Gaussian Elimination with Partial Pivoting

While it is true that almost all nonsingular matrices can be triangularized using only Gauss Transforms (add multiple of one row to another), it does *not* make a good general purpose numerical method. The problem is caused, as you might suspect (?), by small pivot elements. Consider the k^{th} step, zeroing the (i,k) entries with multipliers $m_{ik} = -a_{ik}^{(k-1)}/a_{kk}^{(k-1)}, \;\; k{+}1, k{+}2, \ldots, n$:

$$a_i^{(k)} = a_i^{(k-1)} + m_{ik} a_k^{(k-1)},$$

giving

$$A^{(k)} = \begin{bmatrix} \hat{U}^{(k)} & X \\ 0 & \hat{A}^{(k)} \end{bmatrix}.$$

If $a_{kk}^{(k-1)}$ is small, then $|m_{ik}|$ will be large, and two bad things will happen: (i) information in the entries of $A^{(k-1)}$ gets swamped when the large vector $m_{ik}a_k^{(k-1)}$ gets added to $a_i^{(k-1)}$, and (ii) that information is replaced by basically the same value for each row: $a_i^{(k)}$ will be mostly in the direction $a_k^{(k-1)}$ for *all* of the rows $i = k{+}1, k{+}2, \ldots, n$ of $A^{(k)}$, moving $\hat{A}^{(k)}$ closer to the set of singular matrices.

So it's time to bring back row operation R2: Before zeroing the elements in column k, we find $\max_{k \le j \le n} |a_{jk}^{(k-1)}|$ (the |biggest| element of the first column of $\hat{A}^{(k-1)}$). If that max occurs in row p, then we interchange rows k and p of $A^{(k-1)}$. This is called *partial pivoting*. Now the |biggest| entry in the first row of the permuted $\hat{A}^{(k-1)}$ is in its $(1,1)$ position, and thus all of the multipliers for this step satisfy $|m_{ik}| \le 1$.

In the language of matrix operations: Before applying the Gauss transform M_k, we apply the permutation P_{kp}. The k^{th} step of GE with partial pivoting (GEPP) is

$$A^{(k)} = M_k P_k A^{(k-1)},$$

and after $n-1$ steps

$$A^{(n-1)} = M_{n-1}P_{n-1} \cdots M_2 P_2 M_1 P_1 A \equiv U.$$

If A is nonsingular, this can always be done. It does not give the $A = LU$ factorization as before, because the permutations (row interchanges) mess up the lower triangularity of L. In order to see what factorization we do get, we need to interpret the matrix $M_{n-1}P_{n-1} \cdots M_2P_2M_1P_1$. To that end, take $j < k \le p$ and notice that an e_j Gauss transform followed by a (k,p) permutation is that permutation followed by a different (permuted m_j) e_j Gauss transform:

$$P_k M_j = P_k(I + m_j e_j^T) = P_k + P_k m_j e_j^T P_k^T P_k \equiv (I + \tilde{m}_j e_j^T) P_k \equiv \tilde{M}_j P_k.$$

Now define $N_i = I + n_i e_i^T$, where $n_i = P_{n-1} \cdots P_{i+1} m_i$.

$$M_{n-1}P_{n-1} \cdots M_2P_2M_1P_1 = (N_{n-1} \cdots N_2 N_1)(P_{n-1} \cdots P_2 P_1) \equiv L^{-1}P,$$

giving $PA = LU$. This simple change makes GE general purpose; in fact GEPP (and then forward and backward substitution) is the most often used method for solving $Ax = b$.