### Hybrid Fine Grained ILU

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#### Outline

- Iterative Methods
- Incomplete Factorization
- New Parallel ILU Algorithm
- 4 Hybrid Fine Grained ILU
- Current Project State

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### **Iterative Methods**

- Direct methods for solving Ax = b can be unnecessarily expensive
- Iterative methods are "infinite" solution techniques that requires computation of  $x \to Ax$
- Can sometimes be computationally inefficient if too many iterations are required
- Their convergence can be accelerated by preconditioning

## Preconditioning

$$Ax = b$$
Apply preconditioner
$$C^{-1}Ax = C^{-1}b$$

### Preconditioner

A preconditioner is a matrix C such that:

- $\operatorname{cond}(C^{-1}A) < \operatorname{cond}(A)$
- Solution of linear systems Cz = y requires little computational effort
- That is, computation of  $y \to C^{-1}y$  is "easy"

## Challenges

- If we choose C = I
  - no cost associated with solving linear system Cz = y
  - condition number is the same
- If we choose C = A
  - resulting  $C^{-1}A = I$  perfectly conditioned
  - cost required is equal to that of solving the initial linear system with A itself
- Cost of computing C should be taken into account

### No Perfect Answer!

- Optimal C minimizes total computational effort
- Computational effort depends on:
  - Size of the problem
  - Sparsity pattern of A
  - Spectrum of A
- No general answer about how to choose an optimal C
  - One method is Incomplete Factorization

## Incomplete Factorization

- Given general sparse matrix A, an incomplete LU (ILU) factorization is a pair of matrices:
  - Sparse lower triangular matrix L
  - Sparse upper triangular matrix U

such that  $LU \approx A$ 

- Take preconditioner C = LU. Computing  $C^{-1}y = U^{-1}L^{-1}y$  is simple:
  - Solve Lw = y by forward substitution
  - Solve Uv = w by backward substitution

## This paper

- New fine-grained parallel algorithm for ILU factorization
- Computes all nonzero elements in parallel
- Iteratively improves the accuracy of the factorization
- Provides large amounts of parallelism using shared memory

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# Computing Incomplete Factorization

- Given general sparse matrix A, an incomplete LU (ILU) factorization computes:
  - Sparse lower triangular matrix L
  - Sparse upper triangular matrix U

such that  $LU \approx A$ 

- Use Gaussian elimination process but only allow nonzeros in specified locations of L and U
- Define sparsity pattern S such that  $(i,j) \in S$  if:
  - $I_{ij}$  is permitted to be nonzero when  $i \ge j$
  - $u_{ij}$  is permitted to be nonzero when  $i \leq j$

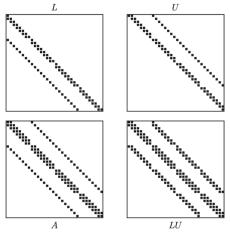
## Incomplete Factorization

#### Algorithm 1 Conventional ILU Factorization

```
1: for i = 2 to n do
2: for k = 1 to i - 1 and (i, k) \in S do
3: a_{ij} = a_{ik}/a_{kk}
4: for j = k + 1 to n and (i, j) \in S do
5: a_{ij} = a_{ij} - a_{ik}a_{kj}
6: end for
7: end for
8: end for
```

## Example: Zero fill-in ILU (ILU(0))

Take S exactly as the sparsity pattern of A



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## New Parallel ILU Algorithm

- Parallelism is very fine-grained
- Individual entries of the factorization can be computed in parallel, using an iterative algorithm

#### Reformulation of ILU

 New algorithm based on the sometimes overlooked property that:

$$(LU)_{ij}=a_{ij}, \qquad (i,j)\in S \tag{1}$$

where  $(LU)_{ij}$  is the (i,j) entry of the ILU factorization of the matrix with entries  $a_{ii}$ 

• i.e. factorization is exact on the sparsity pattern S

### Reformulation of ILU

- New fine-grained algorithm interprets an ILU factorization as a problem of computing unknowns
  - $I_{ii}$  , i > j ,  $(i,j) \in S$
  - $u_{ij}$  ,  $i \leq j$  ,  $(i,j) \in S$

using property (1) as constraint.

