Scalability

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Justification

You have seen how the right use of MPI and OpenMP mechanisms can have a large influence on the performance of your code. However, sometimes you have to make design decisions on a deeper level. Here you will see the effects of a fundamental design choice in a simple algorithm.

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Simple model of parallel computation

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

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:

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

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	$x_0^{(0)}, x_1^{(0)}, x_2^{(0)}, x_3^{(0)}$	$x_0^{(0:1)}, x_1^{(0:1)}, x_2^{(0:1)}, x_3^{(0:1)}$	$x_0^{(0:3)}, x_1^{(0:3)}, x_2^{(0:3)}, x_3^{(0:3)}$
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.

Broadcast

- Run reduce algorithm backwards
- 'Recursive doubling'

Optimal complexity:

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

Attained:

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

Long vector broadcast

Combine scatter and bucket-allgather:

	$t=0$	$t=1$	*etcetera*
p_0	$x_0\downarrow$	$x_0 \quad x_3\downarrow$	$x_0, \quad x_2, x_3$
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	$x_3 \uparrow$	$x_2 x_3 \uparrow$	$x_0 x_1 x_2 x_3$

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

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

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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:

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

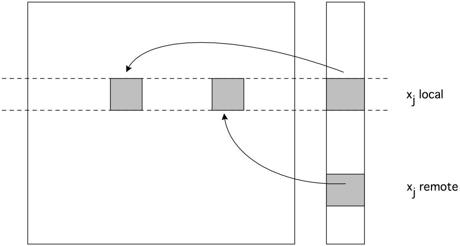
$$\forall_i\colon\ y_i = \sum_q \sum_{j\in I_q} a_{ij}x_j$$

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.



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

Exercise

How much can overlap help you?

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, $p \to \infty$

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

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}	$a_{3,10}$	$a_{3,11}$	y_3
	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}	$a_{7,10}$	$a_{7,11}$	y_7
		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}	$a_{10,9}$	$a_{10,10}$	$a_{10,11}$	
$a_{11,0}$	$a_{11,1}$	$a_{11,2}$		$a_{11,3}$	$a_{11,4}$	$a_{11,5}$		$a_{11,7}$	$a_{11,7}$	$a_{11,8}$		$a_{11,9}$	$a_{11,10}$	$a_{11,11}$	y_{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 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	$\lceil \log_2(c) \rceil \alpha + \frac{c-1}{p} n\beta + \frac{c-1}{p} n\gamma$ $\approx \log_2(r)\alpha + \frac{n}{c}\beta + \frac{n}{c}\gamma$

Efficiency

Let $r = c = \sqrt{n}$, 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)

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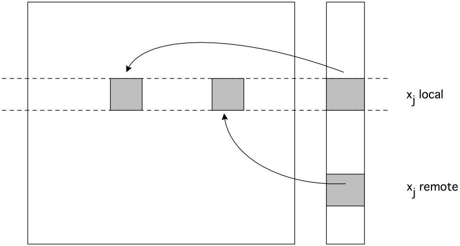
Local and remote operations

Local and remote parts:

$$\forall_i\colon y_i = \sum_{j\in\mathrm{local}} a_{ij}x_j + \sum_{j\in\mathrm{remote}} a_{ij}x_j$$

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



Combine:

Note possible overlap communication and computation;

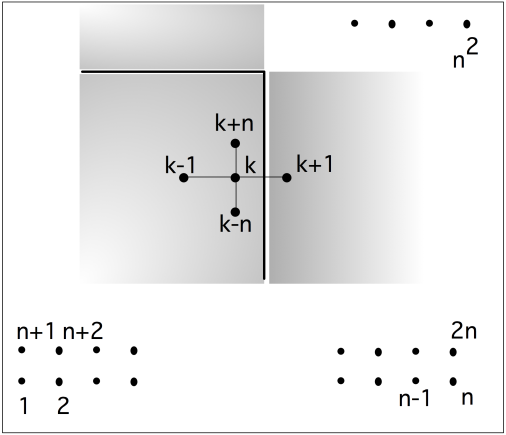
only used in the sparse case

Sparse matrix operations

- Traditional: PDE, discussed next
- New: graph algorithms and big data, discussed later

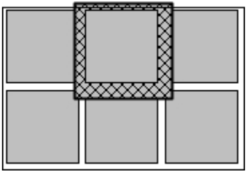
Operator view of spmvp

Difference stencil



Parallel operator view

induces ghost region:



Limited number of neighbours, limited buffer space

Matrix vs operator view

- Domain partitioning: processor 'owns' variable i
- owns all connections from i to other js
- $\Rightarrow$ processor owns whole matrix row
- $\Rightarrow$ 1D partitioning of the matrix, always

