Parallel Gaussian Elimination

1. LU and Cholesky Factorization
   - factoring a square matrix
   - tiled Cholesky factorization
2. Blocked LU Factorization
   - deriving blocked formulations of LU
   - right and left looking LU factorizations
   - tiled algorithm for LU factorization
3. The PLASMA Software Library and the cuSOLVER API
   - Parallel Linear Algebra Software for Multicore Architectures
   - the cuSOLVER library

MCS 572 Lecture 35
Introduction to Supercomputing
Jan Verschelde, 15 November 2024

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solving $A\mathbf{x} = \mathbf{b}$ with the LU factorization

To solve an n-dimensional linear system $A\mathbf{x} = \mathbf{b}$
we factor A as a product of two triangular matrices, $A = LU$:

- L is lower triangular, $L = [\ell_{i,j}]$, $\ell_{i,j} = 0$ if $j > i$ and $\ell_{i,i} = 1$.
- U is upper triangular $U = [u_{i,j}]$, $u_{i,j} = 0$ if $i > j$.

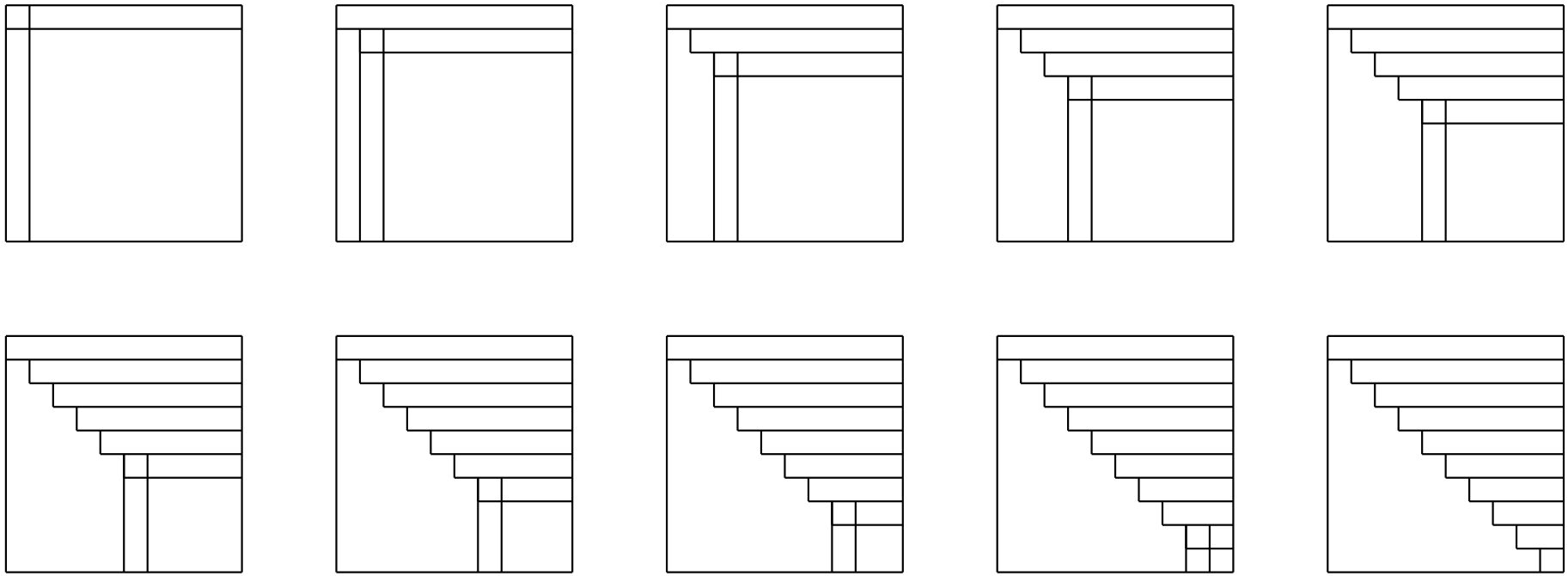
Solving $A\mathbf{x} = \mathbf{b}$ is equivalent to solving $L(U\mathbf{x}) = \mathbf{b}$:

1. Forward substitution: $L\mathbf{y} = \mathbf{b}$.
2. Backward substitution: $U\mathbf{x} = \mathbf{y}$.

Factoring A costs $O(n^3)$, solving triangular systems costs $O(n^2)$.

