### High Performance Numerical Linear Algebra

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• Dense matrix-vector product

• Sparse matrix-vector product

• Nested dissection

Parallel preconditioners



### **Dense matrix-vector product**



### Parallel matrix-vector product; dense

- Assume a division by block rows
- Every processor p has a set of row indices  $I_p$

Mvp on processor p:

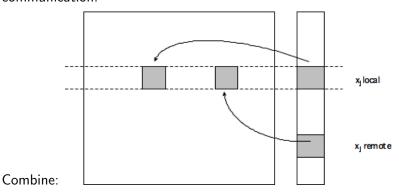
$$\forall_i \colon y_i = \sum_i a_{ij} x_j$$

$$\forall_i \colon y_i = \sum_q \sum_{j \in I_q} a_{ij} x_j$$

#### Local and remote parts:

$$\forall_i \colon y_i = \sum_{j \in I_p} a_{ij} x_j + \sum_{q \neq p} \sum_{j \in I_q} a_{ij} x_j$$

Local part  $I_p$  can be executed right away,  $I_q$  requires communication.





**Input**: Processor number p; the elements  $x_i$  with  $i \in I_p$ ; matrix elements  $A_{ij}$  with  $i \in I_p$ .

**Output**: The elements  $y_i$  with  $i \in I_p$ 

for  $q \neq p$  do

Send elements of x from processor q to p, receive in buffer  $B_{pq}$ .

#### end

$$y_{local} \leftarrow Ax_{local}$$
  
for  $q \neq p$  do  
 $| y_{local} \leftarrow y_{local} + A_{pq}B_q$   
end

**Procedure** Parallel MVP $(A, x_{local}, y_{local}, p)$ 

Note possible overlap communication and computation



# Cost computation 1.

#### Algorithm:

Step	Cost (lower bound)
Allgather $x_i$ so that $x$ is avail-	
able on all nodes	
Locally compute $y_i = A_i x$	$lpha pprox 2rac{n^2}{P}\gamma$



### **Allgather**

Assume that data arrives over a binary tree:

- latency  $\alpha \log_2 P$
- transmission time, receiving n/P elements from P-1 processors



#### Algorithm with cost:

Step	Cost (lower bound)
Allgather $x_i$ so that $x$ is avail-	
able on all nodes	$\log_2(P)\alpha + n\beta$
Locally compute $y_i = A_i x$	$pprox 2rac{n^2}{P}\gamma$



## Parallel efficiency

$$E_p^{\text{1D-row}}(n) = \frac{S_p^{\text{1D-row}}(n)}{p} = \frac{1}{1 + \frac{p \log_2(p)}{2n^2} \frac{\alpha}{\gamma} + \frac{p}{2n} \frac{\beta}{\gamma}}.$$

Strong scaling, weak scaling?



