Scalability of operations

Victor Eijkhout

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Justification

Parallel operations are supposed to be faster than their sequential counterparts. In this section we will explore how to quantify this, and we will see examples where the same result can be computed with diferent efficiencies.

Collectives as building blocks; complexity

Collectives

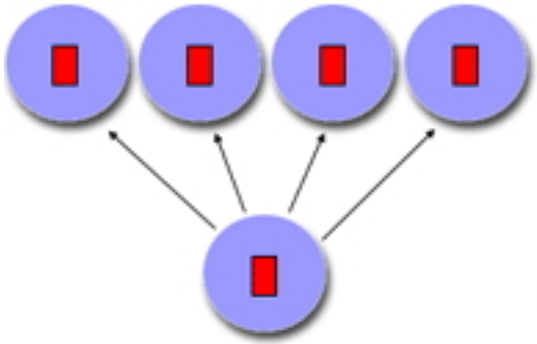
Gathering and spreading information:

- Every process has data, you want to bring it together;
- One process has data, you want to spread it around.

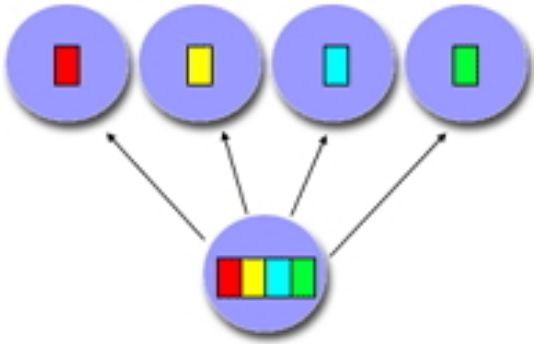
Root process: the one doing the collecting or disseminating.

Basic cases:

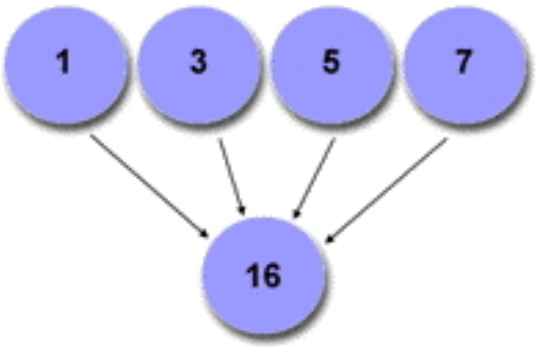
- Collect data: gather.
- Collect data and compute some overall value (sum, max): reduction.
- Send the same data to everyone: broadcast.
- Send individual data to each process: scatter.



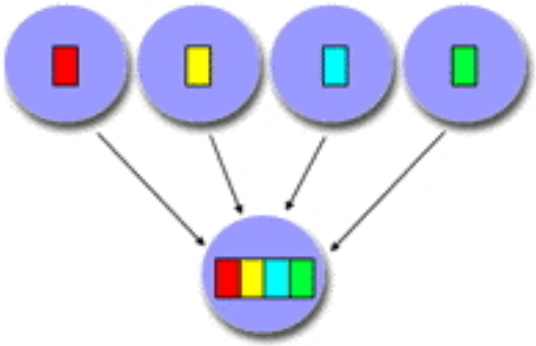
broadcast



scatter



reduction



gather

Collective scenarios

How would you realize the following scenarios with collectives?

- Let each process compute a random number. You want to print the maximum of these numbers to your screen.
- Each process computes a random number again. Now you want to scale these numbers by their maximum.
- Let each process compute a random number. You want to print on what processor the maximum value is computed.

Simple model of parallel computation

- α: message latency
- β: time per word (inverse of bandwidth)
- γ: time per floating point operation