For numerical stability, we apply partial pivoting and compute $PA = LU$,
where P is a permutation matrix.

LU factorization of the matrix A



for column $j = 1, 2, \ldots, n-1$ in A do

1. find the largest element $a_{i,j}$ in column j (for $i \geq j$);
2. if $i \neq j$, then swap rows i and j;
3. for $i = j+1, \ldots n$, for $k = j+1, \ldots, n$ do $a_{i,k} := a_{i,k} - \left(\frac{a_{i,j}}{a_{j,j}} \right) a_{j,k}$.

Cholesky factorization

If A is symmetric, $A^T = A$, and positive semidefinite: $\forall \mathbf{x} : \mathbf{x}^T A\mathbf{x} \geq 0$, then we better compute a Cholesky factorization: $A = LL^T$, where L is a lower triangular matrix.

Because A is positive semidefinite, no pivoting is needed, and we need about half as many operations as LU.

for $j = 1, 2, \ldots, n$ do
  for $k = 1, 2, \ldots, j-1$ do
    $a_{j,j} := a_{j,j} - a_{j,k}^2$;
  $a_{j,j} := \sqrt{a_{j,j}}$;
  for $i = j+1, \ldots, n$ do
    for $k = 1, 2, \ldots, j$ do
      $a_{i,j} := a_{i,j} - a_{i,k} a_{j,k}$
    $a_{i,j} := a_{i,j} / a_{j,j}$

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tiled matrices

Let A be a symmetric, positive definite n-by-n matrix.

For tile size b, let $n = p \times b$ and consider

$$A = \begin{bmatrix} A_{1,1} & A_{2,1} & \cdots & A_{p,1} \\ A_{2,1} & A_{2,2} & \cdots & A_{p,2} \\ \vdots & \vdots & \ddots & \vdots \\ A_{p,1} & A_{p,2} & \cdots & A_{p,p} \end{bmatrix},$$

where $A_{i,j}$ is an b-by-b matrix.

A crude classification of memory hierarchies distinguishes between registers (small), cache (medium), and main memory (large).

To reduce data movements, we want to keep data in registers and cache as much as possible.

tiled Cholesky factorization

for $k = 1, 2, \ldots, p$ do
  DPOTF2$(A_{k,k}, L_{k,k})$ —— $L_{k,k} := \text{Cholesky}(A_{k,k})$
  for $i = k+1, \ldots, p$ do
    DTRSM$(L_{k,k}, A_{i,k}, L_{i,k})$ —— $L_{i,k} := A_{i,k} L_{k,k}^{-T}$
  end for
  for $i = k+1, \ldots, p$ do
    for $j = k+1, \ldots, p$ do
      DGSMM$(L_{i,k}, L_{j,k}, A_{i,j})$ —— $A_{i,j} := A_{i,j} - L_{i,k} L_{j,k}^{T}$
    end for
end for

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blocked LU factorization

The optimal size of the blocks is machine dependent.

$$\begin{bmatrix} A_{1,1} & A_{1,2} & A_{1,3} \\ A_{2,1} & A_{2,2} & A_{2,3} \\ A_{3,1} & A_{3,2} & A_{3,3} \end{bmatrix} = \begin{bmatrix} L_{1,1} & & \\ L_{2,1} & L_{2,2} & \\ L_{3,1} & L_{3,2} & L_{3,3} \end{bmatrix} \begin{bmatrix} U_{1,1} & U_{1,2} & U_{1,3} \\ & U_{2,2} & U_{2,3} \\ & & U_{3,3} \end{bmatrix}$$

Expanding the right hand side and equating to the matrix at the left gives formulations for the LU factorization.