## Two-dimensional partitioning

			<i>x</i> <sub>3</sub>				<i>x</i> <sub>6</sub>				X9	
a <sub>01</sub>	a <sub>02</sub>	<i>y</i> 0	a <sub>03</sub>	a <sub>04</sub>	a <sub>05</sub>		a <sub>06</sub>	a <sub>07</sub>	a <sub>08</sub>		a <sub>09</sub>	ao
a <sub>11</sub>	a <sub>12</sub>		a <sub>13</sub>	a <sub>14</sub>	a <sub>15</sub>	<i>y</i> 1	a <sub>16</sub>	a <sub>17</sub>	a <sub>18</sub>		a <sub>19</sub>	$a_1$
a <sub>21</sub>	a <sub>22</sub>		a <sub>23</sub>	a <sub>24</sub>	a <sub>25</sub>		a <sub>26</sub>	a <sub>27</sub>	a <sub>28</sub>	$y_2$	a <sub>29</sub>	$a_2$
a <sub>31</sub>	a <sub>32</sub>		a <sub>33</sub>	a <sub>34</sub>	a <sub>35</sub>		a <sub>37</sub>	a <sub>37</sub>	a <sub>38</sub>		a39	a <sub>3</sub>
<i>x</i> <sub>1</sub>				<i>x</i> <sub>4</sub>				<i>x</i> <sub>7</sub>				X
a <sub>41</sub>	a <sub>42</sub>	<i>y</i> 4	a43	a44	a <sub>45</sub>		a46	a47	a <sub>48</sub>		a49	a4
a <sub>51</sub>	a <sub>52</sub>		a <sub>53</sub>	a <sub>54</sub>	a55	<i>y</i> 5	a <sub>56</sub>	a <sub>57</sub>	a <sub>58</sub>		a59	a <sub>5</sub>
a <sub>61</sub>	a <sub>62</sub>		a <sub>63</sub>	a <sub>64</sub>	a <sub>65</sub>		a <sub>66</sub>	a <sub>67</sub>	a <sub>68</sub>	<i>y</i> <sub>6</sub>	a <sub>69</sub>	a <sub>6</sub>
a <sub>71</sub>	a <sub>72</sub>		a <sub>73</sub>	a <sub>74</sub>	a <sub>75</sub>		a <sub>77</sub>	a <sub>77</sub>	a <sub>78</sub>		a <sub>79</sub>	a <sub>7</sub>
	<i>x</i> <sub>2</sub>				<i>x</i> <sub>5</sub>				<i>x</i> <sub>8</sub>			
a <sub>81</sub>	a <sub>82</sub>	<i>y</i> 8	a <sub>83</sub>	a <sub>84</sub>	a <sub>85</sub>		a <sub>86</sub>	a <sub>87</sub>	a <sub>88</sub>		a <sub>89</sub>	a <sub>8</sub>
a <sub>91</sub>	a <sub>92</sub>		a93	a94	a95	<i>y</i> 9	a <sub>96</sub>	a97	a98		a99	ag
$a_{10,1}$	a <sub>10,2</sub>		a <sub>10,3</sub>	a <sub>10,4</sub>	a <sub>10,5</sub>		a <sub>10,6</sub>	a <sub>10,7</sub>	a <sub>10,8</sub>	<i>y</i> 10	a <sub>10,9</sub>	a <sub>10</sub>
a <sub>11,1</sub>	a <sub>11,2</sub>		a <sub>11,3</sub>	a <sub>11,4</sub>	a <sub>11,5</sub>		a <sub>11,7</sub>	a <sub>11,7</sub>	a <sub>11,8</sub>		a <sub>11,9</sub>	a <sub>1</sub> :
	a <sub>11</sub> a <sub>21</sub> a <sub>31</sub> x <sub>1</sub> a <sub>41</sub> a <sub>51</sub> a <sub>61</sub> a <sub>71</sub> a <sub>81</sub> a <sub>91</sub> a <sub>10,1</sub>	a11         a12           a21         a22           a31         a32           X1         a41         a42           a51         a52           a61         a62         a71         a72           x2         a81         a82           a91         a92         a10,1         a10,2	a11         a12           a21         a22           a31         a32           X1         a41           a51         a52           a61         a62           a71         a72           x2         a81         a82         y8           a91         a92           a10,1         a10,2	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	a01         a02         y0         a03         a04           a11         a12         a13         a14           a21         a22         a23         a24           a31         a32         a33         a34           x1         x4         x4         x4           a51         a52         a53         a54           a61         a62         a63         a64           a71         a72         a73         a74           x2         a81         a82         y8         a83         a84           a91         a92         a93         a94         a91         a93         a94           a10,1         a10,2         a10,3         a10,4         a10,4         a10,3         a10,4	a01         a02         y0         a03         a04         a05           a11         a12         a13         a14         a15         a25         a23         a24         a25           a31         a32         a33         a34         a35           x1         x4         x4         x4         a45           a51         a52         a53         a54         a55           a61         a62         a63         a64         a65           a71         a72         a73         a74         a75           x2         x8         a83         a84         a85           a91         a92         a93         a94         a95           a10,1         a10,2         a10,3         a10,4         a10,4         a10,5	a01         a02         y0         a03         a04         a05           a11         a12         a13         a14         a15         y1           a21         a22         a23         a24         a25           a31         a32         a33         a34         a35           x1         x4         x4         x4           a51         a52         a53         a54         a55         y5           a61         a62         a63         a64         a65         a5           a71         a72         a73         a74         a75           x2         x5         x5         x6         a85         a91         a92         a93         a94         a95         y9         a10,1         a10,2         a10,3         a10,4         a10,5         a10,5         a10,5         a10,5         a10,3         a10,4         a10,5         a10,5         a10,3         a10,4         a10,5         a26         a26         a26         a26         a26         a26         a26         a26 <td>a01         a02         y0         a03         a04         a05         a06           a11         a12         a13         a14         a15         y1         a16           a21         a22         a23         a24         a25         a26           a31         a32         a33         a34         a35         a37           X1         X4         X4         A45         A46           a51         a52         a53         a54         a55         y5         a56           a61         a62         a63         a64         a65         a66         a66           a71         a72         a73         a74         a75         a77           X2         X8         a83         a84         a85         a86           a91         a92         a93         a94         a95         y9         a96           a10,1         a10,2         a10,3         a10,4         a10,5         b10,6         a10,6</td> <td>a01         a02         y0         a03         a04         a05         a06         a07           a11         a12         a13         a14         a15         y1         a16         a17           a21         a22         a23         a24         a25         a26         a27         a37         a37           x1         x4         x4         x4         x7         x6         a46         a47           a51         a52         a53         a54         a55         y5         a56         a57           a61         a62         a63         a64         a65         a66         a67           a71         a72         a73         a74         a75         a77         a77         a77           x2         x2         x8         a83         a84         a85         a66         a86         a87           a91         a92         a93         a94         a95         y9         a96         a97           a10,1         a10,2         a10,3         a10,4         a10,5         a10,6         a10,7</td> <td>a01         a02         y0         a03         a04         a05         a06         a07         a08           a11         a12         a13         a14         a15         y1         a16         a17         a18           a21         a22         a23         a24         a25         a26         a27         a28           x1         x4         x4         x7         