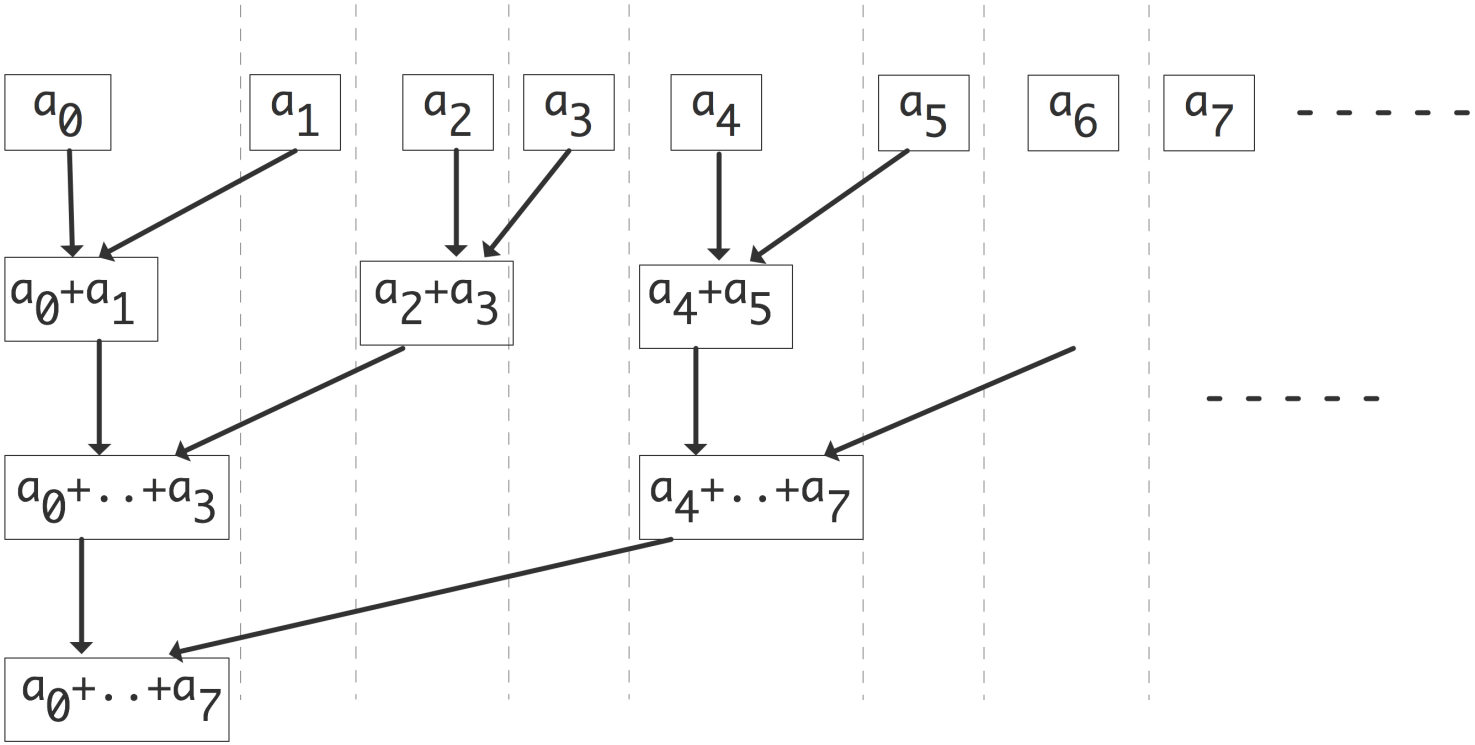
Send n items and do m operations:

$$cost = \alpha + \beta \cdot n + \gamma \cdot m$$

Pure sends: no γ term,
pure computation: no α, β terms,
sometimes mixed: reduction

Model for collectives

- One simultaneous send and receive:
- doubling of active processors
- collectives have a $\alpha \log_2 p$ cost component



Broadcast

	$t=0$	$t=1$	$t=2$
p_0	$x_0\downarrow, x_1\downarrow, x_2\downarrow, x_3\downarrow$	$x_0\downarrow, x_1\downarrow, x_2\downarrow, x_3\downarrow$	x_0, x_1, x_2, x_3
p_1		$x_0\downarrow, x_1\downarrow, x_2\downarrow, x_3\downarrow$	x_0, x_1, x_2, x_3
p_2			x_0, x_1, x_2, x_3
p_3			x_0, x_1, x_2, x_3

On $t=0$, p_0 sends to p_1; on $t=1$ p_0, p_1 send to p_2, p_3.

Optimal complexity:

$$\lceil \log_2 p \rceil \alpha + n\beta.$$

Actual complexity:

$$\lceil \log_2 p \rceil (\alpha + n\beta).$$

Good enough for short vectors.

