Parallel Numerical Algorithms

Chapter 6 – LU Factorization

Prof. Michael T. Heath

Department of Computer Science
University of Illinois at Urbana-Champaign

CS 554 / CSE 512

Outline

LU Factorization

- System of linear algebraic equations has form

$$\boldsymbol{Ax} = \boldsymbol{b}$$

  where $\boldsymbol{A}$ is given $n \times n$ matrix, $\boldsymbol{b}$ is given n-vector, and $\boldsymbol{x}$ is unknown solution n-vector to be computed

- Direct method for solving general linear system is by computing *LU factorization*

$$\boldsymbol{A} = \boldsymbol{LU}$$

  where $\boldsymbol{L}$ is unit lower triangular and $\boldsymbol{U}$ is upper triangular

LU Factorization

- System $\boldsymbol{Ax} = \boldsymbol{b}$ then becomes

$$\boldsymbol{LUx} = \boldsymbol{b}$$

- Solve lower triangular system

$$\boldsymbol{Ly} = \boldsymbol{b}$$

  by forward-substitution to obtain vector $\boldsymbol{y}$

- Finally, solve upper triangular system

$$\boldsymbol{Ux} = \boldsymbol{y}$$

  by back-substitution to obtain solution $\boldsymbol{x}$ to original system

Gaussian Elimination Algorithm

LU factorization can be computed by Gaussian elimination as follows, where $\boldsymbol{U}$ overwrites $\boldsymbol{A}$

for $k = 1$ **to** $n - 1$ { loop over columns }
    for $i = k + 1$ **to** n { compute multipliers for current column }
        $\ell_{ik} = a_{ik}/a_{kk}$
    end
    for $j = k + 1$ **to** n
        for $i = k + 1$ **to** n { apply transformation to remaining submatrix }
            $a_{ij} = a_{ij} - \ell_{ik} a_{kj}$
        end
    end
end

Gaussian Elimination Algorithm

- In general, row interchanges (pivoting) may be required to ensure existence of LU factorization and numerical stability of Gaussian elimination algorithm, but for simplicity we temporarily ignore this issue
- Gaussian elimination requires about $n^3/3$ paired additions and multiplications, so model serial time as

$$T_1 = t_c\, n^3/3$$

where t_c is time required for multiply-add operation

- About $n^2/2$ divisions also required, but we ignore this lower-order term

Loop Orderings for Gaussian Elimination

- Gaussian elimination has general form of triple-nested loop in which entries of $\boldsymbol{L}$ and $\boldsymbol{U}$ overwrite those of $\boldsymbol{A}$

for ____________
    for ____________
        for ____________
            $a_{ij} = a_{ij} - (a_{ik}/a_{kk})\, a_{kj}$
        end
    end
end

- Indices i, j, and k of **for** loops can be taken in any order, for total of $3! = 6$ different ways of arranging loops

Loop Orderings for Gaussian Elimination

- Different loop orders have different memory access patterns, which may cause their performance to vary widely, depending on architectural features such as cache, paging, vector registers, etc.
- Perhaps most promising for parallel implementation are kij and kji forms, which differ only in accessing matrix by rows or columns, respectively

Gaussian Elimination Algorithm

- kji form of Gaussian elimination

for $k = 1$ **to** $n - 1$
    for $i = k + 1$ **to** n
        $\ell_{ik} = a_{ik} / a_{kk}$
    end
    for $j = k + 1$ **to** n
        for $i = k + 1$ **to** n
            $a_{ij} = a_{ij} - \ell_{ik}\, a_{kj}$
        end
    end
end

- Multipliers ℓ_{ik} computed outside inner loop for greater efficiency

Parallel Algorithm

Partition

- For $i, j = 1, \ldots, n$, fine-grain task (i, j) stores a_{ij} and computes and stores