x7           a41         a42         y4         a43         a44         a45         a46         a47         a48           a51         a52         a53         a54         a55         y5         a56         a57         a58           a61         a62         a63         a64         a65         a66         a67         a68           a71         a72         a73         a74         a75         a77         a77         a78           x2         x3         a84         a85         a86         a86         a87         a88           a71         a72         a73         a34         a35         a94         a95         a9         a96         a97         a78           x2         x3         a88         a88         <td< td=""><td>a01         a02         y0         a03         a04         a05         a06         a07         a08           a11         a12         a13         a14         a15         y1         a16         a17         a18           a21         a22         a23         a24         a25         a26         a27         a28         y2           a31         a32         a33         a34         a35         a37         a37         a38         x           x1         x4         x4         x5         x7         x         x         x         x         x         x         a46         a47         a48         a48         a53         a54         a55         y5         a56         a57         a58         a6         a57         a58         a6         a67         a68         y6         a67         a68         y6</td><td>a01         a02         y0         a03         a04         a05         a06         a07         a08         a09           a11         a12         a13         a14         a15         y1         a16         a17         a18         a19           a21         a22         a23         a24         a25         a26         a26         a27         a28         y2         a29           a31         a32         a33         a34         a35         a37         a37         a38         y2         a29           a21         a22         a23         a24         a25         a26         a27         a28         y2         a29           a31         a22         a23         a24         a25         a26         a27         a28         y2         a29           a31         a32         x4         a25         a36         a37         a37         a38         x8         a49           a51         a52         a53         a54         a55         y5         a56         a57         a58         a68         a49           a61         a62         a63         a64         a65         a66         a57         a58</td></td<></td>	a01         a02         y0         a03         a04         a05         a06           a11         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 a24         a25         a26         a27         a37         a37           x1         x4         x4         x4         x7         x6         a46         a47           a51         a52         a53         a54         a55         y5         a56         a57           a61         a62         a63         a64         a65         a66         a67           a71         a72         a73         a74         a75         a77         a77         a77           x2         x2         x8         a83         a84         a85         a66         a86         a87           a91         a92         a93         a94         a95         y9         a96         a97           a10,1         a10,2         a10,3         a10,4         a10,5         a10,6         a10,7	a01         a02         y0         a03         a04         a05         a06         a07         a08           a11         a12         a13         a14         a15         y1         a16         a17         a18           a21         a22         a23         a24         a25         a26         a27         a28           x1         x4         x4         x7         x7           a41         a42         y4         a43         a44         a45         a46         a47         a48           a51         a52         a53         a54         a55         y5         a56         a57         a58           a61         a62         a63         a64         a65         a66         a67         a68           a71         a72         a73         a74         a75         a77         a77         a78           x2         x3         a84         a85         a86         a86         a87         a88           a71         a72         a73         a34         a35         a94         a95         a9         a96         a97         a78           x2         x3         a88         a88 <td< td=""><td>a01         a02         y0         a03         a04         a05         a06         a07         a08           a11         a12         a13         a14         a15         y1         a16        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    a33         a34         a35         a37         a37         a38         y2         a29           a21         a22         a23         a24         a25         a26         a27         a28         y2         a29           a31         a22         a23         a24         a25         a26         a27         a28         y2         a29           a31         a32         x4         a25         a36         a37         a37         a38         x8         a49           a51         a52         a53         a54         a55         y5         a56         a57         a58         a68         a49           a61         a62         a63         a64         a65         a66         a57         a58</td></td<>	a01         a02         y0         a03         a04         a05         a06         a07         a08           a11         a12         a13         a14         a15         y1         a16         a17         a18           a21         a22         a23         a24         a25         a26         a27         a28         y2           a31         a32         a33         a34         a35         a37         a37         a38         x           x1         x4         x4         x5         x7         x         x         x         x         x         x         a46         a47         a48         a48         a53         a54         a55         y5         a56         a57         a58         a6         a57         a58         a6         a67         a68         y6         a67         a68         y6	a01         a02         y0         a03         a04         a05         a06         a07         a08         a09           a11         a12         a13         a14         a15         y1         a16         a17         a18         a19           a21         a22         a23         a24         a25         a26         a26         a27         a28         y2         a29           a31         a32         a33         a34         a35         a37         a37         a38         y2         a29           a21         a22         a23         a24         a25         a26         a27         a28         y2         a29           a31         a22         a23         a24         a25         a26         a27         a28         y2         a29           a31         a32         x4         a25         a36         a37         a37         a38         x8         a49           a51         a52         a53         a54         a55         y5         a56         a57         a58         a68         a49           a61         a62         a63         a64         a65         a66         a57         a58