Long vector broadcast

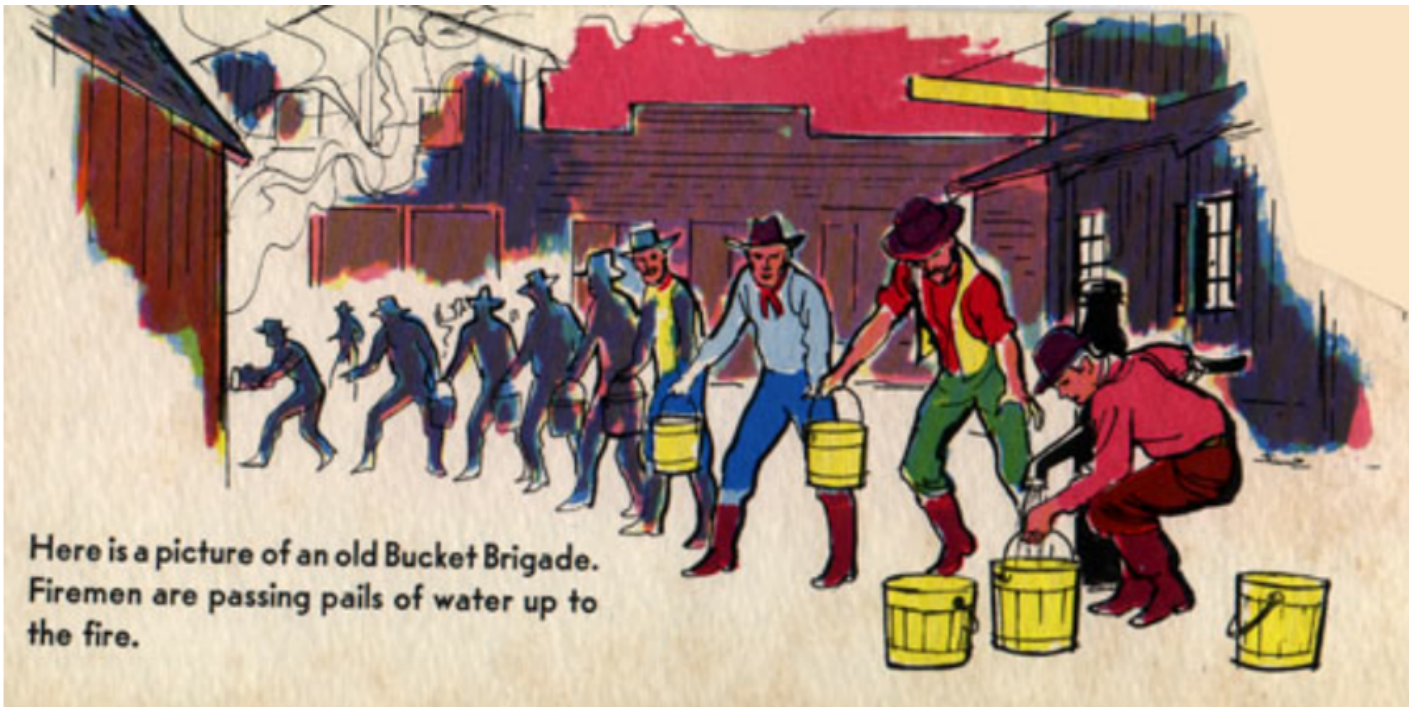
Start with a scatter:

	$t=0$	$t=1$	$t=2$	$t=3$
p_0	$x_0\downarrow, x_1, x_2, x_3$	$x_0, x_1\downarrow, x_2, x_3$	$x_0, x_1, x_2\downarrow, x_3$	$x_0, x_1, x_2, x_3\downarrow$
p_1		x_1		
p_2			x_2	
p_3				x_3

takes $p-1$ messages of size N/p, for a total time of

$$T_{\text{scatter}}(N,P) = (p-1)\alpha + (p-1)\cdot\frac{N}{p}\cdot\beta.$$

Bucket brigade



Long vector broadcast

After the scatter do a bucket-allgather:

	$t=0$	$t=1$	*etcetera*
p_0	$x_0\downarrow$	$x_0 \qquad x_3\downarrow$	$x_0, \quad x_2, x_3$
p_1	$x_1\downarrow$	$x_0\downarrow, x_1$	$x_0, x_1, \quad x_3$
p_2	$x_2\downarrow$	$x_1\downarrow, x_2$	x_0, x_1, x_2
p_3	$x_3\downarrow$	$x_2\downarrow, x_3$	x_1, x_2, x_3

Each partial message gets sent $p-1$ times, so this stage also has a complexity of

$$T_{\text{bucket}}(N,P) = (p-1)\alpha + (p-1)\cdot\frac{N}{p}\cdot\beta.$$

Better if N large.

Reduce

Optimal complexity:

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

Spanning tree algorithm:

	$t=1$	$t=2$	$t=3$
p_0	$x_0^{(0)}, x_1^{(0)}, x_2^{(0)}, x_3^{(0)}$	$x_0^{(0:1)}, x_1^{(0:1)}, x_2^{(0:1)}, x_3^{(0:1)}$	$x_0^{(0:3)}, x_1^{(0:3)}, x_2^{(0:3)}, x$
p_1	$x_0^{(1)} \uparrow, x_1^{(1)} \uparrow, x_2^{(1)} \uparrow, x_3^{(1)} \uparrow$		
p_2	$x_0^{(2)}, x_1^{(2)}, x_2^{(2)}, x_3^{(2)}$	$x_0^{(2:3)} \uparrow, x_1^{(2:3)} \uparrow, x_2^{(2:3)} \uparrow, x_3^{(2:3)} \uparrow$	
p_3	$x_0^{(3)} \uparrow, x_1^{(3)} \uparrow, x_2^{(3)} \uparrow, x_3^{(3)} \uparrow$		

Running time

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

Good enough for short vectors.

Allreduce

Allreduce $\equiv$ Reduce+Broadcast

	$t = 1$	$t = 2$	$t = 3$
p_0	$x_0 \downarrow$	$x_0 x_1 \downarrow$	$x_0 x_1 x_2 x_3$
p_1	$x_1 \uparrow$	$x_0 x_1 \downarrow$	$x_0 x_1 x_2 x_3$
p_2	$x_2 \downarrow$	$x_2 x_3 \uparrow$	$x_0 x_1 x_2 x_3$
p_3	$x_3 \uparrow$	$x_2 x_3 \uparrow$	$x_0 x_1 x_2 x_3$

Same running time as regular reduce!

