Scalability of operations

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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.

Simple model of parallel computation

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

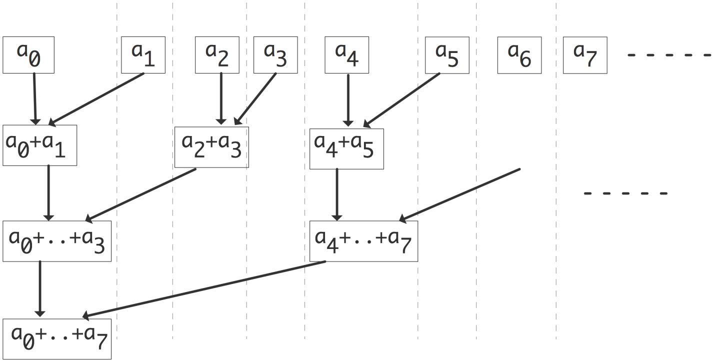
Send *n* items and do *m* operations:

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

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.

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.

Long vector broadcast

Combine scatter and 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

Complexity becomes

$$p\alpha + \beta n(p-1)/p$$

better if n large

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

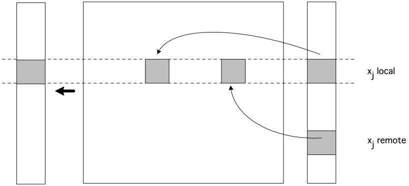
- F_s sequential fraction, F_p parallelizable fraction
- $F_s + F_p = 1$
- $T_1 = (F_s + F_p)T_1 = F_s T_1 + F_p T_1$
- Amdahl's law: $T_p = F_s T_1 + F_p T_1 / p$
- $P \rightarrow \infty$: $T_P \downarrow T_1 F_s$
- Speedup is limited by $S_P \leq 1/F_s$, efficiency is a decreasing function $E \sim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

Parallel matrix-vector product; general

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

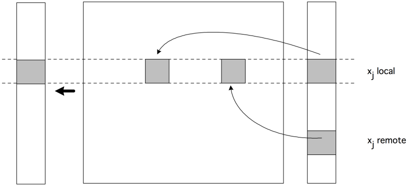


Mvp on processor p:

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

Local and remote operations

Local and remote parts:



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

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

Note possible overlap communication and computation;
only used in the sparse case

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

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

Strong scaling, weak scaling?

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, $p \rightarrow \infty$

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

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

x_0 a_{00} a_{01} a_{02} y_0 a_{10} a_{11} a_{12} a_{20} a_{21} a_{22} a_{30} a_{31} a_{32}	x_3 y_1	x_6 y_2	x_9 y_3
$x_1 \uparrow$ y_4	x_4 y_5	x_7 y_6	x_{10} y_7
$x_2 \uparrow$ y_8	x_5 y_9	x_8 y_{10}	x_{11} y_{11}

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 multi-ply	$\approx 2\frac{n^2}{p}\gamma$
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 multi-ply	$\approx 2\frac{n^2}{p}\gamma$
Reduce-scatter y_i's within rows	$\lceil \log_2(c) \rceil \alpha + \frac{c-1}{p} n\beta + \frac{c-1}{p} n\gamma$ $\approx \log_2(r)\alpha + \frac{n}{c}\beta + \frac{n}{c}\gamma$

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)