$$\begin{array}{lll} A_{1,1} = L_{1,1}U_{1,1} & A_{1,2} = L_{1,1}U_{1,2} & A_{1,3} = L_{1,1}U_{1,3} \\ A_{2,1} = L_{2,1}U_{1,1} & A_{2,2} = L_{2,1}U_{1,2} + L_{2,2}U_{2,2} & A_{2,3} = L_{2,1}U_{1,3} + L_{2,2}U_{2,3} \\ A_{3,1} = L_{3,1}U_{1,1} & A_{3,2} = L_{3,1}U_{1,2} + L_{3,2}U_{2,2} & A_{3,3} = L_{3,1}U_{1,3} + L_{3,2}U_{2,3} \\ & & \quad + L_{3,3}U_{3,3} \end{array}$$

right looking LU

We store the $L_{i,j}$'s and $U_{i,j}$'s in the original matrix:

$$\begin{bmatrix} A_{1,1} & A_{1,2} & A_{1,3} \\ A_{2,1} & A_{2,2} & A_{2,3} \\ A_{3,1} & A_{3,2} & A_{3,3} \end{bmatrix} = \begin{bmatrix} L_{1,1} & & \\ L_{2,1} & I & \\ L_{3,1} & & I \end{bmatrix} \begin{bmatrix} U_{1,1} & U_{1,2} & U_{1,3} \\ & B_{2,2} & B_{2,3} \\ & B_{3,2} & B_{3,3} \end{bmatrix}$$

The matrices $B_{i,j}$'s are obtained after a first block LU step.
To find $L_{2,2}$, $L_{3,2}$, and $U_{2,2}$ we use

$$\begin{cases} A_{2,2} = L_{2,1}U_{1,2} + L_{2,2}U_{2,2} \\ A_{3,2} = L_{3,1}U_{1,2} + L_{3,2}U_{2,2} \end{cases} \quad \text{and} \quad \begin{cases} A_{2,2} = L_{2,1}U_{1,2} + B_{2,2} \\ A_{3,2} = L_{3,1}U_{1,2} + B_{3,2} \end{cases}$$

Eliminating $A_{2,2} - L_{2,1}U_{1,2}$ and $A_{3,2} - L_{3,1}U_{1,2}$ gives

$$\begin{cases} B_{2,2} = L_{2,2}U_{2,2} \\ B_{3,2} = L_{3,2}U_{2,2} \end{cases}$$

Via LU on $B_{2,2}$ we obtain $L_{2,2}$ and $U_{2,2}$. Then: $L_{3,2} := B_{3,2}U_{2,2}^{-1}$.

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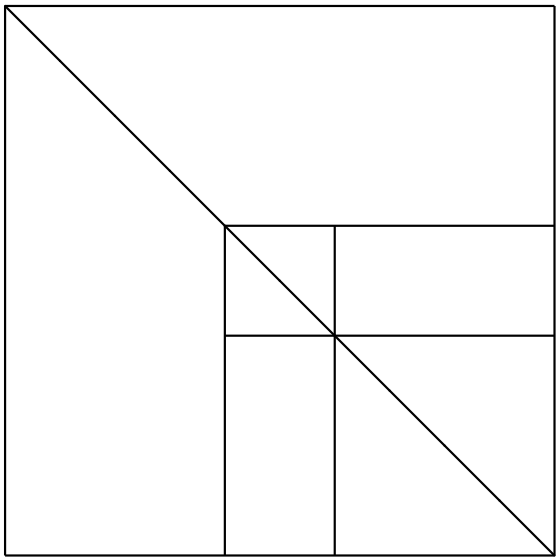
right and left looking

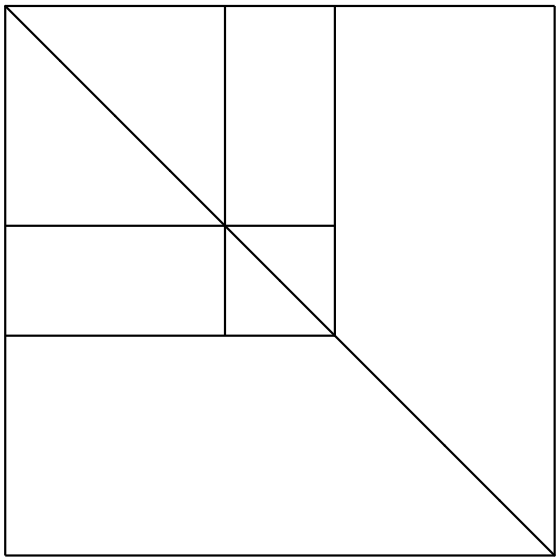
The formulas we derived are similar to the scalar case and are called *right looking*.