Allgather

Gather n elements: each processor owns n/p; optimal running time

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

	$t=1$	$t=2$	$t=3$
p_0	$x_0 \downarrow$	$x_0 x_1 \downarrow$	$x_0 x_1 x_2 x_3$
p_1	$x_1 \uparrow$	$x_0 x_1 \downarrow$	$x_0 x_1 x_2 x_3$
p_2	$x_2 \downarrow$	$x_2 x_3 \uparrow$	$x_0 x_1 x_2 x_3$
p_3	$x_3 \uparrow$	$x_2 x_3 \uparrow$	$x_0 x_1 x_2 x_3$

Same time as gather, half of gather-and-broadcast.

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	$x_0^{(1)}, x_1^{(1)}, x_2^{(1)} \downarrow, x_3^{(1)} \downarrow$	$x_0^{(1:3:2)} \uparrow, x_1^{(1:3:2)}$	$x_1^{(0:3)}$
p_2	$x_0^{(2)} \uparrow, x_1^{(2)} \uparrow, x_2^{(2)}, x_3^{(2)}$	$x_2^{(0:2:2)}, x_3^{(0:2:2)} \downarrow$	$x_2^{(0:3)}$
p_3	$x_0^{(3)} \uparrow, x_1^{(3)} \uparrow, x_2^{(3)}, x_3^{(3)}$	$x_0^{(1:3:2)} \uparrow, x_1^{(1:3:2)}$	$x_3^{(0:3)}$

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

Efficiency and scaling

Speedup

- Single processor time T_1, on p processors T_p
- speedup is $S_p = T_1/T_p$, $S_P \leq p$
- efficiency is $E_p = S_p/p$, $0 < E_p \leq 1$

Many caveats

- Is T_1 based on the same algorithm? The parallel code?
- Sometimes superlinear speedup.
- Can the problem be run on a single processor?
- Can the problem be evenly divided?

Limits on speedup/efficiency

- F_s sequential fraction, F_p parallelizable fraction
- $F_s + F_p = 1$
- $T_1 = (F_s + F_p)T_1 = F_s T_1 + F_p T_1$
- Amdahl's law: $T_p = F_s T_1 + F_p T_1 / p$
- $P \to \infty$: $T_P \downarrow T_1 F_s$
- Speedup is limited by $S_P \leq 1/F_s$, efficiency is a decreasing function $E \sim 1/P$.
- loglog plot: straigth line with slope -1

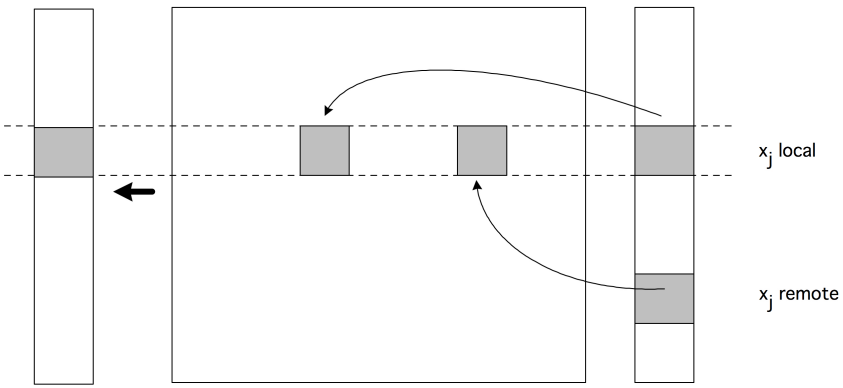
Scaling

- Amdahl's law: strong scaling
  same problem over increasing processors
- Often more realistic: weak scaling
  increase problem size with number of processors,
  for instance keeping memory constant
- Weak scaling: $E_p > c$
- example (below): dense linear algebra

Scalability analysis of dense matrix-vector product

Parallel matrix-vector product; general

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

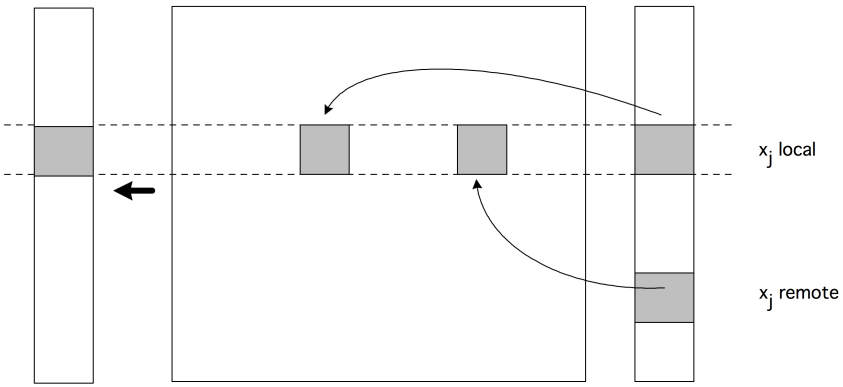


Mvp on processor p:

$$\forall_{i \in I_p} : y_i = \sum_j a_{ij} x_j = \sum_q \sum_{j \in I_q} a_{ij} x_j$$