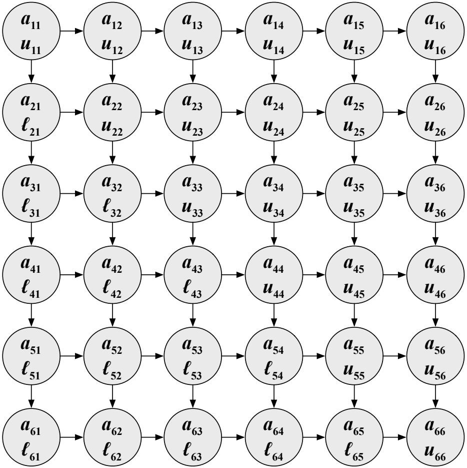
$$\begin{cases} u_{ij}, & \text{if } i \le j \\ \ell_{ij}, & \text{if } i > j \end{cases}$$

yielding 2-D array of n^2 fine-grain tasks

Communicate

- Broadcast entries of A vertically to tasks below
- Broadcast entries of L horizontally to tasks to right

Fine-Grain Tasks and Communication



Fine-Grain Parallel Algorithm

for $k = 1$ **to** $\min(i, j) - 1$
    recv broadcast of a_{kj} from task (k, j) { vert bcast }
    recv broadcast of ℓ_{ik} from task (i, k) { horiz bcast }
    $a_{ij} = a_{ij} - \ell_{ik}\, a_{kj}$ { update entry }
end
if $i \le j$ **then**
    broadcast a_{ij} to tasks (k, j), $k = i + 1, \ldots, n$ { vert bcast }
else
    recv broadcast of a_{jj} from task (j, j) { vert bcast }
    $\ell_{ij} = a_{ij} / a_{jj}$ { multiplier }
    broadcast ℓ_{ij} to tasks (i, k), $k = j + 1, \ldots, n$ { horiz bcast }
end

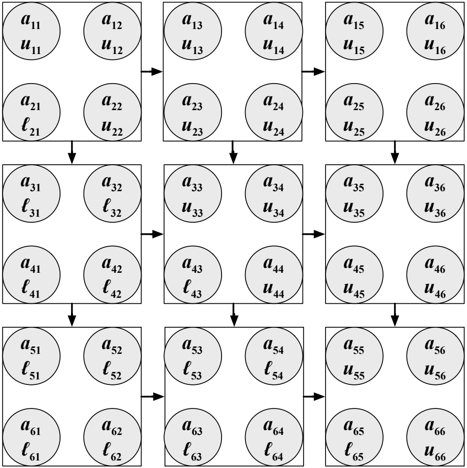
Agglomeration

Agglomerate

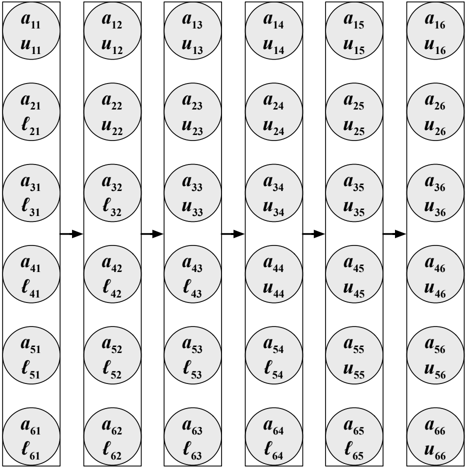
With $n \times n$ array of fine-grain tasks, natural strategies are

- 2-D: combine $k \times k$ subarray of fine-grain tasks to form each coarse-grain task, yielding $(n/k)^2$ coarse-grain tasks
- 1-D column: combine n fine-grain tasks in each column into coarse-grain task, yielding n coarse-grain tasks
- 1-D row: combine n fine-grain tasks in each row into coarse-grain task, yielding n coarse-grain tasks

