

# Iterative solution of linear systems

Victor Eijkhout

Fall 2019

# Justification

As an alternative to Gaussian elimination, iterative methods can be an efficient way to solve the linear system from PDEs. We discuss basic iterative methods and the notion of preconditioning.

## Two different approaches

Solve  $Ax = b$

Direct methods:

- Deterministic
- Exact up to machine precision
- Expensive (in time and space)

Iterative methods:

- Only approximate
- Cheaper in space and (possibly) time
- Convergence not guaranteed

# Stationary iteration

# Iterative methods

Choose any  $x_0$  and repeat

$$x^{k+1} = Bx^k + c$$

until  $\|x^{k+1} - x^k\|_2 < \varepsilon$  or until  $\frac{\|x^{k+1} - x^k\|_2}{\|x^k\|} < \varepsilon$

## Example of iterative solution

Example system

$$\begin{pmatrix} 10 & 0 & 1 \\ 1/2 & 7 & 1 \\ 1 & 0 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 21 \\ 9 \\ 8 \end{pmatrix}$$

with solution  $(2, 1, 1)$ .

Suppose you know (physics) that solution components are roughly the same size, and observe the dominant size of the diagonal, then

$$\begin{pmatrix} 10 & & \\ & 7 & \\ & & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 21 \\ 9 \\ 8 \end{pmatrix}$$

might be a good approximation: solution  $(2.1, 9/7, 8/6)$ .

## Iterative example'

Example system

$$\begin{pmatrix} 10 & 0 & 1 \\ 1/2 & 7 & 1 \\ 1 & 0 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 21 \\ 9 \\ 8 \end{pmatrix}$$

with solution  $(2, 1, 1)$ .

Also easy to solve:

$$\begin{pmatrix} 10 & 0 & 1 \\ 1/2 & 7 & 1 \\ 1 & 0 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 21 \\ 9 \\ 8 \end{pmatrix}$$

with solution  $(2.1, 7.95/7, 5.9/6)$ .

# Abstract presentation

- To solve  $Ax = b$ ; too expensive; suppose  $K \approx A$  and solving  $Kx = b$  is possible
- Define  $Kx_0 = b$ , then error correction  $x_0 = x + e_0$ , and  $A(x_0 - e_0) = b$
- so  $Ae_0 = Ax_0 - b = r_0$ ; this is again unsolvable, so
- $K\tilde{e}_0 = r_0$  and  $x_1 = x_0 - \tilde{e}_0$ .
- In one formula:

$$x_1 = x_0 - K^{-1}r_0$$

- now iterate:  $e_1 = x_1 - x$ ,  $Ae_1 = Ax_1 - b = r_1$  et cetera

Iterative scheme:

$$x_{i+1} = x_i - K^{-1}r_i \quad \text{where } r_i = Ax_i - b$$

# Takeaway

Each iteration involves:

- multiplying by  $A$ ,
- solving with  $K$

# Error analysis

- One step

$$r_1 = Ax_1 - b = A(x_0 - \tilde{e}_0) - b \quad (1)$$

$$= r_0 - AK^{-1}r_0 \quad (2)$$

$$= (I - AK^{-1})r_0 \quad (3)$$

- Inductively:  $r_n = (I - AK^{-1})^n r_0$  so  $r_n \downarrow 0$  if  $|\lambda(I - AK^{-1})| < 1$   
Geometric reduction (or amplification!)
- This is ‘stationary iteration’: no dependence on the iteration number. Simple analysis, limited applicability.

# Takeaway

The iteration process does not have a pre-determined number of operations:  
depends *spectral properties* of the matrix.

# Complexity analysis

- Direct solution is  $O(N^3)$   
except sparse, then  $O(N^{5/2})$  or so
- Iterative per iteration cost  $O(N)$  assuming sparsity.
- Number of iterations is complicated function of spectral properties:
  - Stationary iteration #it =  $O(N^2)$
  - Other methods #it =  $O(N)$   
(2nd order only, more for higher order)
  - Multigrid and fast solvers: #it =  $O(\log N)$  or even  $O(1)$

## Choice of $K$

- The closer  $K$  is to  $A$ , the faster convergence.
- Diagonal and lower triangular choice mentioned above: let

$$A = D_A + L_A + U_A$$

be a splitting into diagonal, lower triangular, upper triangular part, then

- Jacobi method:  $K = D_A$  (diagonal part),
- Gauss-Seidel method:  $K = D_A + L_A$  (lower triangle, including diagonal)
- SOR method:  $K = \omega D_A + L_A$

# Computationally

If

$$A = K - N$$

then

$$Ax = b \Rightarrow Kx = Nx + b \Rightarrow Kx_{i+1} = Nx_i + b$$

Equivalent to the above, and you don't actually need to form the residual.

# Jacobi

$$K = D_A$$

Algorithm:

*for*  $k = 1, \dots$  until convergence, do:

*for*  $i = 1 \dots n$ :

$$\begin{aligned} // a_{ii}x_i^{(k+1)} &= \sum_{j \neq i} a_{ij}x_j^{(k)} + b_i \Rightarrow \\ x_i^{(k+1)} &= a_{ii}^{-1}(\sum_{j \neq i} a_{ij}x_j^{(k)} + b_i) \end{aligned}$$

Implementation:

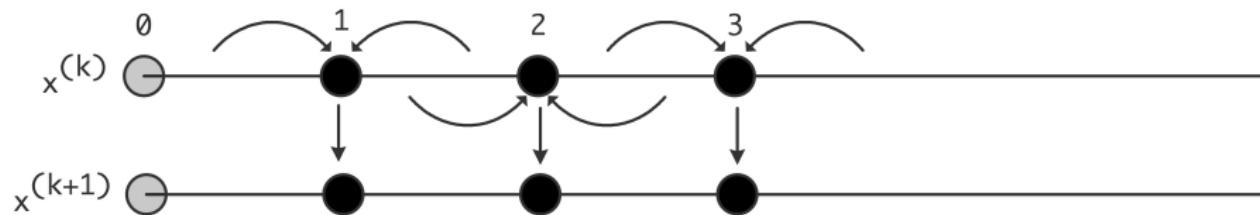
*for*  $k = 1, \dots$  until convergence, do:

*for*  $i = 1 \dots n$ :

$$t_i = a_{ii}^{-1}(-\sum_{j \neq i} a_{ij}x_j + b_i)$$

copy  $x \leftarrow t$

# Jacobi in pictures:



# Gauss-Seidel

$$K = D_A + L_A$$

Algorithm:

*for*  $k = 1, \dots$  until convergence, do:

*for*  $i = 1 \dots n$ :

$$\begin{aligned} // a_{ii}x_i^{(k+1)} + \sum_{j < i} a_{ij}x_j^{(k+1)}) &= \sum_{j > i} a_{ij}x_j^{(k)} + b_i \Rightarrow \\ x_i^{(k+1)} &= a_{ii}^{-1}(-\sum_{j < i} a_{ij}x_j^{(k+1)}) - \sum_{j > i} a_{ij}x_j^{(k)} + b_i \end{aligned}$$

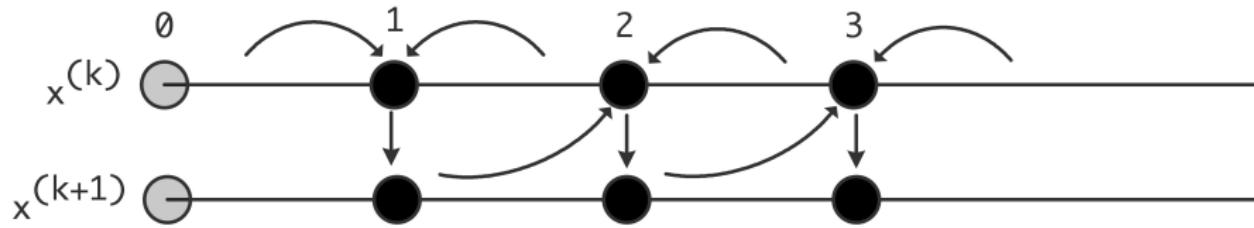
Implementation:

*for*  $k = 1, \dots$  until convergence, do:

*for*  $i = 1 \dots n$ :

$$x_i = a_{ii}^{-1}(-\sum_{j \neq i} a_{ij}x_j + b_i)$$

## GS in pictures:



# Choice of $K$ through incomplete LU

- Inspiration from direct methods: let  $K = LU \approx A$

Gauss elimination:

```
for k,i,j:  
    a[i,j] = a[i,j] - a[i,k] * a[k,j] / a[k,k]
```

Incomplete variant:

```
for k,i,j:  
    if a[i,j] not zero:  
        a[i,j] = a[i,j] - a[i,k] * a[k,j] / a[k,k]
```

$\Rightarrow$  sparsity of  $L + U$  the same as of  $A$

# Applicability

Incomplete factorizations mostly work for M-matrices:  
2nd order FDM and FEM

Can be severe headache for higher order

# Stopping tests

When to stop converging? Can size of the error be guaranteed?