Local and remote operations

Local and remote parts:



$$\forall_{i \in l_p} : y_i = \sum_{j \in l_p} a_{ij} x_j + \sum_{q \neq p} \sum_{j \in l_q} a_{ij} x_j$$

Local part l_p can be executed right away, l_q requires communication.

How to deal with remote parts

- Very flexible: mix of working on local parts, and receiving remote parts.
- More orchestrated:
  1. each process gets a full copy of the input vector (how?)
  2. then operates on the whole input

  Compare?

(Are we making a big assumption here?)

Dense MVP

- Separate communication and computation:
- first allgather
- then matrix-vector product

Cost computation 1.

Algorithm:

Step	Cost (lower bound)
Allgather x_i so that x is available on all nodes	
Locally compute $y_i = A_i x$	$\approx 2\frac{n^2}{P}\gamma$

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 available on all nodes	$\lceil \log_2(P) \rceil \alpha + \frac{P-1}{P} n\beta \approx \log_2(P)\alpha + n\beta$
Locally compute $y_i = A_i x$	$\approx 2\frac{n^2}{P}\gamma$

Parallel efficiency

Speedup:

$$
\begin{aligned}
S_p^{\text{1D-row}}(n) &= \frac{T_1(n)}{T_p^{\text{1D-row}}(n)} \\
&= \frac{2n^2\gamma}{2\frac{n^2}{p}\gamma + \log_2(p)\alpha + n\beta} \\
&= \frac{p}{1 + \frac{p\log_2(p)}{2n^2}\frac{\alpha}{\gamma} + \frac{p}{2n}\frac{\beta}{\gamma}}
\end{aligned}
$$

Efficiency:

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

Strong scaling, weak scaling?

Optimistic scaling

Processors fixed, problem grows:

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

Roughly $E_p \sim 1 - n^{-1}$

Strong scaling

Problem fixed, $p \to \infty$

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

Strong scaling

Problem fixed, $p \to \infty$

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

Roughly $E_p \sim p^{-1}$

Weak scaling

Memory fixed:

$$M = n^2/p$$

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

Weak scaling

Memory fixed:

$$M = n^2/p$$

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

Does not scale: $E_p \sim 1/\sqrt{p}$

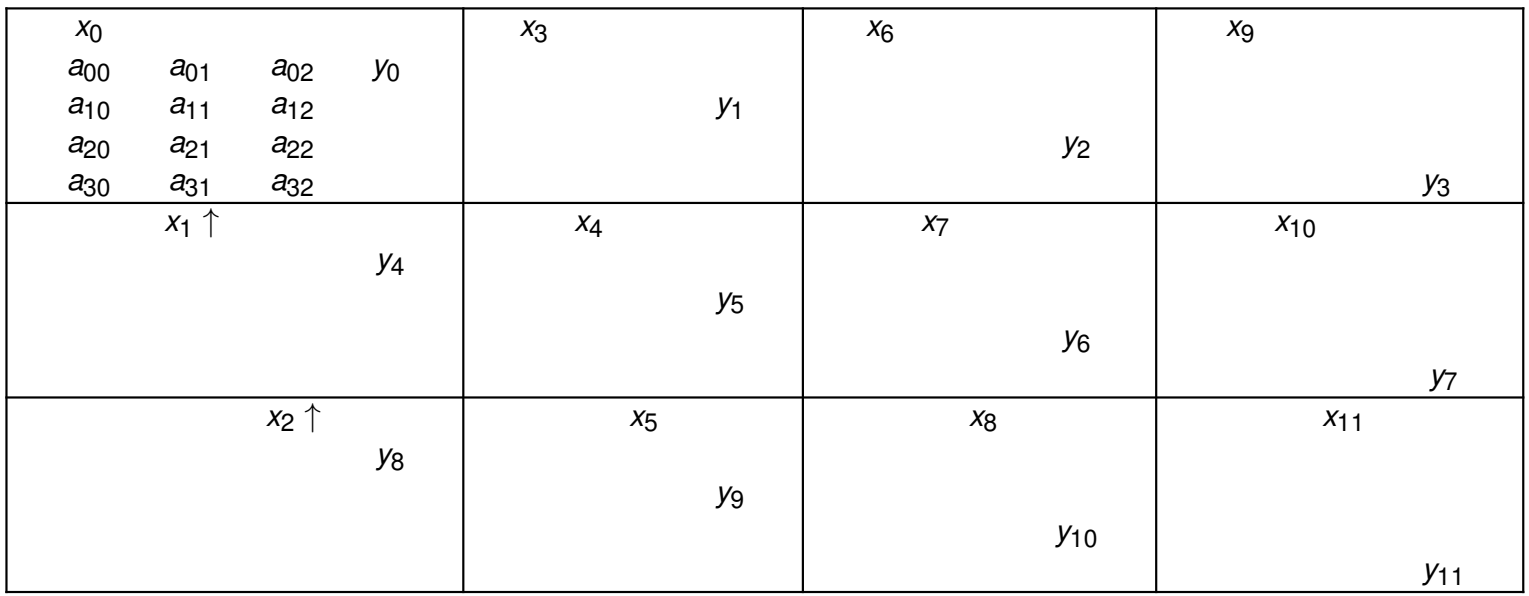
problem in β term: too much communication