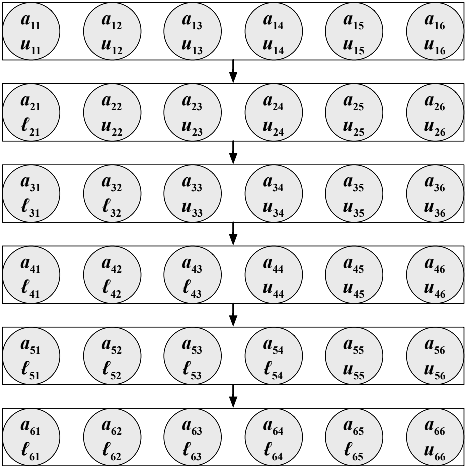
2-D Agglomeration



1-D Column Agglomeration



1-D Row Agglomeration

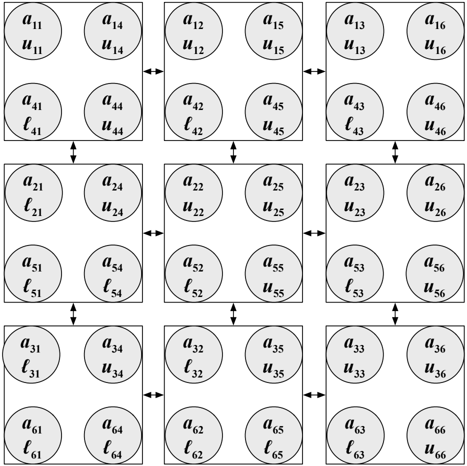


Mapping

Map

- 2-D: assign $(n/k)^2/p$ coarse-grain tasks to each of p processes using any desired mapping in each dimension, treating target network as 2-D mesh
- 1-D: assign n/p coarse-grain tasks to each of p processes using any desired mapping, treating target network as 1-D mesh

2-D Agglomeration with Cyclic Mapping



Coarse-Grain 2-D Parallel Algorithm

for $k = 1$ **to** $n - 1$
  broadcast $\{a_{kj} : \ j \in$ *mycols*, $j \geq k\}$ in process column
  if $k \in$ *mycols* **then**
    for $i \in$ *myrows*, $i > k$
      $\ell_{ik} = a_{ik}/a_{kk}$ { multipliers }
    end
  end
  broadcast $\{\ell_{ik} : \ i \in$ *myrows*, $i > k\}$ in process row
  for $j \in$ *mycols*, $j > k$
    for $i \in$ *myrows*, $i > k$,
      $a_{ij} = a_{ij} - \ell_{ik}\, a_{kj}$ { update }
    end
  end
end

Performance Enhancements

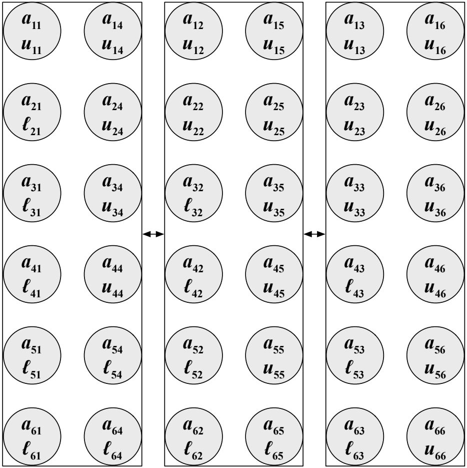
- Each process becomes idle as soon as its last row and column are completed
- With block mapping, in which each process holds contiguous block of rows and columns, some processes become idle long before overall computation is complete
- Block mapping also yields unbalanced load, as computing multipliers and updates requires successively less work with increasing row and column numbers
- Cyclic or reflection mapping improves both concurrency and load balance

Performance Enhancements

Performance can also be enhanced by overlapping communication and computation

- At step k, each process completes updating its portion of remaining unreduced submatrix before moving on to step $k + 1$
- Broadcast of each segment of row $k + 1$, and computation and broadcast of each segment of multipliers for step $k + 1$, could be initiated as soon as relevant segments of row $k + 1$ and column $k + 1$ have been updated by their owners, before completing remainder of their updating for step k
- This *send ahead* strategy enables other processes to start working on next step earlier than they otherwise could

1-D Column Agglomeration with Cyclic Mapping



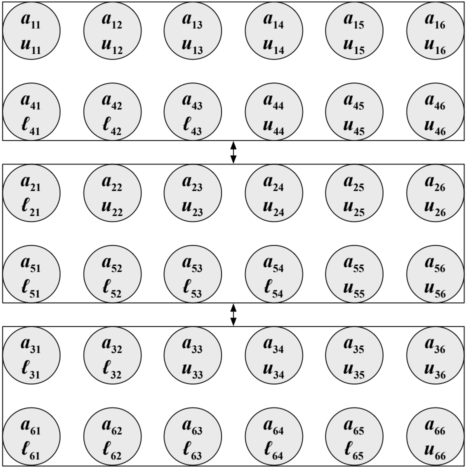
1-D Column Agglomeration

- Matrix rows need not be broadcast vertically, since any given column is contained entirely in only one process
- But there is no parallelism in computing multipliers or updating any given column
- Horizontal broadcasts still required to communicate multipliers for updating