- Direct tests on error  $e_n = x - x_n$  impossible; two choices
- Relative change in the computed solution small:

$$\|x_{n+1} - x_n\| / \|x_n\| < \varepsilon$$

- Residual small enough:

$$\|r_n\| = \|Ax_n - b\| < \varepsilon$$

Without proof: both imply that the error is less than some other  $\varepsilon'$ .

# **Polynomial iterative methods**

# Derivation by hand-waving

- Remember iteration:

$$x_1 = x_0 - K^{-1}r_0, \quad r_0 = Ax_0 - b$$

and conclusion

$$r_n = (I - AK^{-1})^n r_0$$

- Abstract relation between true solution and approximation:

$$x_{\text{true}} = x_{\text{initial}} + K^{-1}\pi(AK^{-1})r_{\text{initial}}$$

- Cayley-Hamilton theorem implies

$$(K^{-1}A)^{-1} = -\pi(K^{-1}A)$$

- inspires us to scheme:

$$x_{i+1} = x_0 + K^{-1}\pi^{(i)}(AK^{-1})r_0$$

Sequence of polynomials of increasing degree

# Residuals

$$x_{i+1} = x_0 + K^{-1}\pi^{(i)}(AK^{-1})r_0$$

Multiply by  $A$  and subtract  $b$ :

$$r_{i+1} = r_0 + \tilde{\pi}^{(i)}(AK^{-1})r_0$$

So:

$$r_i = \hat{\pi}^{(i)}(AK^{-1})r_0$$

where  $\hat{\pi}^{(i)}$  is a polynomial of degree  $i$  with  $\hat{\pi}^{(i)}(0) = 1$ .

⇒ convergence theory

# Computational form

$$x_{i+1} = x_0 + \sum_{j \leq i} K^{-1} r_j \alpha_{ji}.$$

or equivalently:

$$x_{i+1} = x_i + \sum_{j \leq i} K^{-1} r_j \alpha_{ji}.$$

or:

$$\begin{cases} r_i = Ax_i - b \\ x_{i+1}\gamma_{i+1,i} = K^{-1}r_i + \sum_{j \leq i} x_j\gamma_{ji} \\ r_{i+1}\gamma_{i+1,i} = AK^{-1}r_i + \sum_{j \leq i} r_j\gamma_{ji} \end{cases}$$

# Takeaway

Each iteration involves:

- multiplying by  $A$ ,
- solving with  $K$

# Orthogonality

Idea one:

*If you can make all your residuals orthogonal to each other, and the matrix is of dimension  $n$ , then after  $n$  iterations you have to have converged: it is not possible to have an  $n+1$ -st residuals that is orthogonal and nonzero.*

Idea two:

*The sequence of residuals spans a series of subspaces of increasing dimension, and by orthogonalizing the initial residual is projected on these spaces. This means that the errors will have decreasing sizes.*

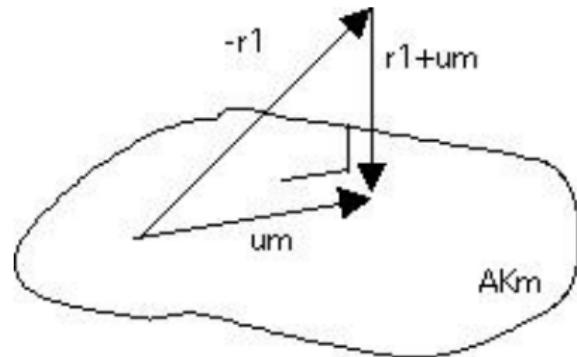
# Minimization

Related concepts:

- Positive definite operator

$$\forall_x: x^t A x > 0$$

- Inner product
- Projection
- Minimization



# Full Orthogonalization Method

Let  $r_0$  be given

For  $i \geq 0$ :

let  $s \leftarrow K^{-1}r_i$

let  $t \leftarrow AK^{-1}r_i$

for  $j \leq i$ :

    let  $\gamma_j$  be the coefficient so that  $t - \gamma_j r_j \perp r_j$

    for  $j \leq i$ :

        form  $s \leftarrow s - \gamma_j x_j$

        and  $t \leftarrow t - \gamma_j r_j$

    let  $x_{i+1} = (\sum_j \gamma_j)^{-1}s$ ,  $r_{i+1} = (\sum_j \gamma_j)^{-1}t$ .

# How do you orthogonalize?

- Given  $x, y$ , can you

$x \leftarrow$  something with  $x, y$

such that  $x \perp y$ ?

(What was that called again in your linear algebra class?)

# How do you orthogonalize?

- Given  $x, y$ , can you

$x \leftarrow$  something with  $x, y$

such that  $x \perp y$ ?

(What was that called again in your linear algebra class?)

- Gramm-Schmid method

# How do you orthogonalize?

- Given  $x, y$ , can you

$x \leftarrow$  something with  $x, y$

such that  $x \perp y$ ?

(What was that called again in your linear algebra class?)

- Gramm-Schmid method
- Update

$$x \leftarrow x - \frac{x^t y}{y^t y} y$$

# Takeaway

Each iteration involves:

- multiplying by  $A$ ,
- solving with  $K$
- inner products!

# Coupled recurrences form

$$x_{i+1} = x_i - \sum_{j \leq i} \alpha_{ji} K^{-1} r_j \quad (4)$$

This equation is often split as

- Update iterate with search direction: direction:

$$x_{i+1} = x_i - \delta_i p_i,$$

- Construct search direction from residuals:

$$p_i = K^{-1} r_i + \sum_{j < i} \beta_{ij} K^{-1} r_j.$$

Inductively:

$$p_i = K^{-1} r_i + \sum_{j < i} \gamma_{ij} p_j,$$

# Conjugate Gradients

Basic idea:

$$r_i^t K^{-1} r_j = 0 \quad \text{if } i \neq j.$$

Split recurrences:

$$\begin{cases} x_{i+1} = x_i - \delta_i p_i \\ r_{i+1} = r_i - \delta_i A p_i \\ p_i = K^{-1} r_i + \sum_{j < i} \gamma_{ij} p_j, \end{cases}$$

Residuals and search directions

## Symmetric Positive Definite case

Three term recurrence is enough:

$$\begin{cases} x_{i+1} = x_i - \delta_i p_i \\ r_{i+1} = r_i - \delta_i A p_i \\ p_{i+1} = K^{-1} r_{i+1} + \gamma_i p_i \end{cases}$$

# Preconditioned Conjugate Gradients

Compute  $r^{(0)} = b - Ax^{(0)}$  for some initial guess  $x^{(0)}$

**for**  $i = 1, 2, \dots$

**solve**  $Mz^{(i-1)} = r^{(i-1)}$

$\rho_{i-1} = r^{(i-1)T} z^{(i-1)}$

**if**  $i = 1$

$p^{(1)} = z^{(0)}$

**else**

$\beta_{i-1} = \rho_{i-1} / \rho_{i-2}$

$p^{(i)} = z^{(i-1)} + \beta_{i-1} p^{(i-1)}$

**endif**

$q^{(i)} = Ap^{(i)}$

$\alpha_i = \rho_{i-1} / p^{(i)T} q^{(i)}$

$x^{(i)} = x^{(i-1)} + \alpha_i p^{(i)}$

$r^{(i)} = r^{(i-1)} - \alpha_i q^{(i)}$

    check convergence; continue if necessary

**end**

# **takeaway**

Each iteration involves:

- Matrix-vector product
- Preconditioner solve
- Two inner products
- Other vector operations.

# Three popular iterative methods

- Conjugate gradients: constant storage and inner products; works only for symmetric systems
- GMRES (like FOM): growing storage and inner products: restarting and numerical cleverness
- BiCGstab and QMR: relax the orthogonality

# CG derived from minimization

Special case of SPD:

For which vector  $x$  with  $\|x\| = 1$  is  $f(x) = 1/2x^tAx - b^t x$  minimal?  
(5)

Taking derivative:

$$f'(x) = Ax - b.$$

Optimal solution:

$$f'(x) = 0 \Rightarrow Ax = b.$$

Traditional: variational formulation

New: error of neural net

## Minimization by line search

Assume full minimization  $\min_x: f(x) = 1/2x^t Ax - b^t x$  too expensive.