### Algorithm

- Collecting x<sub>j</sub> on each processor p<sub>ij</sub> by an allgather inside the processor columns.
- Each processor  $p_{ij}$  then computes  $y_{ij} = A_{ij}x_j$ .
- Gathering together the pieces y<sub>ij</sub> in each processor row to form y<sub>i</sub>, distribute this over the processor row: combine to form a reduce-scatter.
- Setup for the next A or A<sup>t</sup> product



# Analysis 1.

Step	Cost (lower bound)					
Allgather $x_i$ 's within columns	$\lceil \log_2(r) \rceil \alpha + \frac{r-1}{p} n\beta \approx \log_2(r) \alpha + \frac{n}{c} \beta$					
Perform local matrix-vector multiply	$ \log_2(r)\alpha + \frac{1}{c}\rho  \approx 2\frac{n^2}{\rho}\gamma$					
Reduce-scatter $y_i$ 's within rows						



#### Reduce-scatter

	t = 1	t = 2	t=3
$p_0$	$x_0^{(0)}, x_1^{(0)}, x_2^{(0)} \downarrow, x_3^{(0)} \downarrow$	$x_0^{(0:2:2)}, x_1^{(0:2:2)} \downarrow$	$x_0^{(0:3)}$
$p_1$	$x_0^{(1)}, x_1^{(1)}, x_2^{(1)} \downarrow, x_3^{(1)} \downarrow$	$x_0^{(1:3:2)} \uparrow, x_1^{(1:3:2)}$	$x_1^{(0:3)}$
<b>p</b> <sub>2</sub>	$x_0^{(2)} \uparrow, x_1^{(2)} \uparrow, x_2^{(2)}, x_3^{(2)}$	$x_2^{(0:2:2)}, x_3^{(0:2:2)} \downarrow$	$x_2^{(0:3)}$
<b>p</b> <sub>3</sub>	$x_0^{(3)} \uparrow, x_1^{(3)} \uparrow, x_2^{(3)}, x_3^{(3)}$	$x_0^{(1:3:2)} \uparrow, x_1^{(1:3:2)}$	$x_3^{(0:3)}$