Scaling

- Same phenomenon as with dense matrix:
- n^2 variables, memory needed is cn^2/p
- 1D partitioning *of domain* does not weakly scale
  - Message size is one line: n
  - is $\sqrt{p}\sqrt{M}$, goes up with processors
- 2D partitioning *of domain* scales weakly.
  - message size $n/\sqrt{p} = \sqrt{M}$
  - constant in M

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Cholesky algorithm

$$\mathrm{Chol}\begin{pmatrix}A_{11} & A_{21}^t\\ A_{21} & A_{22}\end{pmatrix} = LL^t \qquad \text{where} \quad L = \begin{pmatrix}L_{11} & 0\\ \tilde{A}_{21} & \mathrm{Chol}(A_{22}-\tilde{A}_{21}\tilde{A}_{21}^t)\end{pmatrix}$$

and where $\tilde{A}_{21} = A_{21}L_{11}^{-t}$, $A_{11} = L_{11}L_{11}^t$.

Implementation

for $k = 1, \mathrm{nblocks}$:

`Chol`: factor $L_k L_k^t \leftarrow A_{kk}$

`Trsm`: solve $\tilde{A}_{>k,k} \leftarrow A_{>k,k} L_k^{-t}$

`Gemm`: form the product $\tilde{A}_{>k,k} \tilde{A}^t_{>k,k}$

`Syrk`: symmmetric rank-k update $A_{>k,>k} \leftarrow A_{>k,>k} - \tilde{A}_{>k,k} \tilde{A}^t_{>k,k}$

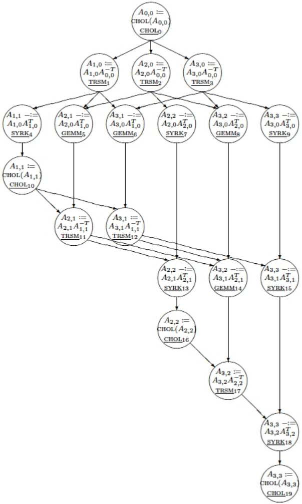
Blocked implementation

$$\left(\begin{array}{c|c|cc} & \multicolumn{3}{c}{\text{finished}} \\ \hline & A_{kk} & A_{k,k+1} & A_{k,k+2}\cdots \\ \hline & A_{k+1,k} & A_{k+1,k+1} & A_{k+1,k+2}\cdots \\ & A_{k+2,k} & A_{k+2,k+2} & \\ & \vdots & \vdots & \end{array}\right)$$

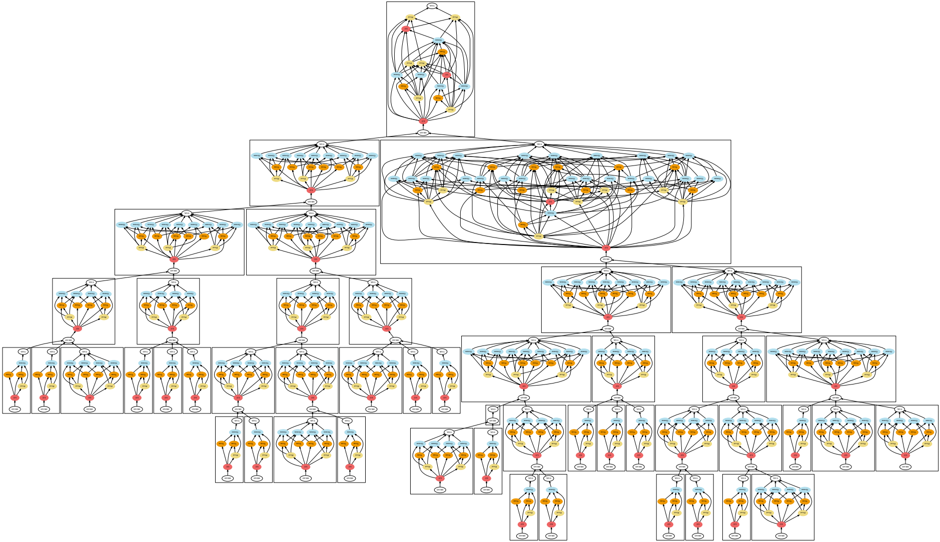
Extra level of inner loops:

for $k = 1, \mathrm{nblocks}$:
  `Chol`: factor $L_k L_k^t \leftarrow A_{kk}$
  for $\ell > k$:
    `Trsm`: solve $\tilde{A}_{\ell,k} \leftarrow A_{\ell,k} L_k^{-t}$
  for $\ell_1, \ell_2 > k$:
    `Gemm`: form the product $\tilde{A}_{\ell_1,k} \tilde{A}^t_{\ell_2,k}$
  for $\ell_1, \ell_2 > k$, $\ell_1 \leq \ell_2$:
    `Syrk`:symmmetric rank-k update
$$A_{\ell_1,\ell_2} \leftarrow A_{\ell_1,\ell_2} - \tilde{A}_{\ell_1,k} \tilde{A}^t_{\ell_2,k}$$