Iterative update

$$x_{i+1} = x_i + p_i \delta_i$$

where  $p_i$  is search direction.

Finding optimal value  $\delta_i$  is ‘line search’:

$$\delta_i = \operatorname{argmin}_{\delta} \|f(x_i + p_i \delta)\| = \frac{r_i^t p_i}{p_i^t A p_i}$$

Other constants follow from orthogonality.

# Line search

Also popular in other contexts:

- General non-linear systems
- Machine learning: stochastic gradient descent  
 $p_i$  is ‘block vector’ of training set

$p_1^t A p_i$  is a matrix  $\Rightarrow (p_1^t A p_i)^{-1} r_i^t p_i$  system solving

# Let's go parallel

# What's in an iterative method?

From easy to hard

- Vector updates  
These are trivial
- Inner product
- Matrix-vector product
- Preconditioner solve

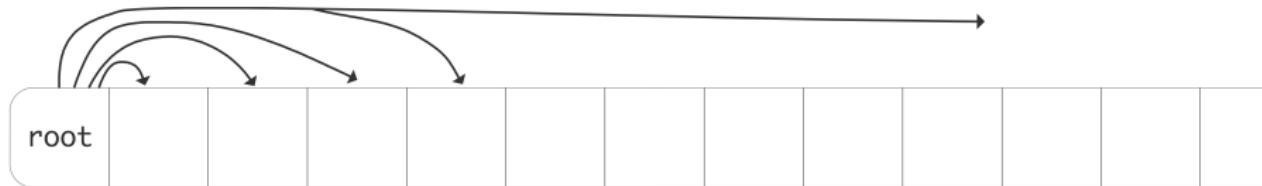
## Inner products: collectives

Collective operation: data from all processes is combined.  
(Is a matrix-vector product a collective?)

Examples: sum-reduction, broadcast  
These are each other's mirror image, computationally.

# Naive realization of collectives

Broadcast:



Single message:

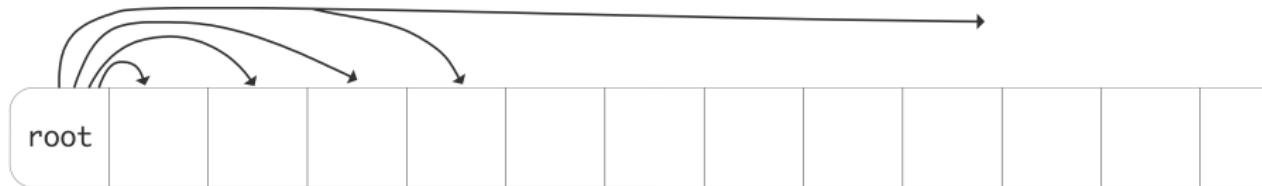
$$\alpha = \text{message startup} \approx 10^{-6} \text{ s}, \quad \beta = \text{time per word} \approx 10^{-9} \text{ s}$$

- Time for message of  $n$  words:

$$\alpha + \beta n$$

# Naive realization of collectives

Broadcast:



Single message:

$$\alpha = \text{message startup} \approx 10^{-6} \text{ s}, \quad \beta = \text{time per word} \approx 10^{-9} \text{ s}$$

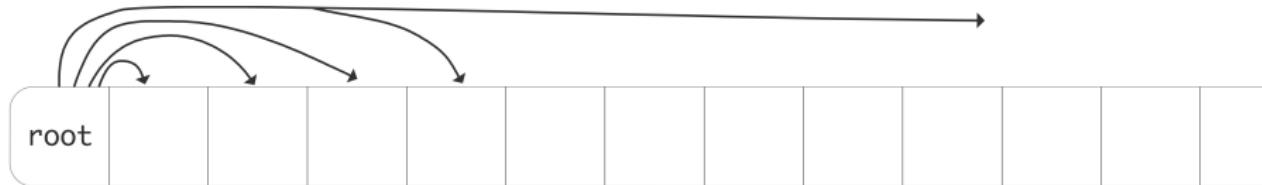
- Time for message of  $n$  words:

$$\alpha + \beta n$$

- Single inner product:  $n = 1$

# Naive realization of collectives

Broadcast:



Single message:

$$\alpha = \text{message startup} \approx 10^{-6} \text{ s}, \quad \beta = \text{time per word} \approx 10^{-9} \text{ s}$$

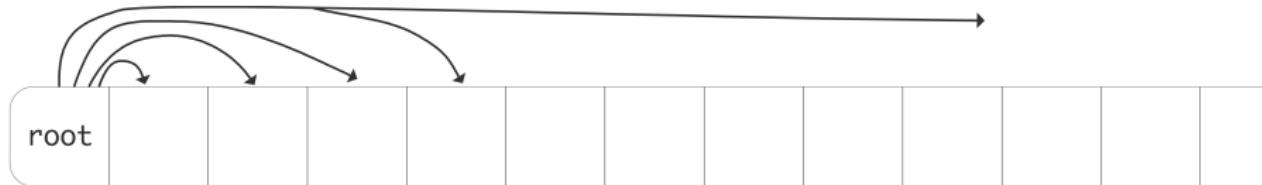
- Time for message of  $n$  words:

$$\alpha + \beta n$$

- Single inner product:  $n = 1$
- Time for collective?

# Naive realization of collectives

Broadcast:



Single message:

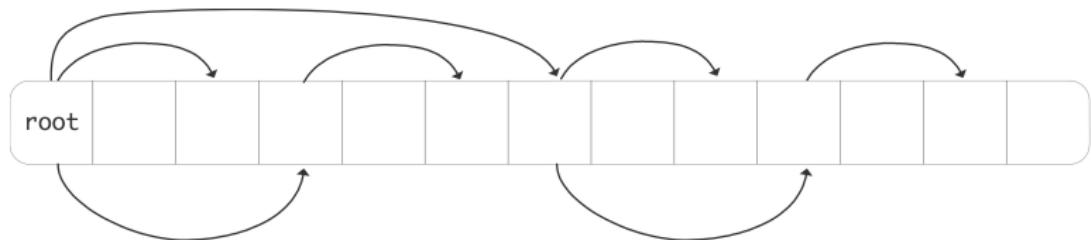
$$\alpha = \text{message startup} \approx 10^{-6} \text{ s}, \quad \beta = \text{time per word} \approx 10^{-9} \text{ s}$$

- Time for message of  $n$  words:

$$\alpha + \beta n$$

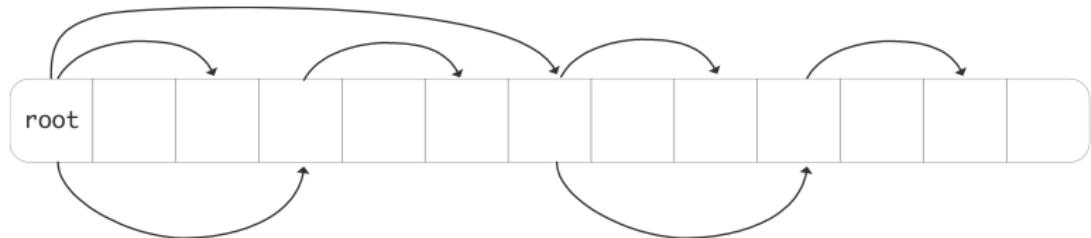
- Single inner product:  $n = 1$
- Time for collective?
- Can you improve on that?

## Better implementation of collective



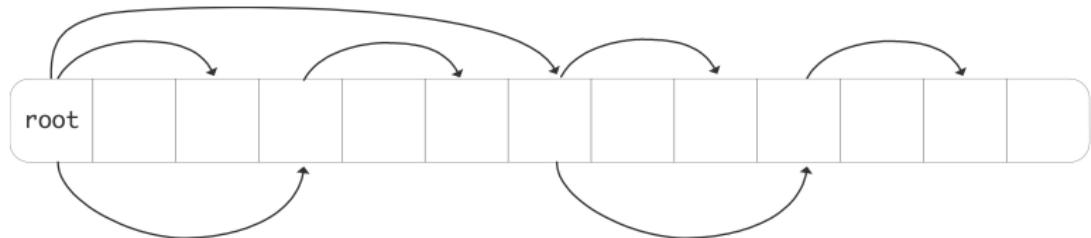
- What is the running time now?