Coarse-Grain 1-D Column Parallel Algorithm

for $k = 1$ **to** $n - 1$
  if $k \in$ *mycols* **then**
    for $i = k + 1$ **to** n
      $\ell_{ik} = a_{ik}/a_{kk}$ { multipliers }
    end
  end
  broadcast $\{\ell_{ik} : k < i \le n\}$ { broadcast }
  for $j \in$ *mycols*, $j > k$
    for $i = k + 1$ **to** n
      $a_{ij} = a_{ij} - \ell_{ik}\, a_{kj}$ { update }
    end
  end
end

1-D Row Agglomeration with Cyclic Mapping



1-D Row Agglomeration

- Multipliers need not be broadcast horizontally, since any given matrix row is contained entirely in only one process
- But there is no parallelism in updating any given row
- Vertical broadcasts still required to communicate each row of matrix to processes below it for updating

Coarse-Grain 1-D Row Parallel Algorithm

```
for k = 1 to n − 1
    broadcast {a_kj : k ≤ j ≤ n}            { broadcast }
    for i ∈ myrows, i > k,
        ℓ_ik = a_ik / a_kk                  { multipliers }
    end
    for j = k + 1 to n
        for i ∈ myrows, i > k,
            a_ij = a_ij − ℓ_ik a_kj         { update }
        end
    end
end
```

Performance Enhancements

- Same performance enhancements as for 2-D agglomeration apply to both 1-D column and 1-D row agglomerations as well, including cyclic mapping and send ahead strategy

Scalability for 2-D Agglomeration

- Updating by each process at step k requires about $(n-k)^2/p$ operations
- Summing over $n-1$ steps

$$\begin{aligned} T_{\text{comp}} &\approx t_c \sum_{k=1}^{n-1} (n-k)^2/p \\ &\approx t_c\, n^3/(3p) \end{aligned}$$

Scalability for 2-D Agglomeration

- Similarly, amount of data broadcast at step k along each process row and column is about $(n-k)/\sqrt{p}$, so on 2-D mesh

$$\begin{aligned} T_{\text{comm}} &\approx \sum_{k=1}^{n-1} 2(t_s + t_w\,(n-k)/\sqrt{p}\,) \\ &\approx 2\,t_s\,n + t_w\,n^2/\sqrt{p} \end{aligned}$$

where we have allowed for overlap of broadcasts for successive steps

Scalability for 2-D Agglomeration

- Total execution time is

$$T_p \approx t_c\, n^3/(3p) + 2\, t_s\, n + t_w\, n^2/\sqrt{p}$$

- To determine isoefficiency function, set

$$t_c\, n^3/3 \approx E\,(t_c\, n^3/3 + 2\, t_s\, n\, p + t_w\, n^2 \sqrt{p}\,)$$

which holds for large p if $n = \Theta(\sqrt{p}\,)$, so isoefficiency function is $\Theta(p\sqrt{p}\,)$, since $T_1 = \Theta(n^3)$

Scalability for 1-D Agglomeration

- With either 1-D column or 1-D row agglomeration, updating by each process at step k requires about $(n-k)^2/p$ operations
- Summing over $n-1$ steps

$$T_{\text{comp}} \approx t_c \sum_{k=1}^{n-1} (n-k)^2/p \approx t_c\, n^3/(3p)$$

Scalability for 1-D Agglomeration

- Amount of data broadcast at step k is about $n-k$, so on 1-D mesh

$$
\begin{aligned}
T_{\text{comm}} &\approx \sum_{k=1}^{n-1} (t_s + t_w\,(n-k)) \\
&\approx t_s\,n + t_w\,n^2/2
\end{aligned}
$$

where we have allowed for overlap of broadcasts for successive steps

Scalability for 1-D Agglomeration

- Total execution time is

$$T_p \approx t_c\, n^3/(3p) + t_s\, n + t_w\, n^2/2$$

- To determine isoefficiency function, set

$$t_c\, n^3/3 \approx E\,(t_c\, n^3/3 + t_s\, n\, p + t_w\, n^2 p/2)$$

  which holds for large p if $n = \Theta(p)$, so isoefficiency function is $\Theta(p^3)$, since $T_1 = \Theta(n^3)$