But we may organize the LU factorization differently:

right looking



left looking



What is good looking? Left is best for data access.

left looking formulas

Going from $P_1 A$ to $P_2 P_1 A$:

$$\begin{bmatrix} L_{1,1} & & \\ L_{2,1} & I & \\ L_{3,1} & & I \end{bmatrix} \begin{bmatrix} U_{1,1} & A_{1,2} & A_{1,3} \\ & A_{2,2} & A_{2,3} \\ & A_{3,2} & A_{3,3} \end{bmatrix} \rightarrow \begin{bmatrix} L_{1,1} & & \\ L_{2,1} & L_{2,2} & \\ L_{3,1} & L_{3,2} & I \end{bmatrix} \begin{bmatrix} U_{1,1} & U_{1,2} & A_{1,3} \\ & U_{2,2} & A_{2,3} \\ & & A_{3,3} \end{bmatrix}$$

We keep the original $A_{i,j}$'s and postpone updating to the right.

1. We get $U_{1,2}$ via $A_{1,2} = L_{1,1} U_{1,2}$ and compute $U_{1,2} = L_{1,1}^{-1} A_{1,2}$.
2. To compute $L_{2,2}$ and $L_{3,2}$ do $\begin{bmatrix} B_{2,2} \\ B_{3,2} \end{bmatrix} = \begin{bmatrix} A_{2,2} \\ A_{3,2} \end{bmatrix} - \begin{bmatrix} L_{2,1} \\ L_{3,1} \end{bmatrix} U_{1,2}$.

   and factor $P_2 \begin{bmatrix} B_{2,2} \\ B_{3,2} \end{bmatrix} = \begin{bmatrix} L_{2,2} \\ L_{3,2} \end{bmatrix} U_{2,2}$ as before.

   Replace $\begin{bmatrix} A_{2,3} \\ A_{3,3} \end{bmatrix} := P_2 \begin{bmatrix} A_{2,3} \\ A_{3,3} \end{bmatrix}$ and $\begin{bmatrix} L_{2,1} \\ L_{3,1} \end{bmatrix} := P_2 \begin{bmatrix} L_{2,1} \\ L_{3,1} \end{bmatrix}$.

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tiled LU factorization

for $k = 1, 2, \ldots, p$ do

  DGETF$(A_{k,k}, L_{k,k}, U_{k,k}, P_{k,k})$ —— $L_{k,k}, U_{k,k}, P_{k,k} := \mathrm{LU}(A_{k,k})$

  for $j = k+1, \ldots, p$ do

    DGESSM$(A_{k,j}, L_{k,k}, P_{k,k}, U_{k,j})$ —— $U_{k,j} := L_{k,k}^{-1} P_{k,k} A_{k,j}$

  end for

  for $i = k+1, \ldots, p$ do

    DTSTRF$(U_{k,k}, A_{i,k}, P_{i,k})$ —— $U_{k,k}, L_{i,k}, P_{i,k} := LU\left(\begin{bmatrix} U_{k,k} \\ A_{i,k} \end{bmatrix}\right)$

    for $j = k+1, \ldots, p$ do

      DSSSM$(U_{k,j}, A_{i,j}, L_{i,k}, P_{i,k})$ —— $\begin{bmatrix} U_{k,j} \\ A_{i,j} \end{bmatrix} := L_{i,k}^{-1} P_{i,k} \begin{bmatrix} U_{k,j} \\ A_{i,j} \end{bmatrix}$

    end for

end for

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the PLASMA software library

Parallel Linear Algebra Software for Multicore Architectures.

- Software using FORTRAN and C.
- Design for efficiency on homogeneous multicore processors and multi-socket systems of multicore processors.
- Built using a small set of sequential routines as building blocks, referred to as *core BLAS*.
- Free to download from `http://icl.cs.utk.edu/plasma`.

Capabilities and limitations:

- Can solve dense linear systems and least squares problems.
- Unlike LAPACK, PLASMA currently does not solve eigenvalue or singular value problems and provide no support for band matrices.