## Better implementation of collective



- What is the running time now?
- Can you come up with lower bounds on the  $\alpha, \beta$  terms? Are these achieved here?

## Better implementation of collective



- What is the running time now?
- Can you come up with lower bounds on the  $\alpha, \beta$  terms? Are these achieved here?
- How about the case of really long buffers?

# Inner products

- Only operation that intrinsically has a  $p$  dependence
- Collective, so induces synchronization
- $\Rightarrow$  exposes load unbalance, can take lots of time
- Research in approaches to hiding: overlapping with other operations

# What do those inner products serve?

- Orthogonality of residuals
- Basic algorithm: Gram-Schmidt
- one step: given  $u, v$

$$v' \leftarrow v - \frac{u^t v}{u^t u} u.$$

then  $v' \perp u$

- bunch of steps: given  $U, v$

$$v' \leftarrow v - \frac{U^t v}{U^t U} U.$$

then  $v' \perp U$ .

Gram-Schmidt algorithm

# Modified Gram-Schmidt

For  $i = 1, \dots, n$ :

$$\text{let } c_i = u_i^t v / u_i^t u_i$$

$$\text{update } v \leftarrow v - c_i u_i$$

More numerical stable

# Full Orthogonalization Method

Let  $r_0$  be given

For  $i \geq 0$ :

let  $s \leftarrow K^{-1}r_i$

let  $t \leftarrow AK^{-1}r_i$

for  $j \leq i$ :

    let  $\gamma_j$  be the coefficient so that  $t - \gamma_j r_j \perp r_j$

    for  $j \leq i$ :

        form  $s \leftarrow s - \gamma_j x_j$

        and  $t \leftarrow t - \gamma_j r_j$

    let  $x_{i+1} = (\sum_j \gamma_j)^{-1}s$ ,  $r_{i+1} = (\sum_j \gamma_j)^{-1}t$ .

# Modified Gramm-Schmidt

Let  $r_0$  be given

For  $i \geq 0$ :

let  $s \leftarrow K^{-1}r_i$

let  $t \leftarrow AK^{-1}r_i$

for  $j \leq i$ :

let  $\gamma_j$  be the coefficient so that  $t - \gamma_j r_j \perp r_j$

form  $s \leftarrow s - \gamma_j x_j$

and  $t \leftarrow t - \gamma_j r_j$

let  $x_{i+1} = (\sum_j \gamma_j)^{-1}s$ ,  $r_{i+1} = (\sum_j \gamma_j)^{-1}t$ .

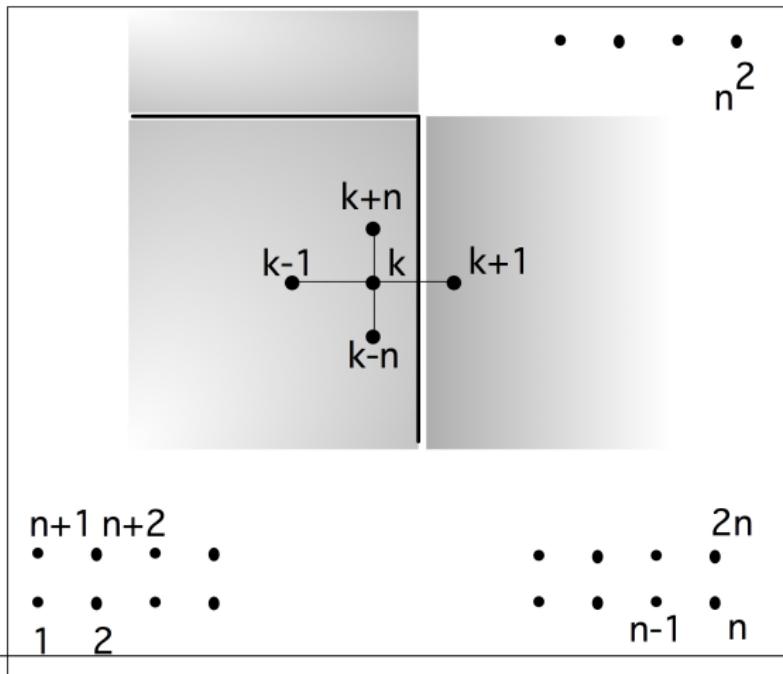
# Practical differences

- Modified GS more stable
- Inner products are global operations: costly

## Matrix-vector product

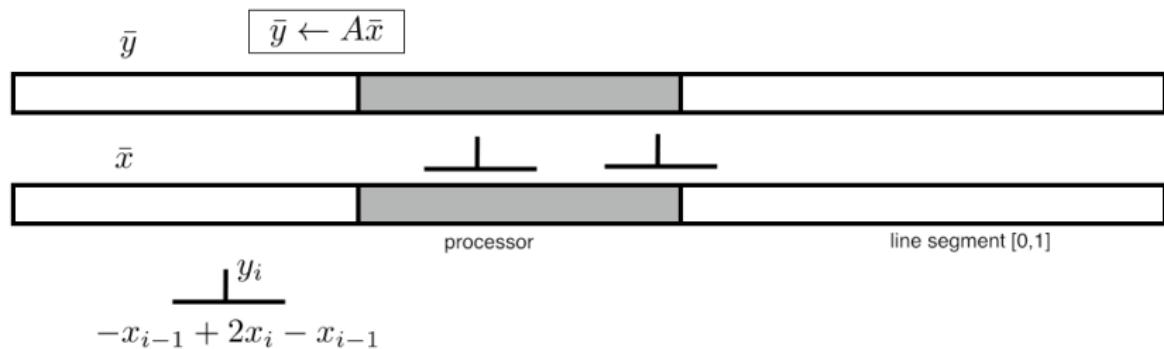
# PDE, 2D case

A difference stencil applied to a two-dimensional square domain, distributed over processors. Each point connects to neighbours  $\Rightarrow$  each process connects to neighbours.



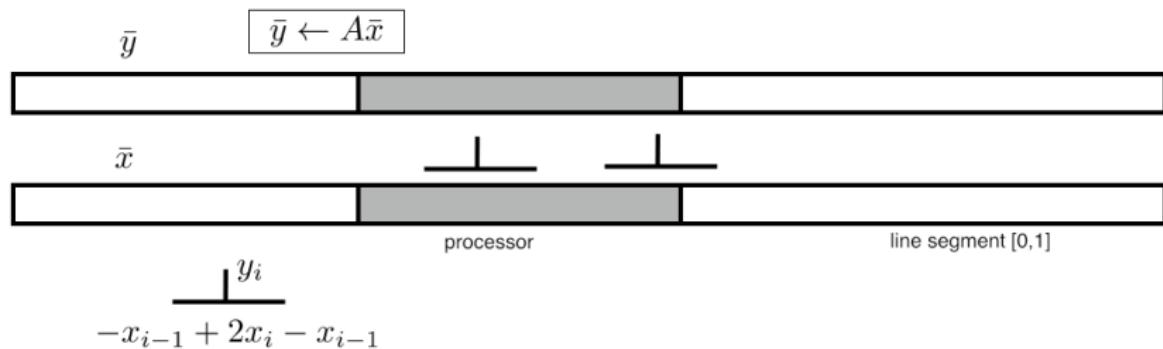
# Parallelization

Assume each process has the matrix values and vector values in part of the domain.