Two-dimensional partitioning

x_0				x_3				x_6				x_9		
a_{00}	a_{01}	a_{02}	y_0	a_{03}	a_{04}	a_{05}		a_{06}	a_{07}	a_{08}		a_{09}	$a_{0,10}$	$a_{0,11}$
a_{10}	a_{11}	a_{12}		a_{13}	a_{14}	a_{15}	y_1	a_{16}	a_{17}	a_{18}		a_{19}	$a_{1,10}$	$a_{1,11}$
a_{20}	a_{21}	a_{22}		a_{23}	a_{24}	a_{25}		a_{26}	a_{27}	a_{28}	y_2	a_{29}	$a_{2,10}$	$a_{2,11}$
a_{30}	a_{31}	a_{32}		a_{33}	a_{34}	a_{35}		a_{37}	a_{37}	a_{38}		a_{39}	$a_{3,10}$	$a_{3,11}$
	x_1				x_4				x_7				x_{10}	
a_{40}	a_{41}	a_{42}	y_4	a_{43}	a_{44}	a_{45}		a_{46}	a_{47}	a_{48}		a_{49}	$a_{4,10}$	$a_{4,11}$
a_{50}	a_{51}	a_{52}		a_{53}	a_{54}	a_{55}	y_5	a_{56}	a_{57}	a_{58}		a_{59}	$a_{5,10}$	$a_{5,11}$
a_{60}	a_{61}	a_{62}		a_{63}	a_{64}	a_{65}		a_{66}	a_{67}	a_{68}	y_6	a_{69}	$a_{6,10}$	$a_{6,11}$
a_{70}	a_{71}	a_{72}		a_{73}	a_{74}	a_{75}		a_{77}	a_{77}	a_{78}		a_{79}	$a_{7,10}$	$a_{7,11}$
		x_2				x_5				x_8				x_{11}
a_{80}	a_{81}	a_{82}	y_8	a_{83}	a_{84}	a_{85}		a_{86}	a_{87}	a_{88}		a_{89}	$a_{8,10}$	$a_{8,11}$
a_{90}	a_{91}	a_{92}		a_{93}	a_{94}	a_{95}	y_9	a_{96}	a_{97}	a_{98}		a_{99}	$a_{9,10}$	$a_{9,11}$
$a_{10,0}$	$a_{10,1}$	$a_{10,2}$		$a_{10,3}$	$a_{10,4}$	$a_{10,5}$		$a_{10,6}$	$a_{10,7}$	$a_{10,8}$	y_{10}	$a_{10,9}$	$a_{10,10}$	$a_{10,11}$
$a_{11,0}$	$a_{11,1}$	$a_{11,2}$		$a_{11,3}$	$a_{11,4}$	$a_{11,5}$		$a_{11,7}$	$a_{11,7}$	$a_{11,8}$		$a_{11,9}$	$a_{11,10}$	$a_{11,11}$

Two-dimensional partitioning

Processor grid $p = r \times c$, assume $r, c \approx \sqrt{p}$.



Key to the algorithm

- Consider block (i, j)
- it needs to multiple by the xs in column j
- it produces part of the result of row i

Algorithm

- Collecting x_j on each processor p_{ij} by an *allgather* inside the processor columns.
- Each processor p_{ij} then computes $y_{ij} = A_{ij}x_j$.
- Gathering together the pieces y_{ij} in each processor row to form y_i, distribute this over the processor row: combine to form a *reduce-scatter*.
- Setup for the next A or A^t 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	$\approx 2\frac{n^2}{p}\gamma$
Reduce-scatter y_i's within rows	

Reduce-scatter

Time:

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

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

Efficiency

Let $r = c = \sqrt{p}$, then

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

Strong scaling

Same story as before for $p \to \infty$:

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

No strong scaling

Weak scaling

Constant memory $M = n^2/p$:

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

Weak scaling

Constant memory $M = n^2/p$:

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

Weak scaling

Constant memory $M = n^2/p$:

