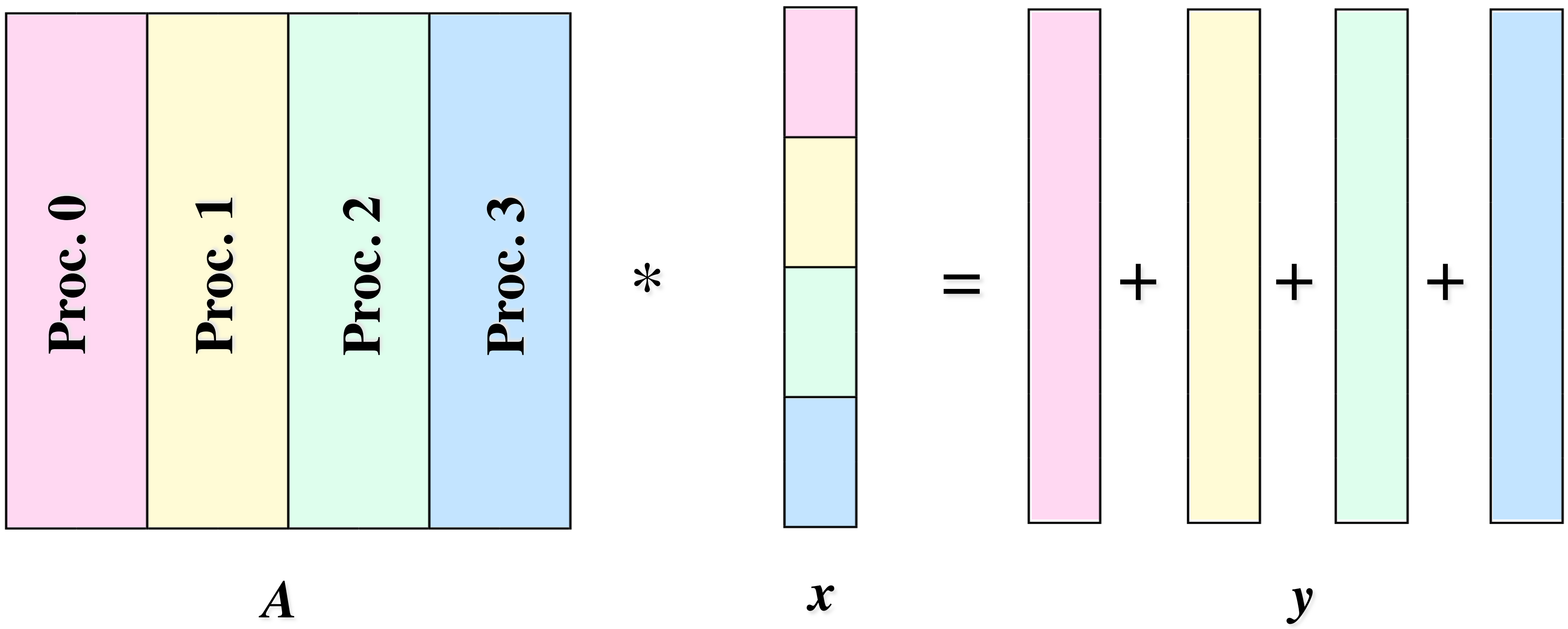


x is stored in all processes

Gather to Proc. 0 by MPI_Gather

Parallelization of matrix-vector multiplication

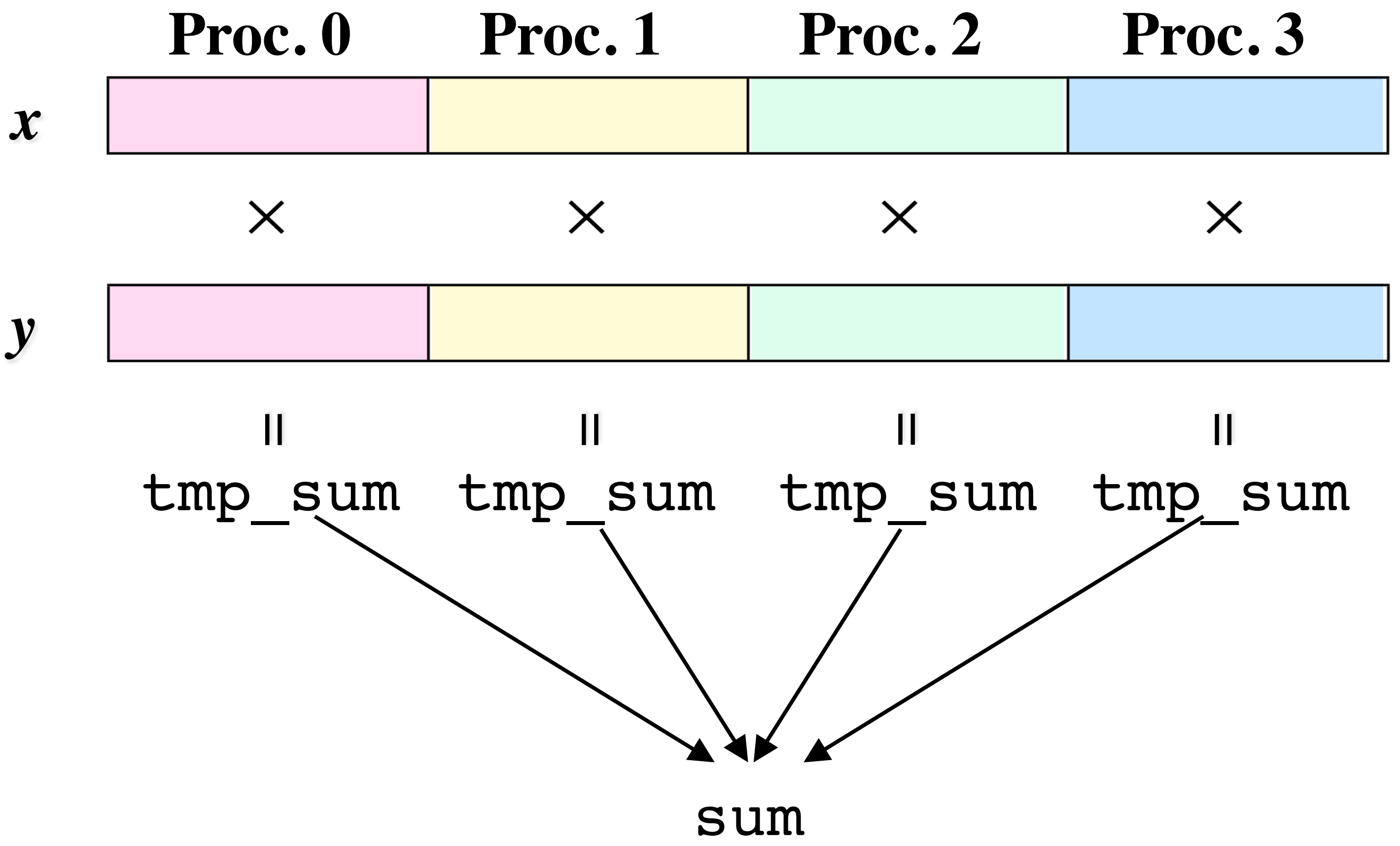
- $y = Ax$ in CCS format



Sum results by MPI_Reduce
and send to Proc. 0

Parallelization of inner products

$$(\boldsymbol{x}, \boldsymbol{y}) = \sum_{j=1}^{n} \bar{x}_j y_j$$