Basic Linear Algebra Subprograms: BLAS

1. Level-1 BLAS: vector-vector operations, $O(n)$ cost.
   inner products, norms, $\mathbf{x} \pm \mathbf{y}$, $\alpha\mathbf{x} + \mathbf{y}$.
2. Level-2 BLAS: matrix-vector operations, $O(mn)$ cost.
   - $\mathbf{y} = \alpha A\mathbf{x} + \beta\mathbf{y}$
   - $A = A + \alpha\mathbf{x}\mathbf{y}^T$, rank one update
   - $\mathbf{x} = T^{-1}\mathbf{b}$, for T a triangular matrix
3. Level-3 BLAS: matrix-matrix operations, $O(kmn)$ cost.
   - $C = \alpha AB + \beta C$
   - $C = \alpha AA^T + \beta C$, rank k update of symmetric matrix
   - $B = \alpha TB$, for T a triangular matrix
   - $B = \alpha T^{-1}B$, solve linear system with many right hand sides

graph driven asynchronous execution

We view a blocked algorithm as a Directed Acyclic Graph (DAG):

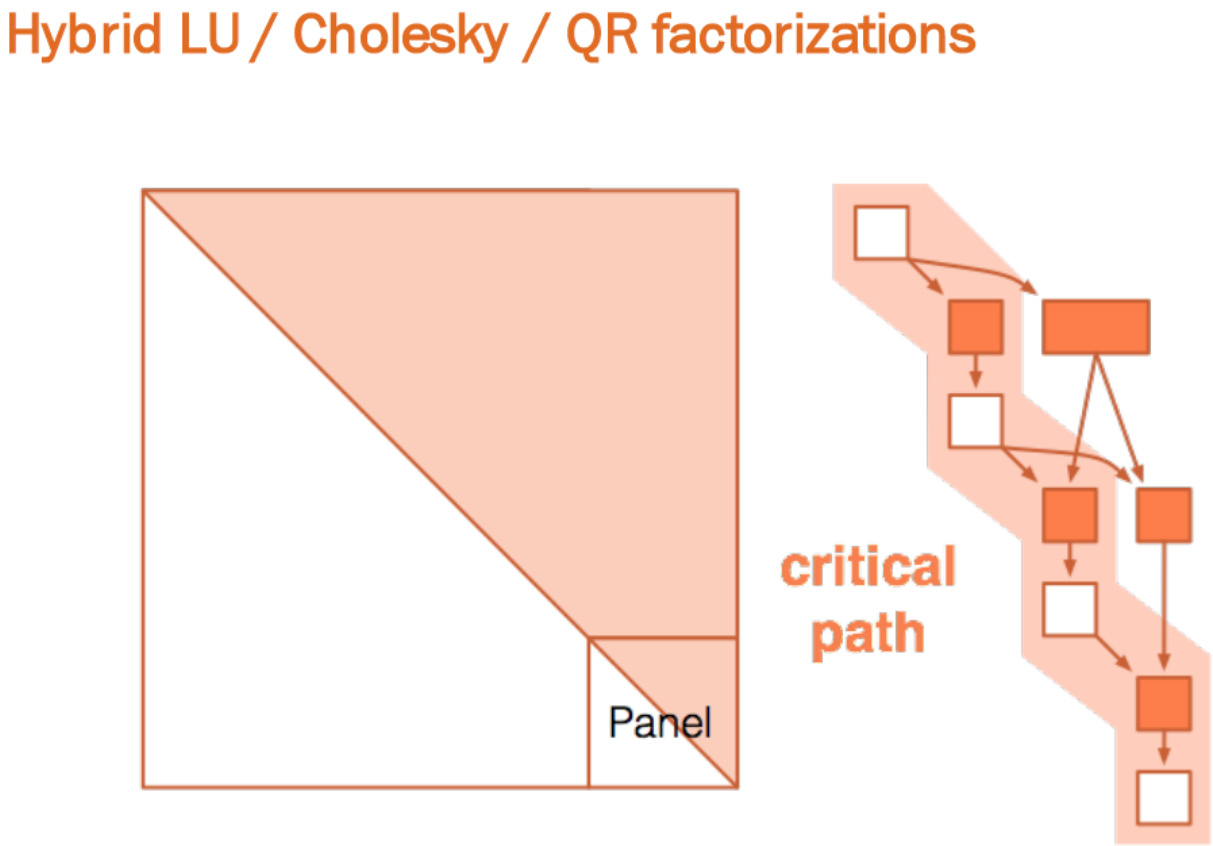
- nodes are computational tasks performed in kernel subroutines;
- edges represent the dependencies among the tasks.