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

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

LU factorizations

- Needs a cyclic distribution
- This is very hard to program, so:
- Scalapack, 1990s product, not extendible, impossible interface
- Elemental: 2010s product, extendible, nice user interface (and it is way faster)

Boundary value problems

Consider in 1D

$$\begin{cases} -u''(x) = f(x, u, u') & x \in [a, b] \\ u(a) = u_a,\, u(b) = u_b \end{cases}$$

in 2D:

$$\begin{cases} -u_{xx}(\bar{x}) - u_{yy}(\bar{x}) = f(\bar{x}) & x \in \Omega = [0, 1]^2 \\ u(\bar{x}) = u_0 & \bar{x} \in \delta\Omega \end{cases}$$

Approximation of 2nd order derivatives

Taylor series (write h for δx):

$$u(x+h) = u(x) + u'(x)h + u''(x)\frac{h^2}{2!} + u'''(x)\frac{h^3}{3!} + u^{(4)}(x)\frac{h^4}{4!} + u^{(5)}(x)\frac{h^5}{5!} + \cdots$$

and

$$u(x-h) = u(x) - u'(x)h + u''(x)\frac{h^2}{2!} - u'''(x)\frac{h^3}{3!} + u^{(4)}(x)\frac{h^4}{4!} - u^{(5)}(x)\frac{h^5}{5!} + \cdots$$

Subtract:

$$u(x+h) + u(x-h) = 2u(x) + u''(x)h^2 + u^{(4)}(x)\frac{h^4}{12} + \cdots$$

so

$$u''(x) = \frac{u(x+h) - 2u(x) + u(x-h)}{h^2} - u^{(4)}(x)\frac{h^4}{12} + \cdots$$

Numerical scheme:

$$-\frac{u(x+h) - 2u(x) + u(x-h)}{h^2} = f(x, u(x), u'(x))$$

(2nd order PDEs are very common!)

This leads to linear algebra

$$-u_{xx} = f \rightarrow \frac{2u(x) - u(x+h) - u(x-h)}{h^2} = f(x, u(x), u'(x))$$

Equally spaced points on $[0,1]$: $x_k = kh$ where $h = 1/(n+1)$, then

$$-u_{k+1} + 2u_k - u_{k-1} = -1/h^2 \, f(x_k, u_k, u_k') \quad \text{for } k = 1, \ldots, n$$

Written as matrix equation:

$$\begin{pmatrix} 2 & -1 & & \\ -1 & 2 & -1 & \\ & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} f_1 + u_0 \\ f_2 \\ \vdots \end{pmatrix}$$

Matrix properties

- Very sparse, banded
- Symmetric (only because 2nd order problem)
- Sign pattern: positive diagonal, nonpositive off-diagonal (true for many second order methods)
- Positive definite (just like the continuous problem)
- Constant diagonals (from constant coefficients in the DE)

Sparse matrix in 2D case

Sparse matrices so far were tridiagonal: only in 1D case.

Two-dimensional: $-u_{xx} - u_{yy} = f$ on unit square $[0,1]^2$

Difference equation:

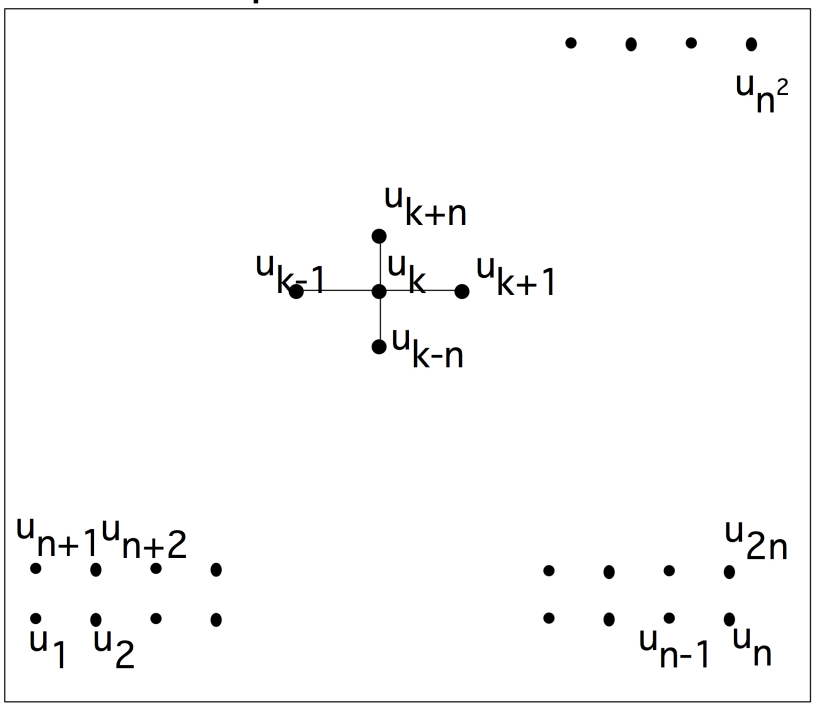
$$4u(x,y) - u(x+h,y) - u(x-h,y) - u(x,y+h) - u(x,y-h) = h^2 f(x,y)$$

$$4u_k - u_{k-1} - u_{k+1} - u_{k-n} - u_{k+n} = f_k$$

Consider a graph where $\{u_k\}_k$ are the edges
and (u_i, u_j) is an edge iff $a_{ij} \neq 0$.