Time:

$$\lceil \log_2 p \rceil \alpha + \frac{p-1}{p} n(\beta + \gamma).$$



Step	Cost (lower bound)				
Allgather $x_i$ 's within columns	$\lceil \log_2(r) \rceil \alpha + \frac{r-1}{p} n\beta \approx \rceil$				
	$\log_2(r)\alpha + \frac{n}{c}\beta$				
Perform local matrix-vector multiply	$ \lceil \log_2(r) \rceil \alpha + \frac{r-1}{p} n\beta \approx \log_2(r) \alpha + \frac{n}{c} \beta \\ \approx 2 \frac{n^2}{p} \gamma $				
Reduce-scatter $y_i$ 's within rows	$ \lceil \log_2(c) \rceil \alpha + \frac{c-1}{p} n\beta + \frac{c-1}{p} n\gamma \approx                                  $				



## **Efficiency**

$$E_p^{\sqrt{p}\times\sqrt{p}}(n) = \frac{1}{1 + \frac{p\log_2(p)}{2n^2}\frac{\alpha}{\gamma} + \frac{\sqrt{p}}{2n}\frac{(2\beta + \gamma)}{\gamma}}$$

Weak scaling: for  $p \to \infty$  this is  $\approx 1/\log_2 P$ : only slowly decreasing.



# LU factorization scaling

Needs a cyclic distribution

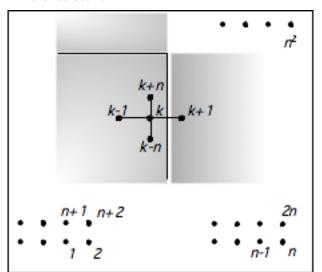


### **Sparse matrix-vector product**



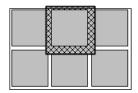
## **Sparse matrix-vector product**

Difference stencil





#### induces ghost region:



Limited number of neighbours, limited buffer space



# **Scaling**

Separately 1D and 2D partitioning of the domain.



#### **Nested dissection**



### Fill-in during LU

Fill-in: index (i,j) where  $a_{ij} = 0$  but  $\ell_{ij} \neq 0$  or  $u_{ij} \neq 0$ .

2D BVP:  $\Omega$  is  $n \times n$ , gives matrix of size  $N = n^2$ , with bandwidth n.

Matrix storage O(N)

LU storage  $O(N^{3/2})$ 

LU factorization work  $O(N^2)$ 

Cute fact: storage can be computed linear in #nonzeros



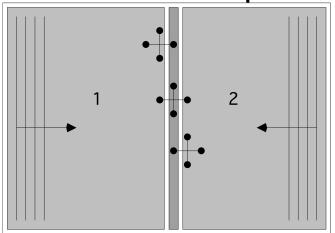
## Fill-in is a function of ordering

$$\begin{pmatrix} * & * & \cdots & * \\ * & * & & \emptyset \\ \vdots & & \ddots & \\ * & \emptyset & & * \end{pmatrix}$$

After factorization the matrix is dense. Can this be permuted?



**Domain decomposition** 



3



1	/ *	*									0 \	١,	
1	*	*	*								:		
		٠	٠	٠				Ø			:	}	$(n^2 - n)/2$
١			*	*	*						0		
١				*	*						*	l Į	
١						*	*				0	1 1	
						*	*	*			:		$(n^2 - n)/2$
١			Ø				•	٠.	٠.		:		
1								*	*	*	0	l J	
									*	*	*	}	n
١	0			0	*	0	• • •		0	*	* /	/	



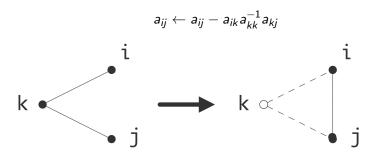
### **DD** factorization

$$A^{\text{DD}} = \begin{pmatrix} A_{11} & \emptyset & A_{13} \\ \emptyset & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} = \begin{pmatrix} I & & & & \\ \emptyset & I & & & \\ A_{31}A_{11}^{-1} & A_{32}A_{22}^{-1} & I \end{pmatrix} \begin{pmatrix} A_{11} & \emptyset & A_{13} \\ & A_{22} & A_{23} \\ & & S \end{pmatrix}$$
$$S = A_{33} - A_{31}A_{11}^{-1}A_{13} - A_{32}A_{22}^{-1}A_{23}$$

Parallelism. . .