Gather to Proc. 0 by MPI_Reduce

Example of MPI code

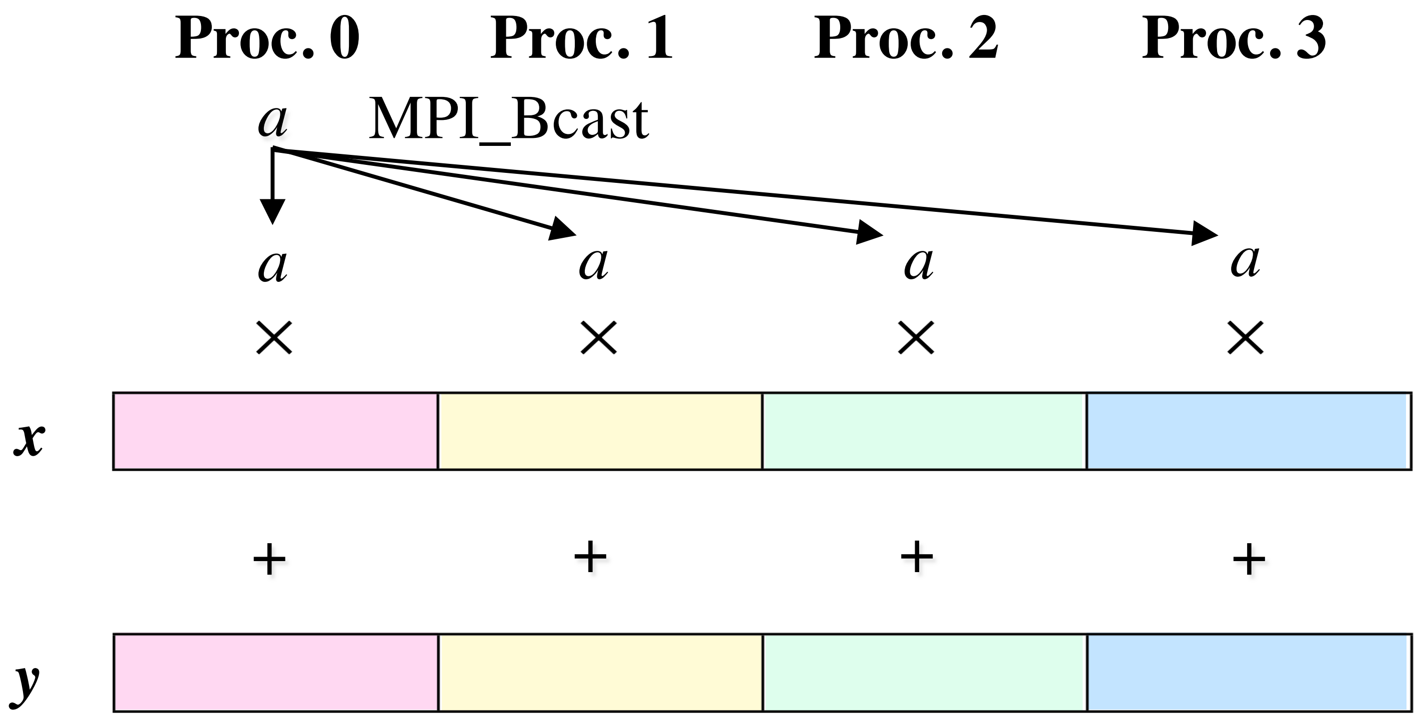
$$(\boldsymbol{x}, \boldsymbol{y}) = \sum_{j=1}^{n} \bar{x}_j y_j$$

```
program main
include 'mpif.h'
...
call mpi_init(ierr)
call mpi_comm_size(mpi_comm_world, npu, ierr)
call mpi_comm_rank(mpi_comm_world, mype, ierr)
...
tmp_sum = (0.0D0, 0.0D0)
do i=istart(mype+1), iend(mype+1)
  tmp_sum = tmp_sum + conj(x(i)) * y(i)
end do
call mpi_reduce(tmp_sum, sum, 1, mpi_double_complex,
mpi_sum, 0, mpi_comm_world, ierr)
...
call mpi_finalize(ierr)
```

Parallelization of constant times a vector plus a vector

$\boldsymbol{y} = \boldsymbol{y} + a\boldsymbol{x}$, a : scalar, $\boldsymbol{x}, \boldsymbol{y}$: vector.