Given a DAG, tasks are scheduled asynchronously and independently, considering the dependencies imposed by the edges in the DAG.

A critical path in the DAG connects those nodes that have the highest number of outgoing edges.

The scheduling policy assigns higher priority to those tasks that lie on the critical path.

copied from tutorial slides



From ISC High Performance 2017, Frankfurt
Tutorial 03: Linear Algebra Software for High Performance Computing
Hartwig Anzt

running example_cposv

Adjusted dimensions:

```
int cores = 2;
int N     = 10000;
int LDA   = 10000;
int NRHS  = 5;
int LDB   = 10000;
```

Cholesky factorization with the dimension equal to 10,000.

```
$ time ./example_cposv
-- PLASMA is initialized to run on 2 cores.
============
Checking the Residual of the solution
-- ||Ax-B||_oo/((||A||_oo||x||_oo+||B||_oo).N.eps) = 2.846077e-03
-- The solution is CORRECT !
-- Run of CPOSV example successful !

real 2m48.451s
user 5m29.606s
sys 0m2.830s
$
```

checking the speedups

The wall clock times for Cholesky on dimension 10,000:

#cores	real time	speedup
1	2m 40.913s	
2	1m 22.271s	1.96
4	42.621s	3.78
8	23.480s	6.85
16	12.647s	12.72

Ran on two 8-core Intel Xeon E5-2670 Sandy Bridge at 2.60GHz, 128GB of internal memory at 1600MHz.

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the cuSOLVER library

The cuSOLVER library is a high level package

- based on cuBLAS and cuSPARSE,
- offering two APIs: for single and multiple GPUs.

The cuSolverDN is for dense matrices,
while cuSolverSP is for sparse matrices.

Offers solvers for eigenvalue problems and
singular value decompositions can be computed.

a sample from the CUDA Libraries

The folder `cuSolverDn_LinearSolver` in
`/usr/local/cuda/samples/7_CUDALibraries/`
has an example that demonstrates cuSolverDN's LU, QR,
and Cholesky factorization.

The example solves $A\mathbf{x} = \mathbf{b}$, where $\mathbf{b}$ is a vector of ones.

The matrix A comes from the Florida Sparse Matrix Collection,
at `http://www.cise.ufl.edu/research/sparse/matrices`.

running on the V100 gpu

```
$ ./cuSolverDn_LinearSolver
GPU Device 0: "Quadro GV100" with compute capability 7.0

step 1: read matrix market format
Using default input file [./gr_900_900_crg.mtx]
sparse matrix A is 900 x 900 with 7744 nonzeros, base=1
step 2: convert CSR(A) to dense matrix
step 3: set right hand side vector (b) to 1
step 4: prepare data on device
step 5: solve A*x = b
timing: cholesky =   0.001399 sec
step 6: evaluate residual
|b - A*x| = 1.136868E-13
|A| = 1.600000E+01
|x| = 2.357708E+01
|b - A*x|/(|A|*|x|) = 3.013701E-16
$
```

suggested reading

- E. Agullo, J. Dongarra, B. Hadri, J. Kurzak, J. Langou, J. Langou, H. Ltaief, P. Luszczek, and A. YarKhan. **PLASMA Users' Guide. Parallel Linear Algebra Software for Multicore Architectures. Version 2.0**.
- A. Buttari, J. Langou, J. Kurzak, and J. Dongarra. **A class of parallel tiled linear algebra algorithms for multicore architectures.** *Parallel Computing* 35: 38-53, 2009.
- V. Volkov and J. W. Demmel. **Benchmarking GPUs to tune dense linear algebra.** In *Proceedings of the 2008 ACM/IEEE conference on Supercomputing*. IEEE Press, 2008. Article No. 31.

Summary + Exercises

In Wilkinson and Allen, parallel linear system solving is in §11.3.2.

Exercises:

1. Write your own parallel shared memory version of the Cholesky factorization, using OpenMP, Pthreads, or the Intel TBB.
2. Derive right looking LU factorization formulas with pivoting, i.e.: introducing permutation matrices P. Develop first the formulas for a 3-by-3 block matrix and then generalize the formulas into an algorithm for any p-by-p block matrix.
3. Take an appropriate example from the PLASMA installation to test the speedup of the multicore LU factorization routines.