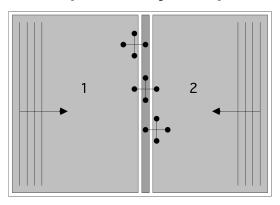


## **Graph theory of sparse elimination**





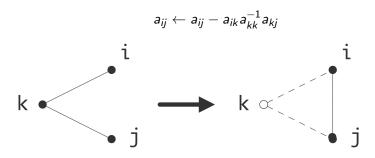
## Graph theory of sparse elimination



3



## **Graph theory of sparse elimination**



So inductively S is dense



### **Recursive bisection**

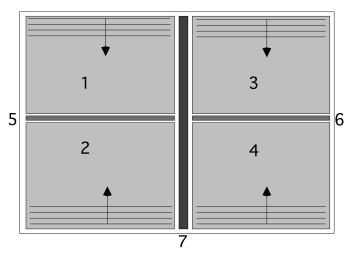


Figure: A four-way domain decomposition

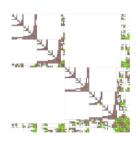


$$A^{\mathrm{DD}} = \left( \begin{array}{ccccccc} A_{11} & & & & A_{15} & & A_{17} \\ & A_{22} & & & A_{25} & & A_{27} \\ & & A_{33} & & & A_{36} & A_{37} \\ & & & A_{44} & & A_{46} & A_{47} \\ A_{51} & A_{52} & & & A_{55} & & A_{57} \\ & & A_{63} & A_{64} & & A_{66} & A_{67} \\ A_{71} & A_{72} & A_{73} & A_{74} & A_{75} & A_{76} & A_{77} \end{array} \right)$$

The domain/operator/graph view is more insightful, don't you think?



## How does this look in reality?





### Complexity

#### With $n = \sqrt{N}$ :

- one dense matrix on a separator of size n, plus
- two dense matrices on separators of size n/2
- $\rightarrow 3/2 \, n^2$  space and  $5/12 \, n^3$  time
- and then four times the above with  $n \to n/2$

space = 
$$3/2n^2 + 4 \cdot 3/2(n/2)^2 + \cdots$$
  
=  $N(3/2 + 3/2 + \cdots)$  log  $n$  terms  
=  $O(N \log N)$   
time =  $5/12n^3/3 + 4 \cdot 5/12(n/2)^3/3 + \cdots$   
=  $5/12N^{3/2}(1 + 1/4 + 1/16 + \cdots)$   
=  $O(N^{3/2})$ 

### More direct factorizations

Minimum degree, multifrontal,...

Finding good separators and domain decompositions is tough in general.



### Parallel preconditioners



## Sparse operations in parallel: mvp

```
Mvp y = Ax

for i=1..n
   y[i] = sum over j=1..n a[i,j]*x[j]

In parallel:

for i=myfirstrow..mylastrow
   y[i] = sum over j=1..n a[i,j]*x[j]
```



#### How about ILU solve?

```
Consider Lx = y
```

```
for i=1..n x[i] = (y[i] - sum over j=1..i-1 ell[i,j]*x[j]) / a[i,i]
```

#### Parallel code:

```
for i=myfirstrow..mylastrow
  x[i] = (y[i] - sum over j=1..i-1 ell[i,j]*x[j])
     / a[i,i]
```

#### Problems?



### **Block method**

```
for i=myfirstrow..mylastrow
  x[i] = (y[i] - sum over j=myfirstrow..i-1 ell[i,j]*x[j]
      / a[i,i]
```

Block Jacobi with local GS solve



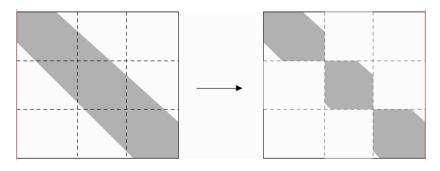


Figure: Sparsity pattern corresponding to a block Jacobi preconditioner



### Multicolour ILU