 ⇒ total number of unknowns is n<sub>S</sub> = |S|, the number of elements in the sparsity pattern S

#### Reformulation of ILU

• To find these  $n_S$  unknowns, rewrite constraints (1) as:

$$\sum_{k=1}^{\min(i,j)} I_{ik} u_{kj} = a_{ij}, \quad (i,j) \in S$$
 (2)

- Each constraint can be associated with an element in S ⇒ there are n<sub>S</sub> constraints
- Thus problem of solving for n<sub>S</sub> unknowns using n<sub>S</sub> nonlinear equations

## Solution of constraint equations

 Write explicit formula for each unknown in terms of the other unknowns:

$$I_{ij} = \frac{1}{u_{jj}} \left( a_{ij} - \sum_{k=1}^{j-1} I_{ik} u_{kj} \right), \quad \text{if } i > j$$
 (3)

$$u_{ij} = a_{ij} - \sum_{k=1}^{i-1} l_{ik} u_{kj}, \quad \text{if } i \leq j$$
 (4)

 Equations are in the form x = G(x) where x is a vector containing the unknowns I<sub>ij</sub> and u<sub>ij</sub>

## Solution of constraint equations

Solve equations via fixed-point iteration:

$$x^{(p+1)} = G(x^{(p)}), \quad p = 0, 1, ...$$
 (5)

with an initial guess  $x^{(0)}$ 

• Each component of new iterate  $x^{(p+1)}$  can be computed in parallel

### **Initial Guess**

- To begin the fixed point iterations, we need an initial guess for the unknowns
- Simple initial guess:

  - $(L^{(0)})_{ij} = (A)_{ij}$  , i > j ,  $(i,j) \in S$   $(U^{(0)})_{ij} = (A)_{ij}$  ,  $i \le j$  ,  $(i,j) \in S$

### **New Parallel ILU**

#### Algorithm 2 Fine-Grained Parallel Incomplete Factorization

```
1: Set unknowns l_{ii} and u_{ii} to initial values
 2: for sweep = 1, 2, ... until convergence do
         for (i, j) \in S, in parallel do
 3:
              if i > i then
 4:
                  I_{ii} = (a_{ii} - \sum_{k=1}^{j-1} I_{ik} u_{ki}) / u_{ii}
 5:
 6:
              else
                  u_{ii} = a_{ii} - \sum_{k=1}^{i-1} I_{ik} u_{ki}
 7:
              end if
 8:
         end for
 9:
10: end for
```

#### **New Parallel ILU**

- Each fixed-point iteration updating all unknowns is called a sweep
- Algorithm parallelized across elements of S
- Given p compute threads, partition set S into p parts, one for each thread
- Threads run in parallel updating the components of the vector of unknowns x, asynchronously

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## **Distributed Memory Implementation**

- To take advantage of available computing resources, algorithm should be adapted to distributed memory systems
- May want to increase problem size, where a matrix may no longer fit in a single node's memory

### Block Jacobi Preconditioner

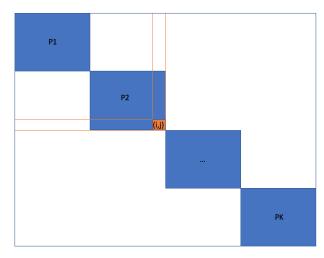
- A simple preconditioner is the diagonal of A, i.e. use  $D = \text{diag}(a_{11}, a_{22}, \dots, a_{nn})$
- Can generalize this if we write A in block format:

$$A = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1K} \\ A_{21} & A_{22} & \cdots & A_{2K} \\ \vdots & \vdots & \ddots & \vdots \\ A_{K1} & A_{K2} & \cdots & A_{KK} \end{bmatrix}$$

• Use the *block diagonal* of *A* as a preconditioner:

$$D = \begin{bmatrix} A_{11} & 0 & \cdots & 0 \\ 0 & A_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & A_{KK} \end{bmatrix}$$

### Block Jacobi - Hybrid Implementation



## **Hybrid Implementation**

- Distribute blocks across processors/nodes
- Compute ILU factorization for each block using OpenMP on each node
- Gather blocks on single processor in order to use preconditioner in iterative method
- Alternatively, could perform iterative method in parallel no need to gather blocks

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### Work so far

- Have finished shared memory ILU implementation using OpenMP
- Have finished PCG (an iterative method) code utilizing forward/backward substitution and matrix multiply routines
- Currently finishing Hybrid Block Jacobi-ILU implementation using MPI across nodes

#### References

- [1] Edmond Chow and Aftab Patel. Fine-grained parallel incomplete lu factorization. *SIAM Journal on Scientific Computing*, 37(2):C169–C193, 2015.
- [2] Yousef Saad. *Iterative methods for sparse linear systems*. SIAM, 2003.