# Parallelization

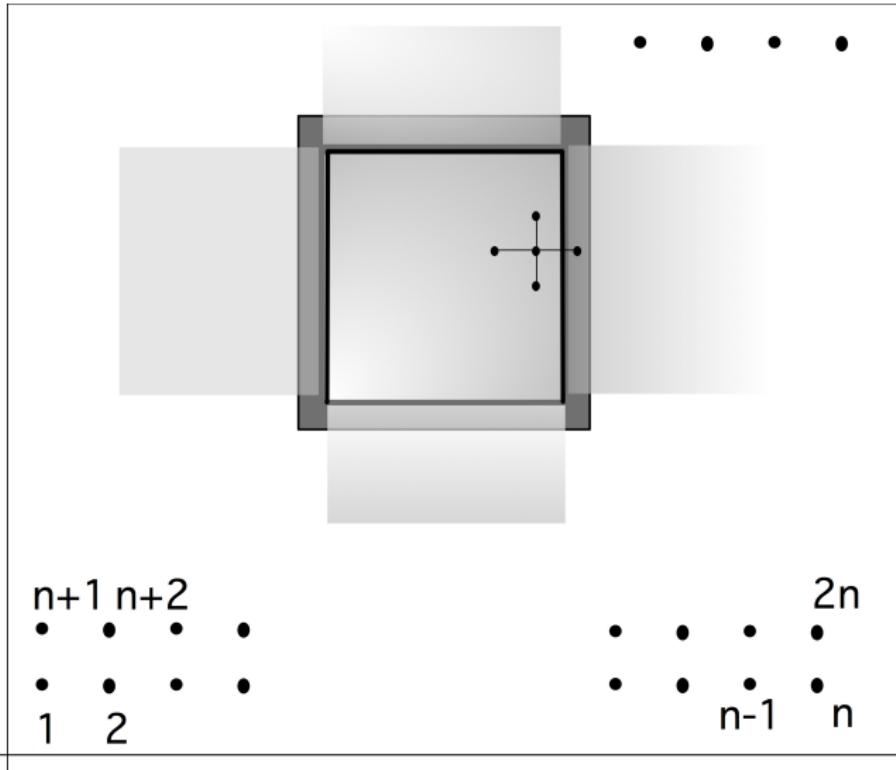
Assume each process has the matrix values and vector values in part of the domain.



Processor needs to get values from neighbors.

# Halo region

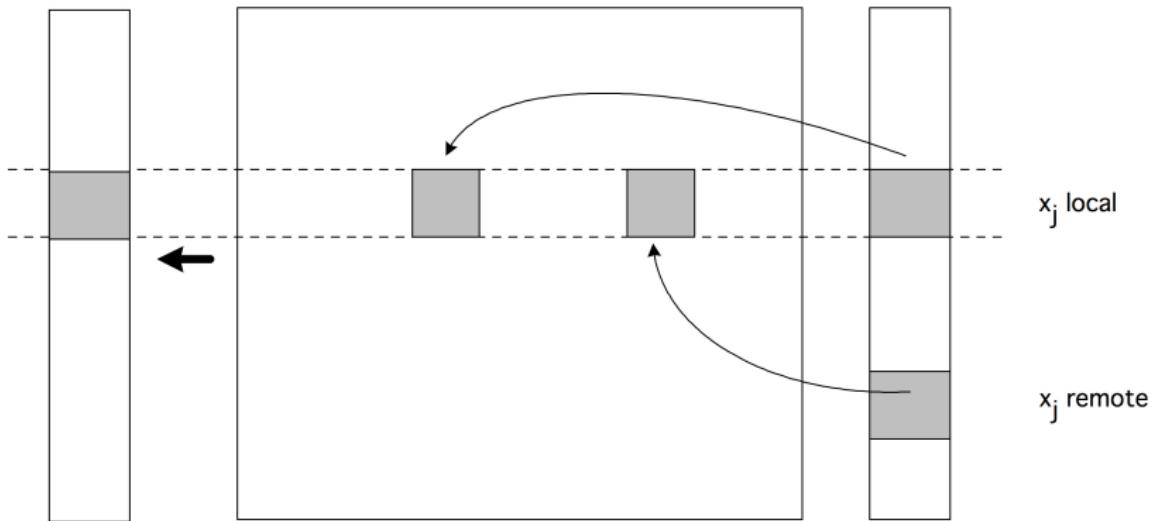
The 'halo' region of a process, induced by a stencil



# Matrices in parallel

$$y \leftarrow Ax$$

and  $A, x, y$  all distributed:



# Matrix-vector product performance

- Large scale:
  - partition for scalability
  - minimize communication (Metis, Zoltan: minimize edge cuts)
  - dynamic load balancing? requires careful design
- Processor scale:
  - Performance largely bounded by bandwidth
  - Some optimization possible

Beware of optimizations that change the math!

## Preconditioners

# Preconditioners

- There's much that can be said here.
- Some comments to follow
- There is intrinsic dependence in solvers, hence in preconditioners:
  - parallelism is very tricky.
  - approximate inverses

## 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

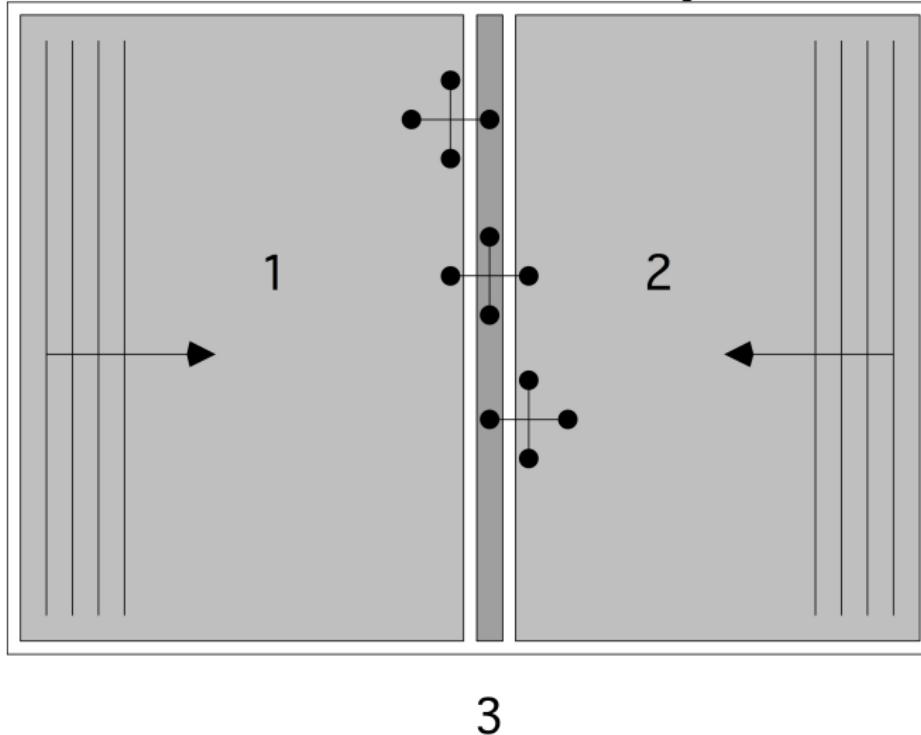
# Fill-in is a function of ordering

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

After factorization the matrix is dense.

Can this be permuted?

# Domain decomposition



$$\left( \begin{array}{cc|cc} \begin{matrix} \star & \star \\ \star & \star & \star \\ \ddots & \ddots & \ddots \\ \star & \star & \star \\ \star & \star \end{matrix} & & \emptyset & \begin{matrix} 0 \\ \vdots \\ 0 \\ \star \end{matrix} \\ \hline & \begin{matrix} \star & \star \\ \star & \star & \star \\ \ddots & \ddots & \ddots \\ \star & \star & \star \\ \star & \star \end{matrix} & \begin{matrix} 0 \\ \vdots \\ \vdots \\ 0 \\ \star \end{matrix} \\ \hline \emptyset & \begin{matrix} 0 & \dots & \dots & 0 & \star \end{matrix} & \begin{matrix} 0 & \dots & \dots & 0 & \star & \star \end{matrix} & \end{array} \right) \quad \left. \begin{array}{l} (n^2 - n)/2 \\ (n^2 - n)/2 \\ n \end{array} \right\}$$

## DD factorization

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

$$S = A_{33} - A_{31}A_{11}^{-1}A_{13} - A_{32}A_{22}^{-1}A_{23}$$

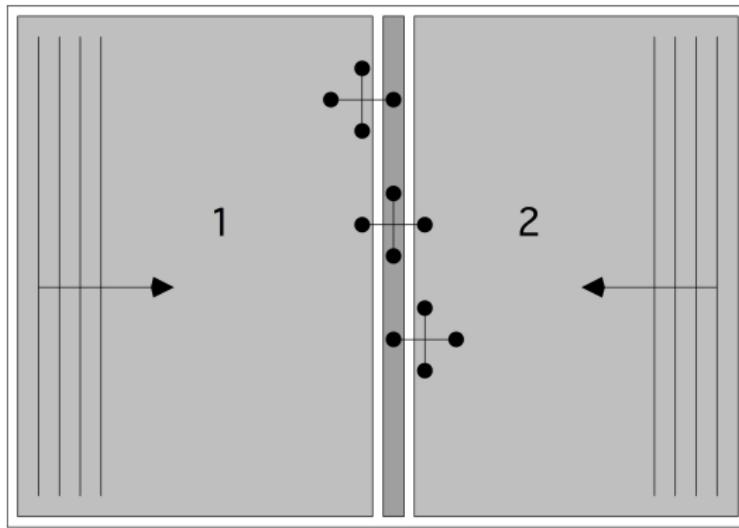
Parallelism...

