Parallel Computing Advanced Computing

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$$\begin{cases} a_{11}x_1 + a_{12}x_2 + \dots + a_{1N}x_N &= b_1 \\ a_{21}x_1 + a_{22}x_2 + \dots + a_{2N}x_N &= b_2 \\ & \dots & & \dots \\ a_{M1}x_1 + a_{M2}x_2 + \dots + a_{MN}x_N &= b_M \end{cases}$$

N=*M*: the problem has a solution **if** the equations are linearly independent

- When solving a linear system of equations numerically, we may be confronted with two effects caused by the same numerical problem:
 - Equations can "become" linearly dependent due to rounding errors.
 - Accumulation of rounding errors can lead to a "wrong" solution.

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + a_{14}x_4 &= \omega_1 \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + a_{24}x_4 &= \omega_2 \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + a_{34}x_4 &= \omega_3 \\ a_{41}x_1 + a_{42}x_2 + a_{43}x_3 + a_{44}x_4 &= \omega_4 \end{cases}$$

$$\Leftrightarrow \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \\ \omega_4 \end{pmatrix}$$

 The basic idea to solve such a system is a straight-forward substitution:

$$\begin{cases} 3x + 2y &= 5 \\ x + y &= 3 \end{cases} \Leftrightarrow \begin{cases} x &= \frac{5-2y}{3} \Leftrightarrow x + y &= 3 \end{cases}$$

$$\Leftrightarrow \left\{ \begin{array}{ccc} x & = & \frac{5-2y}{3} \\ \frac{5-2y}{3} + y & = & 3 \end{array} \right. \Leftrightarrow \left\{ \begin{array}{ccc} x & = & \frac{5-2y}{3} \\ y & = & 4 \end{array} \right. \Leftrightarrow \left\{ \begin{array}{ccc} x & = & -1 \\ y & = & 4 \end{array} \right.$$

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ 0 & a_{22} - \frac{a_{21}a_{12}}{a_{11}} & a_{23} - \frac{a_{21}a_{13}}{a_{11}} & a_{24} - \frac{a_{21}a_{14}}{a_{11}} \\ 0 & a_{32} - \frac{a_{31}a_{12}}{a_{11}} & a_{33} - \frac{a_{31}a_{13}}{a_{11}} & a_{34} - \frac{a_{31}a_{14}}{a_{11}} \\ 0 & a_{42} - \frac{a_{41}a_{12}}{a_{11}} & a_{43} - \frac{a_{41}a_{13}}{a_{11}} & a_{44} - \frac{a_{41}a_{14}}{a_{11}} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} \omega_1 \\ \omega_2 - \frac{a_{21}\omega_1}{a_{11}} \\ \omega_3 - \frac{a_{31}\omega_1}{a_{11}} \\ \omega_4 - \frac{a_{41}\omega_1}{a_{11}} \end{pmatrix}$$

Upper triangular matrix:

$$\begin{pmatrix} a_{11}^{(1)} & a_{12}^{(1)} & a_{13}^{(1)} & a_{14}^{(1)} \\ 0 & a_{22}^{(2)} & a_{23}^{(2)} & a_{24}^{(2)} \\ 0 & 0 & a_{33}^{(3)} & a_{34}^{(3)} \\ 0 & 0 & 0 & a_{44}^{(4)} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} \omega_1^{(1)} \\ \omega_2^{(1)} \\ \omega_2^{(2)} \\ \omega_3^{(3)} \\ \omega_4^{(4)} \end{pmatrix}$$

At this point, the problem is solved!

• The general formula for the construction of the upper triangular matrix associated with the Gauss elimination method for a system of n equations is the following:

$$a_{jk}^{(m+1)} = a_{jk}^{(m)} - \frac{a_{jm}^{(m)} a_{mk}^{(m)}}{a_{mm}^{(m)}}$$

$$\omega_j^{(m+1)} = \omega_j^{(m)} - \frac{a_{jm}^{(m)} \omega_m^{(m)}}{a_{mm}^{(m)}}$$

$$a_{jk}^{(1)} = a_{jk}$$
$$j, k = m + 1, \dots, n$$

$$\omega_j^{(1)} = \omega_j$$
 $j = m+1,\ldots,n$

• The solution is then obtained by **Backward Substitution**:

$$x_m = \frac{1}{a_{mm}^{(m)}} \left(\omega_m^{(m)} - \sum_{k=m+1}^n a_{mk}^{(m)} x_k \right)$$

$$m = n, n - 1, n - 2, \dots, 1$$

This method requires *n*³ operations! (of algebraic calculations)

 However, this elimination method has a "weak point":

$$a_{jk}^{(m+1)} = a_{jk}^{(m)} - \frac{a_{jm}^{(m)} a_{mk}^{(m)}}{a_{mm}^{(m)}}$$

If this number is small, the division result can be a large number that will be added to a potentially small number...

One way to avoid this type of problems is to "move" the small numbers away from the diagonal, exchanging lines and/or columns of the matrices/vectors of the problem.

Partial pivoting (per column):

exchange the lines of A and the vector/matrix on the right side in order to place the largest value in the "problematic" column, i.e. in the diagonal.

$$\begin{pmatrix} 1 & 3 & 4 & 6 \\ 0 & 10^{-8} & 198 & 19 \\ 0 & -91 & 51 & 9 \\ 0 & 7 & 76 & 541 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \\ \omega_4 \end{pmatrix}$$

$$\begin{bmatrix}
1 & 3 & 4 & 6 \\
0 & -91 & 51 & 9 \\
0 & 10^{-8} & 198 & 19 \\
0 & 7 & 76 & 541
\end{bmatrix}
\begin{pmatrix}
x_1 \\
x_2 \\
x_3 \\
x_4
\end{pmatrix} = \begin{pmatrix}
\omega_1 \\
\omega_3 \\
\omega_2 \\
\omega_4
\end{pmatrix}$$

- In order to minimise rounding errors, the pivoting operation should be performed at each step of the triangularisation process, systematically placing the highest value element of the column under analysis on the diagonal.
- But this can bring a lot of overhead to the process, so it's sometimes more efficient to only pivot when a problematic small number appears in the diagonal.
- The choice depends on the balance between required precision and available computing resources.

Complete pivoting (both by row and column): exchange the rows and columns of A and the vectors X and ω in order to place the largest diagonal value in the column and row of the "problematic" element.

$$\begin{pmatrix} 1 & 3 & 4 & 6 \\ 0 & 10^{-8} & 198 & 19 \\ 0 & -91 & 51 & 9 \\ 0 & 7 & 76 & 541 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \\ \omega_4 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 4 & 3 & 6 \\ 0 & 198 & 10^{-8} & 19 \\ 0 & 51 & -91 & 9 \\ 0 & 76 & 7 & 541 \end{pmatrix} \begin{pmatrix} x_1 \\ x_3 \\ x_2 \\ x_4 \end{pmatrix} = \begin{pmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \\ x_2 \\ x_4 \end{pmatrix}$$

- Ideally, from the point of view of numerical accuracy, we should do a complete pivoting in order to ensure that the largest element of the sub-matrix still to be treated is always in the diagonal...
- But we can choose to pivot only when there is a very small number on the diagonal...
- Be sure to keep a record of all line and column exchange operations!