Send a scalar *a* to all processes by MPI_Bcast



Methods for linear systems with multiple right-hand sides

$$AX = B$$

Linear systems with multiple right-hand sides

Linear systems with L right-hand sides

$$AX = B$$

where, A is a matrix of order n and

$$X = \left[\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \ldots, \boldsymbol{x}^{(L)}\right], \; B = \left[\boldsymbol{b}^{(1)}, \boldsymbol{b}^{(2)}, \ldots, \boldsymbol{b}^{(L)}\right]$$

Solution by Direct methods

- Complete factorization (e.g., $A = LU$) of the matrix A is required.
- If complete factorization is possible, then we can solve the system by L forward and backward substitutions.
- Large computational complexity and memory usage are required for complete factorization.

Block Krylov subspace methods

Types of Block Krylov subspace methods

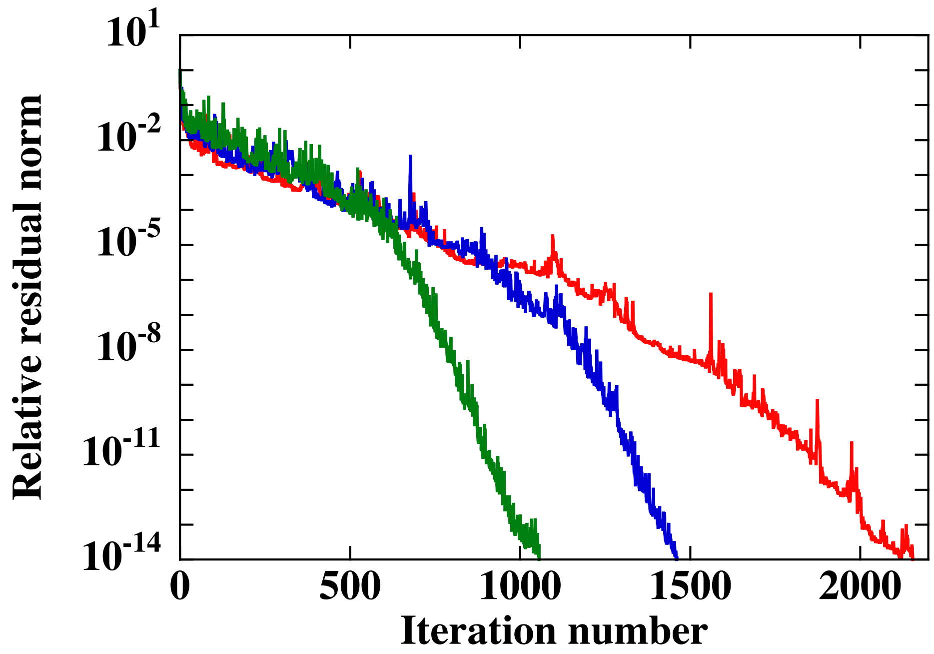
• Block BiCG	O'Leary (1980)
• Block GMRES	Vital (1990)
• Block QMR	Freund (1997)
• Block BiCGSTAB	Guennouni (2003)
• Block BiCGGR	Tadano (2009)

We can efficiently obtain solution vectors by using Block Krylov subspace methods.

Block Krylov subspace methods

What is the meaning of “**good efficiency**” ?

Residual may converge in fewer iterations than Krylov subspace methods for single right-hand side.



Relatrive residual histories of the Block BiCGSTAB methods.

■ : $L = 1$, ■ : $L = 2$, ■ : $L = 4$.

Block CG method

$X_0 \in \mathbb{R}^{n\times L}$ is an initial guess,

Compute $R_0 = B - AX_0$,

Set $P_0 = R_0$,

For $k = 0, 1, \ldots,$ until $\|R_k\|_F \leq \varepsilon_{TOL}\|B\|_F$ **do**:

$Q_k = AP_k$,

Solve $(P_k^T Q_k)\alpha_k = R_k^T R_k$ for α_k,

$X_{k+1} = X_k + P_k\alpha_k$,

$R_{k+1} = R_k - Q_k\alpha_k$,

Solve $(R_k^T R_k)\beta_k = R_{k+1}^T R_{k+1}$ for β_k,

$P_{k+1} = R_{k+1} + P_k\beta_k$,

End For

Differences from CG method

1. The number of matrix-vector multiplications is increased from 1 to L.
2. α_k and β_k become matrices of order L.
3. AXPY calculation becomes matrix-matrix multiplications.