# Graph theory of sparse elimination

$$a_{ij} \leftarrow a_{ij} - a_{ik} a_{kk}^{-1} a_{kj}$$



# Graph theory of sparse elimination



# Graph theory of sparse elimination

$$a_{ij} \leftarrow a_{ij} - a_{ik} a_{kk}^{-1} a_{kj}$$



So inductively  $S$  is dense

## More about separators

- This is known as ‘domain decomposition’ or ‘substructuring’
- Separators have better spectral properties

# Recursive bisection

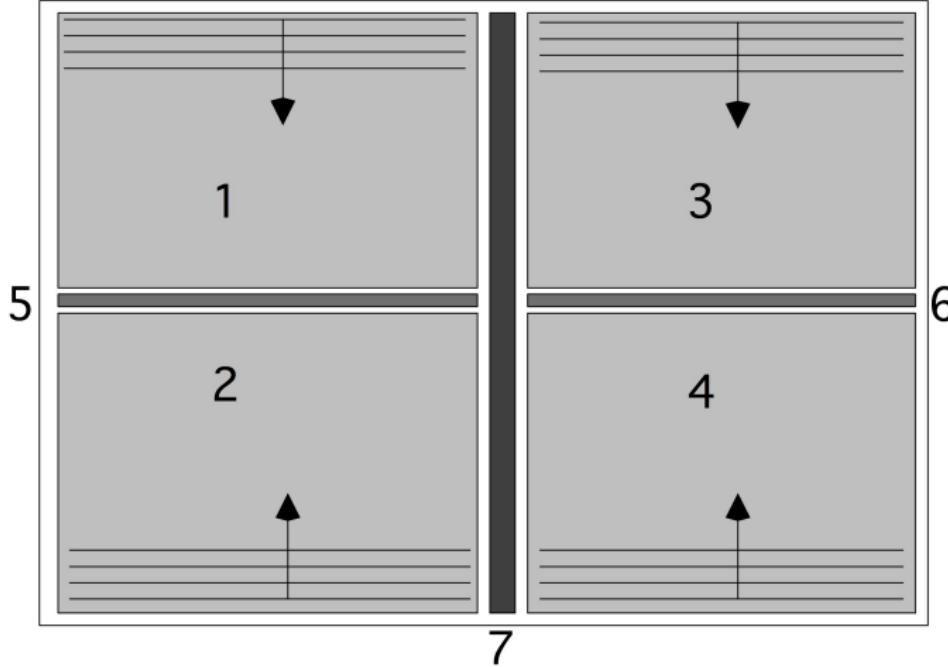
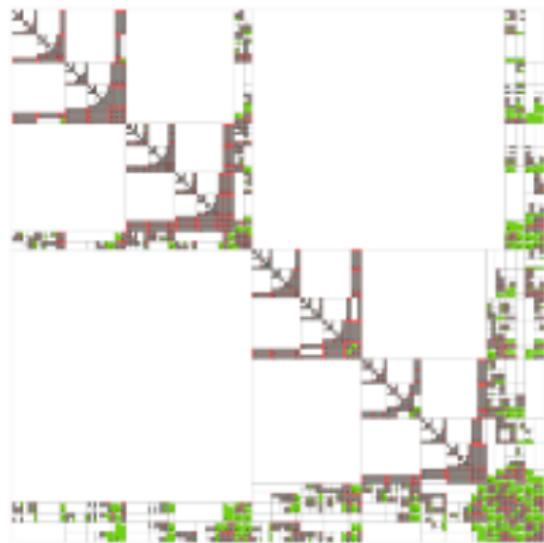


Figure: A four-way domain decomposition

$$A^{DD} = \begin{pmatrix} A_{11} & & A_{15} & A_{17} \\ & A_{22} & & A_{25} \\ & & A_{33} & A_{36} \\ & & & A_{44} \\ A_{51} & A_{52} & & A_{55} \\ & & A_{63} & A_{64} \\ A_{71} & A_{72} & A_{73} & A_{74} & A_{75} & A_{76} & A_{77} \end{pmatrix}$$

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  $n \rightarrow n/2$

$$\begin{aligned}\text{space} &= 3/2n^2 + 4 \cdot 3/2(n/2)^2 + \dots \\ &= N(3/2 + 3/2 + \dots) \quad \log n \text{ terms} \\ &= O(N \log N)\end{aligned}$$

$$\begin{aligned}\text{time} &= 5/12n^3/3 + 4 \cdot 5/12(n/2)^3/3 + \dots \\ &= 5/12N^{3/2}(1 + 1/4 + 1/16 + \dots) \\ &= O(N^{3/2})\end{aligned}$$

Unfortunately only in 2D.

## More direct factorizations

Minimum degree, multifrontal,...

Finding good separators and domain decompositions is tough in general.

# 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

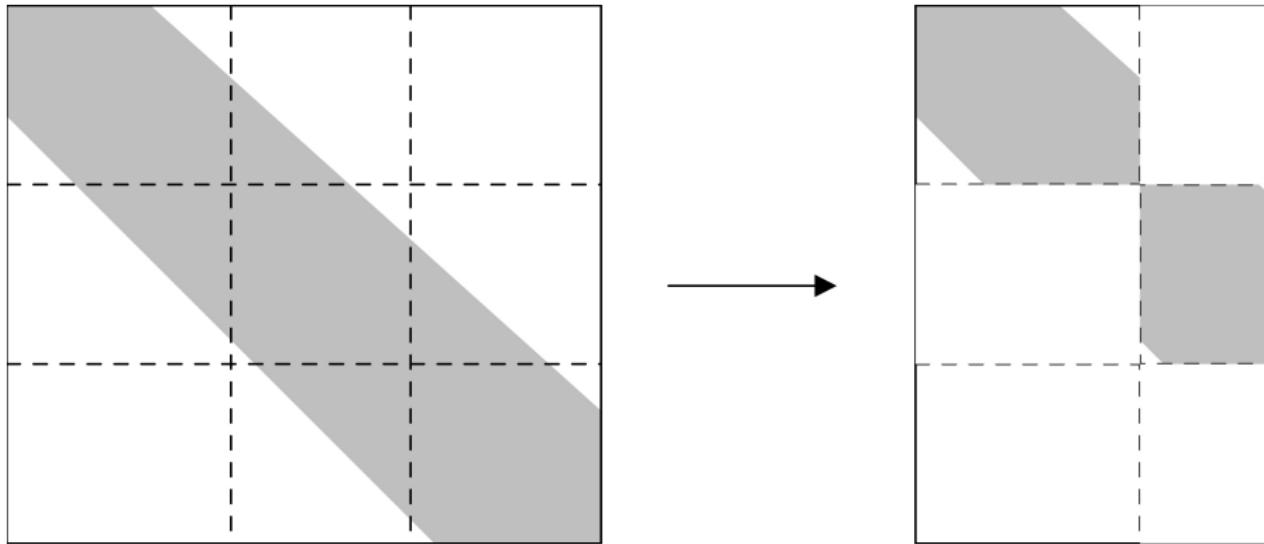


Figure: Sparsity pattern corresponding to a block Jacobi preconditioner

# Variable reordering

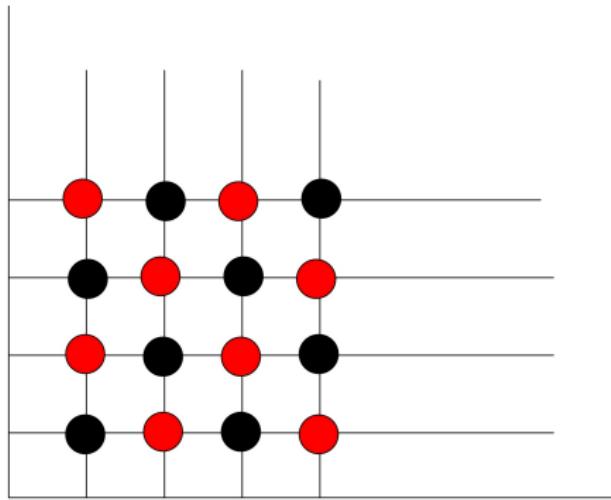
$$\begin{pmatrix} a_{11} & a_{12} & & & \emptyset \\ a_{21} & a_{22} & a_{23} & & \\ & a_{32} & a_{33} & a_{34} & \\ \emptyset & \ddots & \ddots & \ddots & \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \end{pmatrix}$$

with redblack

$$\begin{pmatrix} a_{11} & & a_{12} & & \\ & a_{33} & a_{32} & a_{34} & \\ & & a_{55} & \ddots & \ddots \\ & & & \ddots & \ddots \\ a_{21} & a_{23} & & a_{22} & \\ & a_{43} & a_{45} & & a_{44} \\ & & \ddots & & \ddots \end{pmatrix} \begin{pmatrix} x_1 \\ x_3 \\ x_5 \\ \vdots \\ x_2 \\ x_4 \\ \vdots \end{pmatrix} = \begin{pmatrix} y_1 \\ y_3 \\ y_5 \\ \vdots \\ y_2 \\ y_4 \\ \vdots \end{pmatrix}$$