Partial Pivoting

- Row ordering of A is irrelevant in system of linear equations
- Partial pivoting takes rows in order of largest entry in magnitude of leading column of remaining unreduced matrix
- This choice ensures that multipliers do not exceed 1 in magnitude, which reduces amplification of rounding errors
- In general, partial pivoting is required to ensure existence and numerical stability of LU factorization

Partial Pivoting

- Partial pivoting yields factorization of form

  $$PA = LU$$

  where P is permutation matrix

- If $PA = LU$, then system $Ax = b$ becomes

  $$PAx = LUx = Pb$$

  which can be solved by forward-substitution in lower triangular system $Ly = Pb$, followed by back-substitution in upper triangular system $Ux = y$

Parallel Partial Pivoting

- Partial pivoting complicates parallel implementation of Gaussian elimination and significantly affects potential performance
- With 2-D algorithm, pivot search is parallel but requires communication within process column and inhibits overlapping of successive steps
- With 1-D column algorithm, pivot search requires no communication but is purely serial
- Once pivot is found, index of pivot row must be communicated to other processes, and rows must be explicitly or implicitly interchanged in each process

Parallel Partial Pivoting

- With 1-D row algorithm, pivot search is parallel but requires communication among processes and inhibits overlapping of successive steps
- If rows are explicitly interchanged, then only two processes are involved
- If rows are implicitly interchanged, then mapping of rows to processes is altered, which may degrade concurrency and load balance
- Tradeoff between column and row algorithms with partial pivoting depends on relative speeds of communication and computation

Alternatives to Partial Pivoting

- Because of negative effects of partial pivoting on parallel performance, various alternatives have been proposed that limit pivot search
  - tournament pivoting
  - threshold pivoting
  - pairwise pivoting
- Such strategies are not foolproof and may trade off some degree of stability and accuracy for speed
- Stability and accuracy may be recovered via iterative refinement, but this has its own cost

Communication vs. Memory Tradeoff

- If explicit replication of storage is allowed, then lower communication volume is possible
- As with matrix multiplication, "2.5-D" algorithms have recently been developed that use partial storage replication to reduce communication volume to whatever extent available memory allows
- If sufficient memory is avaiable, then these algorithms can achieve provably optimal communication

References

- J. W. Demmel, M. T. Heath, and H. A. van der Vorst, Parallel numerical linear algebra, *Acta Numerica* 2:111-197, 1993
- G. A. Geist and C. H. Romine, LU factorization algorithms on distributed-memory multiprocessor architectures, *SIAM J. Sci. Stat. Comput.* 9:639-649, 1988
- L. Grigori, J. Demmel, and H. Xiang, CALU: A communication optimal LU factorization algorithm, *SIAM J. Matrix Anal. Appl.* 32:1317-1350, 2011
- B. A. Hendrickson and D. E. Womble, The torus-wrap mapping for dense matrix calculations on massively parallel computers, *SIAM J. Sci. Stat. Comput.* 15:1201-1226, 1994

References

- J. M. Ortega, *Introduction to Parallel and Vector Solution of Linear Systems*, Plenum Press, 1988
- J. M. Ortega and C. H. Romine, The ijk forms of factorization methods II: parallel systems, *Parallel Comput.* 7:149-162, 1988
- Y. Robert, *The Impact of Vector and Parallel Architectures on the Gaussian Elimination Algorithm*, Wiley, 1990
- E. Solomonik and J. Demmel, Communication-optimal parallel 2.5D matrix multiplication and LU factorization algorithms, 17th Euro-Par Conf. on Parallel Processing, LNCS 6853, Springer, 2011
- S. A. Vavasis, Gaussian elimination with pivoting is P-complete, *SIAM J. Disc. Math.* 2:413-423, 1989