The graph view of things

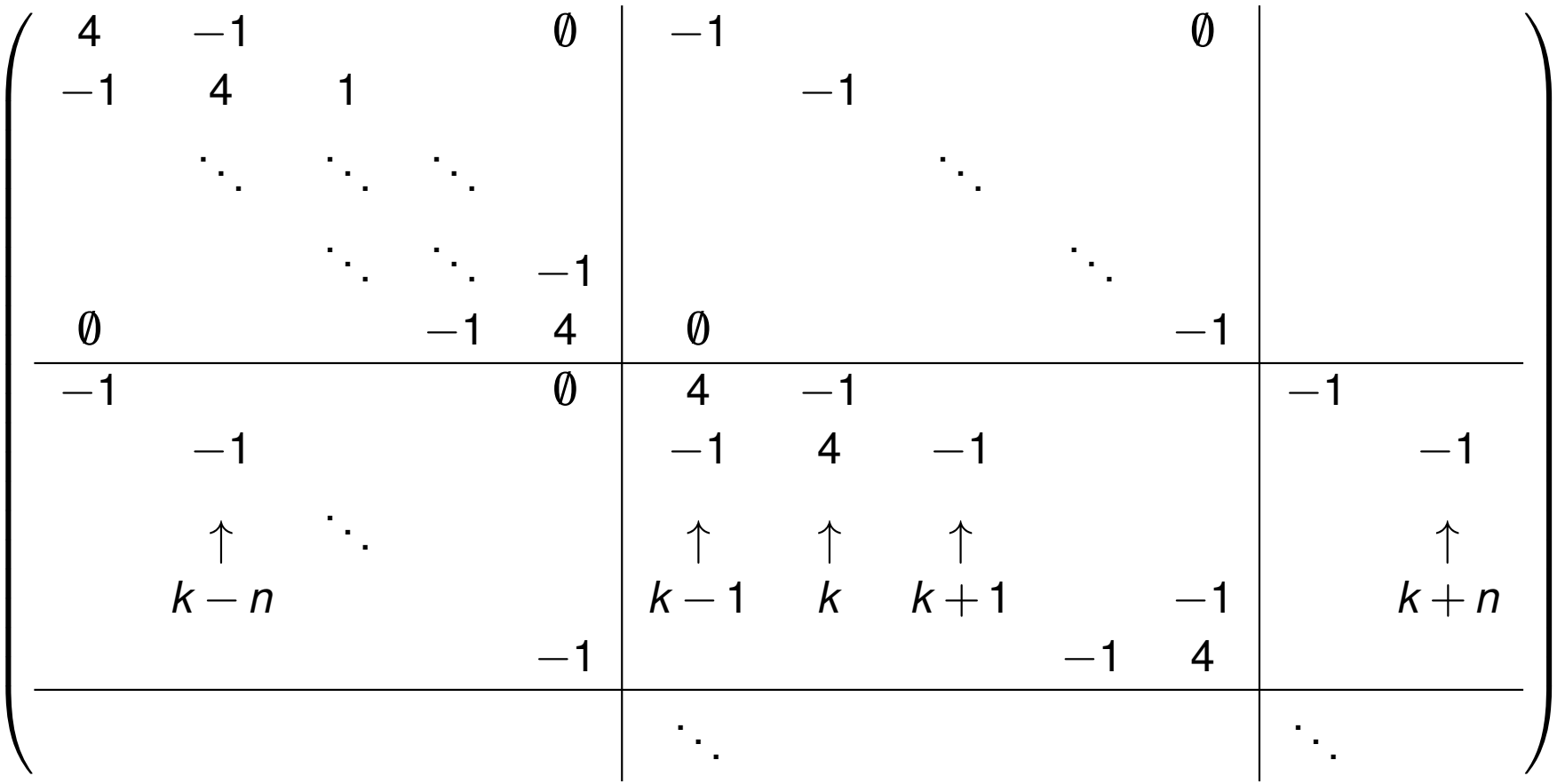
Poisson eq:



This is a graph!

This is the (adjacency) graph of a sparse matrix.

Sparse matrix from 2D equation



Matrix properties

- Very sparse, banded
- Factorization takes less than n^2 space, n^3 work
- Symmetric (only because 2nd order problem)
- Sign pattern: positive diagonal, nonpositive off-diagonal (true for many second order methods)
- Positive definite (just like the continuous problem)
- Constant diagonals: only because of the constant coefficient differential equation
- Factorization: lower complexity than dense, recursion length less than N.

Realistic meshes