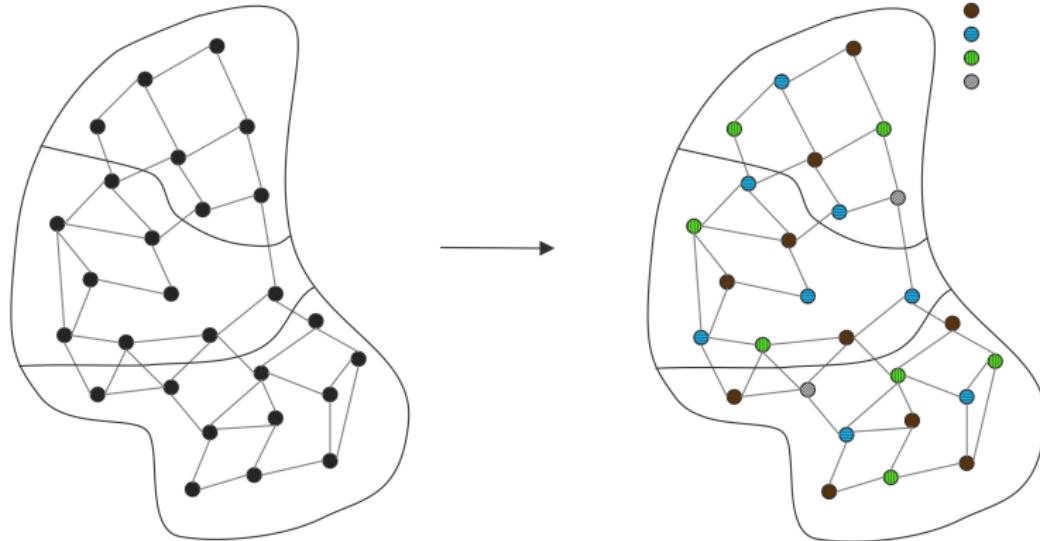
Two-processor parallel Gauss-Seidel or ILU

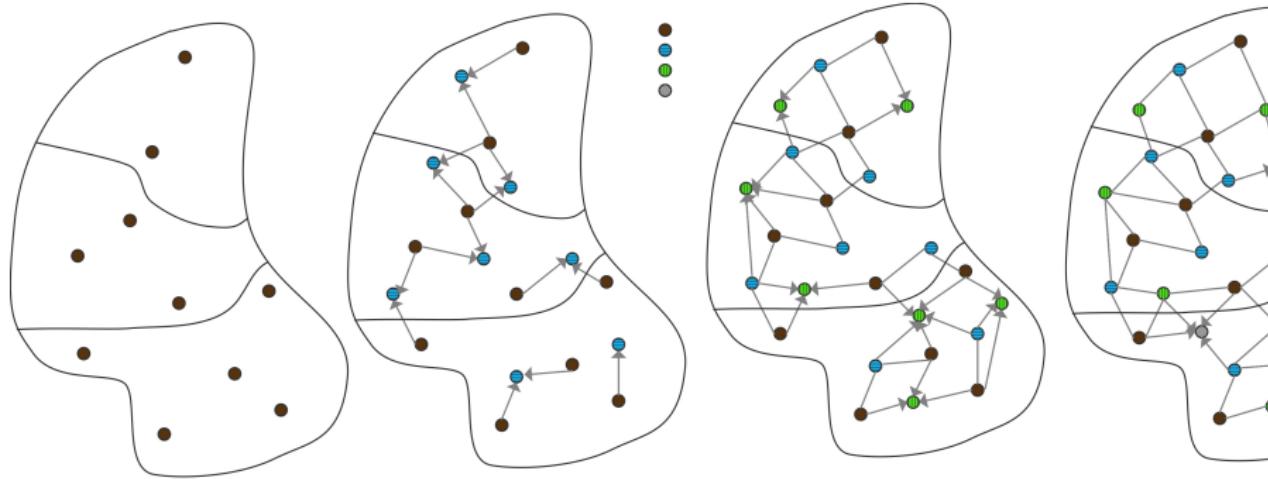
## 2D redblack



In general, colouring, colour number

# Multicolour ILU





# How do you get a multi-colouring?

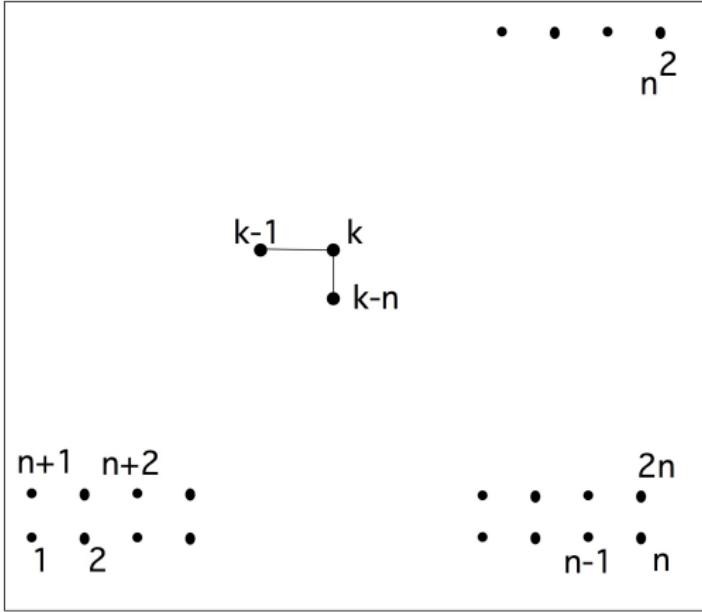
Exactly colour number is NP-completely: don't bother.

For preconditioner an approximation is good enough:

Luby / Jones-Plassman algorithm

- Give every node a random value
- First colour: all nodes with a higher value than all their neighbours
- Second colour: higher value than all neighbours except in first colour
- et cetera