Efficient matrix-vector multiplication

- Let the matrix *A* be stored in CRS format.
- Compute $Y = AX$. *Y* and *X* are *n*-row *L*-column arrays.

```
do k=1,L
 do i=1,n
  do j=row_ptr(i), row_ptr(i+1)-1
   Y(i,k)=Y(i,k)+A(j)*X(col_ind(j),k)
  end do
 end do
end do
```

[**Problems**]

- Continuous memory access for *X* is not available.
  (In Fortran, arrays are stored in column major order.)
- Coefficient matrix data must be read *L* times from memory.

Efficient matrix-vector multiplication

[**Modification**]

- We store *X* and *Y* in transposed form. (*L*-row *n*-column array).

```
do i=1,n
 do j=row_ptr(i), row_ptr(i+1)-1
  do k=1,L
   Y(k,i)=Y(k,i)+A(j)*X(k,col_ind(j))
  end do
 end do
end do
```

- Continuous access (at least *L* times) can be provided for *X*.
- Matrix data are read in just once from memory.
- Continuous access can also be provided for *Y*.

Computation of $n \times L$ matrix by $L \times L$ matrix multiplication

- The vectors are transposed, for efficient matrix-vector multiplication.

Transposition

$$X_{k+1} = X_k + P_k \alpha_k \quad \Rightarrow \quad X_{k+1}^{\mathrm{T}} = X_k^{\mathrm{T}} + \alpha_k^{\mathrm{T}} P_k^{\mathrm{T}}$$

```
do j=1,n
 do i=1,L
  do k=1,L
   X(k,j)=X(k,j)+Alpha(k,i)*P(i,j)
  end do
 end do
end do
```

Continuous access is enabled by transposing.

The matrix `Alpha` is transposed in advance.

Computation of $L\times n$ matrix by $n\times L$ matrix multiplication

- This computation is required to compute α_k and β_k.
- Let us consider the computation of $C_k = P_k^{\mathrm{T}} Q_k$.

```
do j=1,n
 do i=1,L
  do k=1,L
   C(k,i) = C(k,i) + P(k,j) * Q(i,j)
  end do
 end do
end do
```

- We can also maintain continuous memory access in computation of C_k.

Parallelization with OpenMP

- Parallelization interface for shared memory.
- Parallelization can be obtained simply by adding a few lines to the exist program.

```
!$OMP PARALLEL
      [   program   ]
!$OMP END PARALLEL
```

Writing as above enables thread start and separate processing in each thread.
(We assume that the following codes are enclosed by `!$OMP PARALLEL` and `!$OMP END PARALLEL` directives.)

Parallelization with OpenMP

1. Parallelization of matrix-vector multiplication

```
!$OMP DO PRIVATE(j,k)
do i=1,n
 do j=row_ptr(i), row_ptr(i+1)-1
  do k=1,L
   Y(k,i)=Y(k,i)+A(j)*X(k,col_ind(j))
  end do
 end do
end do
```

Simply add `!$OMP DO` before the first `do` loop.

Parallelization with OpenMP

2. Parallelization of $n \times L$ matrix by $L \times L$ matrix multiplication

```
!$OMP DO PRIVATE(i,k)
do j=1,n
 do i=1,L
  do k=1,L
   X(k,j) = X(k,j) + Alpha(k,i) * P(i,j)
  end do
 end do
end do
```

Simply add `!$OMP DO` before the first `do` loop.