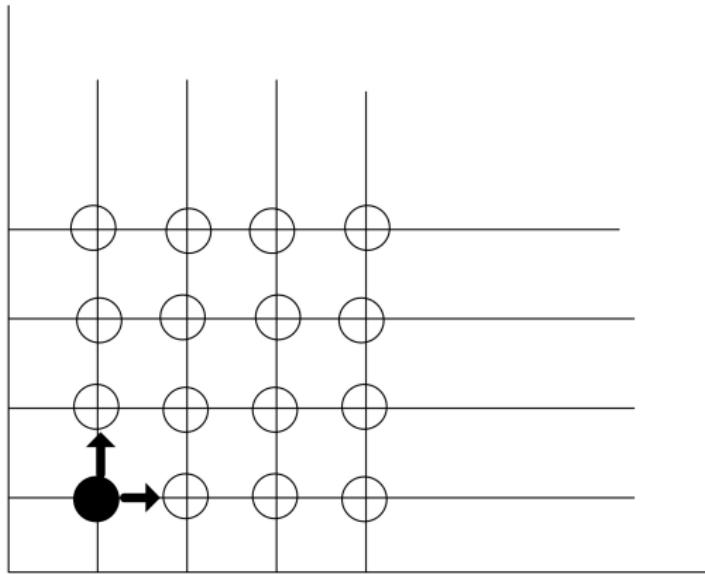
# Recurrences

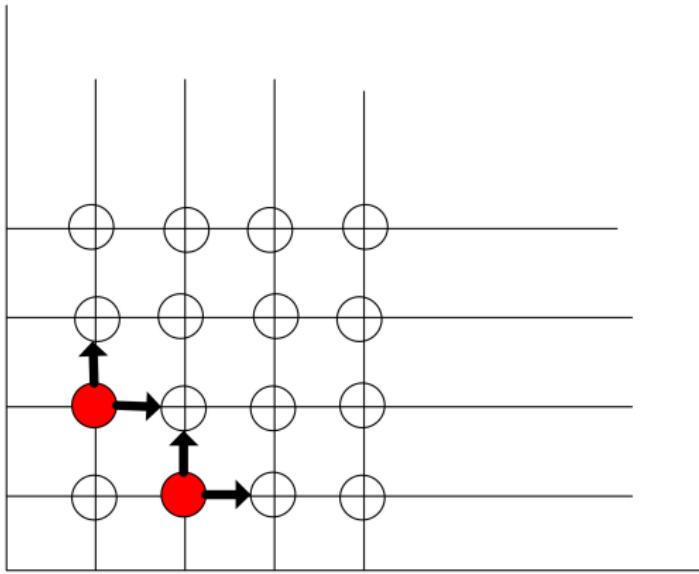


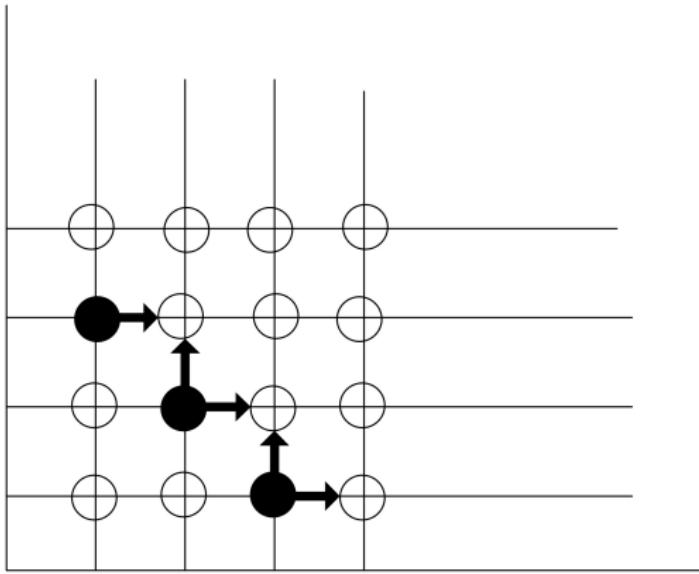
$$x_{i,j} = f(x_{i-1,j}, x_{i,j-1})$$

Intuitively: recursion length  $n^2$

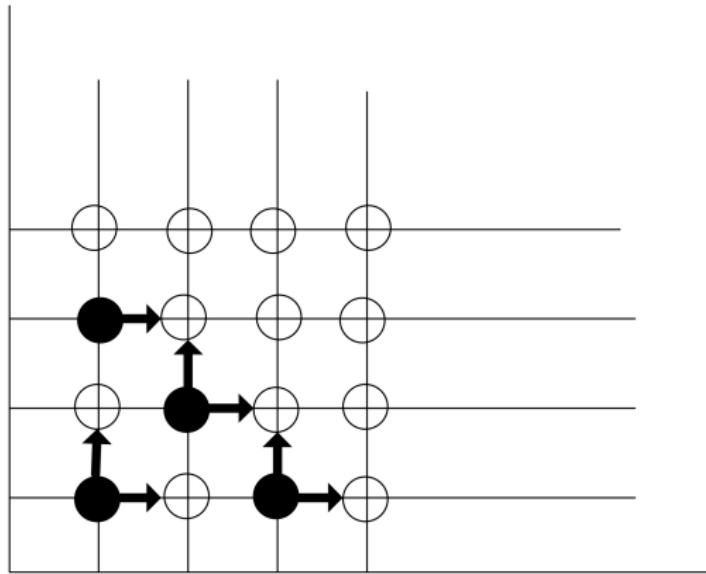
# However...



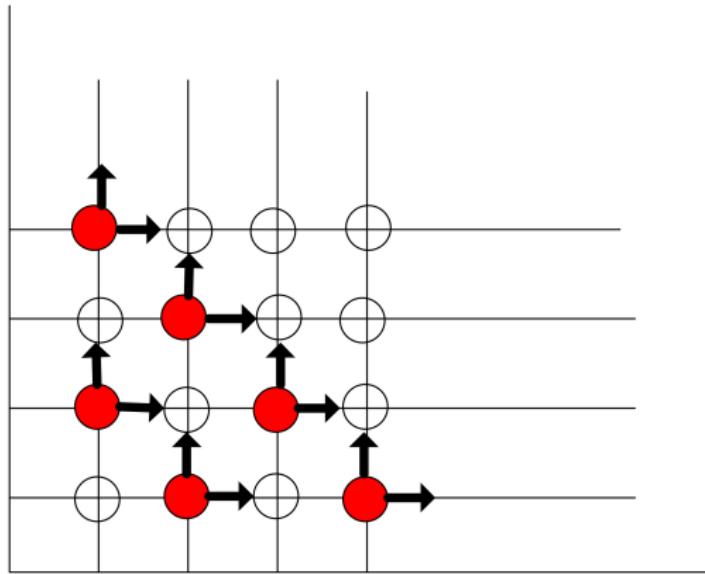




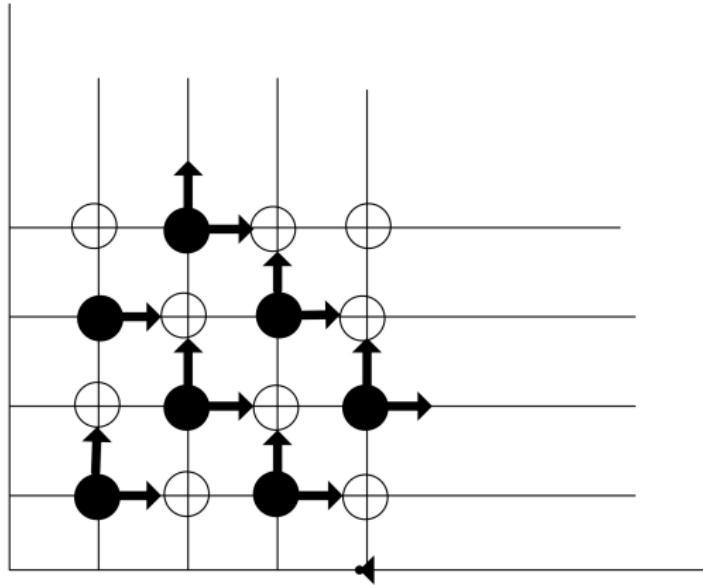
# And in fact



## But then too



# And



# Conclusion

1. Wavefronts have sequential length  $2n$ ,  
average parallelism  $n/2$
2. Equivalency of wavefronts and multicolouring

# Recursive doubling

Write recurrence  $x_i = b_i - a_{i-1}x_{i-1}$  as

$$\begin{pmatrix} 1 & & & \emptyset \\ a_{21} & 1 & & \\ & \ddots & \ddots & \\ \emptyset & & a_{n,n-1} & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

for short:  $A = I + B$

## Transform

$$\begin{pmatrix} 1 & & & & & & & & 0 \\ 0 & 1 & & & & & & & \\ & -a_{32} & 1 & & & & & & \\ & & 0 & 1 & & & & & \\ & & & -a_{54} & 1 & & & & \\ & & & & 0 & 1 & & & \\ & & & & & -a_{76} & 1 & & \\ & & & & & & \ddots & & \\ & & & & & & & \ddots & \\ & & & & & & & & \ddots \end{pmatrix} \times (I + B) =$$

$$\begin{pmatrix} 1 & & & & & & & & 0 \\ a_{21} & 1 & & & & & & & \\ -a_{32} a_{21} & 0 & 1 & & & & & & \\ & & a_{43} & 1 & & & & & \\ & & -a_{54} a_{43} & 0 & 1 & & & & \\ & & & & a_{65} & 1 & & & \\ & & & & -a_{76} a_{65} & 0 & 1 & & \\ & & & & & \ddots & & \ddots & \\ & & & & & & \ddots & & \ddots \end{pmatrix}$$

- Recurrence over half the elements
- Parallel calculation of other half
- Now recurse...

# Turning implicit operations into explicit

Normalize ILU solve to  $(I - L)$  and  $(I - U)$

Approximate  $(I - L)x = y$  by  $x \approx (I + L + L^2)y$

Convergence guaranteed for diagonally dominant