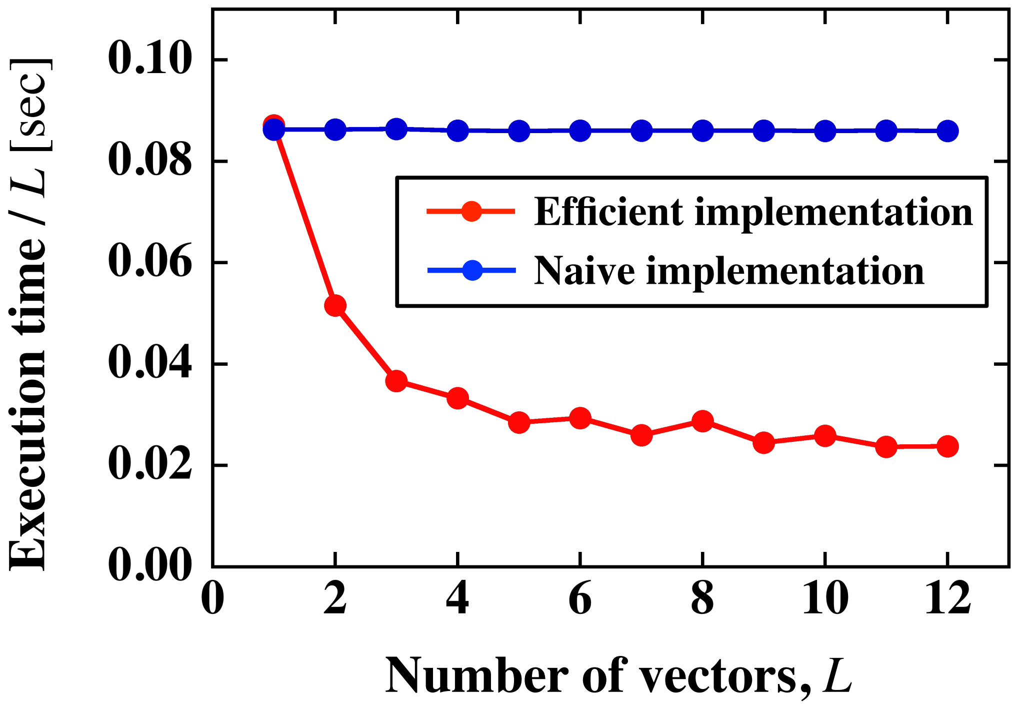
Parallelization with OpenMP

3. Parallelization of *L*×*n* matrix by *n*×*L* matrix multiplication

```
!$OMP SINGLE
 do j=1,L
  do i=1,L
   C(i,j) = 0.0D0
  end do
 end do
!$OMP END SINGLE

!$OMP DO PRIVATE(i,k) REDUCTION(+:C)
do j=1,n
 do i=1,L
  do k=1,L
   C(k,i) = C(k,i) + dconjg(P(k,j)) * Q(i,j)
  end do
 end do
end do
```

Performance of Matrix-vector multiplication



- Execution time of the naive and efficient implementation of Mat-vec mult.
- Matrix size : 1,572,864, #nonzero elements : 80,216,064.
- Experimental environment: CPU : AMD Opteron 2.3GHz × 4.
- Parallelization : 16 OpenMP threads.

Parallelization with OpenMP

[Test linear system]
- Size : 1, 572, 864
- #nonzero elements : 80, 216, 064
- #right-hand sides : 4
- Method: Block BiCGSTAB

[Computing environment]
CPU: Intel Xeon X5550 2.67GHz × 2
Mem: 48GBytes
OS: Cent OS 5.3
Compiler : Intel Fortran ver. 11.1
Option : `-fast -openmp`

#Threads	Time [sec] (#Iterations)	Time / #Iterations	Speedup
1	303.49 (179)	1.6955	1.00
2	183.07 (179)	1.0227	1.66
3	138.07 (179)	0.7713	2.20
4	104.61 (181)	0.5749	2.95
5	80 57 (181)	0.4451	3.81
6	78.56 (181)	0.4340	3.91
7	74.96 (181)	0.4141	4.09
8	68.18 (181)	0.3767	4.50

Summary

In this lecture, we have considered in particular

- Krylov subspace methods for solving linear systems.
- Methods of implementing and parallelizing matrix-vector multiplication for sparse matrices.
- Block Krylov subspace methods, code optimization, and parallelization with OpenMP.