You can graph this



Sometimes…



DAG schedulers

- Directed Acyclic Graph (dataflow)
- Each node has dependence on other nodes, can execute when dependencies available
- Quark/DaGue (TN): dependence on memory area written
  pretty much limited to dense linear algebra
- OpenMP has a pretty good scheduler
- Distributed memory scheduling is pretty hard

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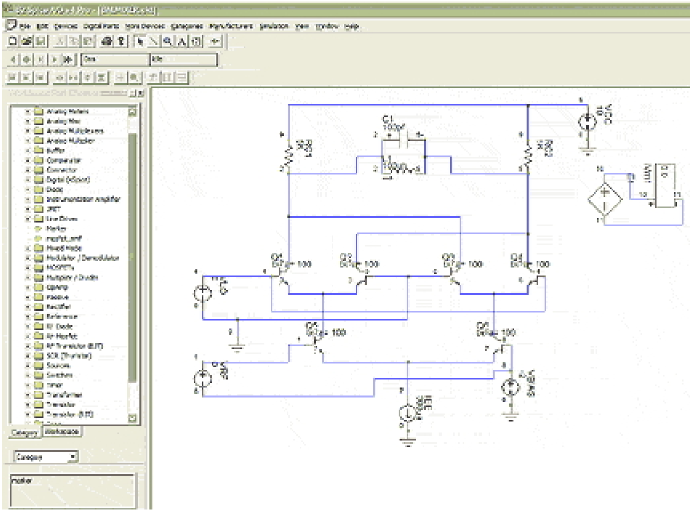
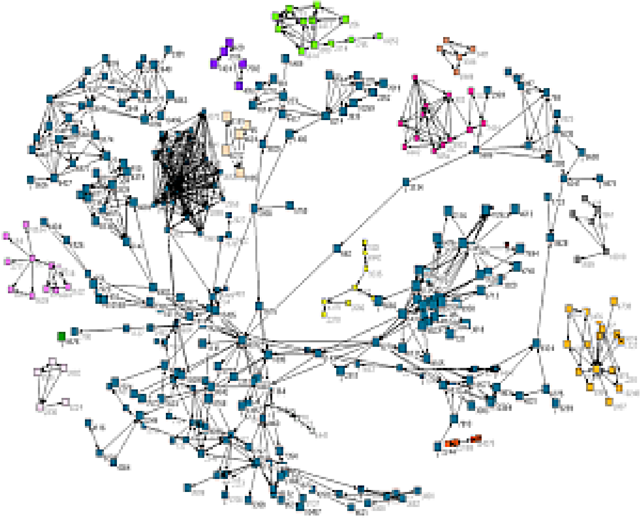
Graph algorithms

- Traditional: search, shortest path, connected components
- New: centrality

Traditional use of graph algorithms



1990s use of graph algorithms



2010 use of graph algorithms

2010 use of graph algorithms

Traditional graph algorithm

Input : A graph, and a starting node s
Output: A function $d(v)$ that measures the distance from s to v
Let s be given, and set $d(s) = 0$
Initialize the finished set as $U = \{s\}$
Set $c = 1$
while *not finished* **do**
    Let V the neighbours of U that are not themselves in U
    if $V = \emptyset$ **then**
        We're done
    else
        Set $d(v) = c + 1$ for all $v \in V$.
        $U \leftarrow U \cup V$
        Increase $c \leftarrow c + 1$

Computational characteristics

- Uses a queue: central storage
- Parallelism not self-evident
- Flexible assignment of work to processors, so no locality

Matrix formulation

Let

$$x_i = \begin{cases} 1 & i = s \\ \infty & \text{otherwise} \end{cases}$$

Let x zero except in i,
then $x^t G$ nonzero in j if there is an edge (i,j)

Matrix algorithm

Define a product as

$$y^t = x^t G \equiv \forall_i \colon (y^t)_j = \min_{i\colon G_{ij} \neq 0} x_i + 1,$$

Iterate

$$x, x^t G, x^t G^2, \ldots$$

After k (diameter) iterations $(x^t G^k)_i$ is the distance $d(s,i)$.

Single Source Shortest Path

Similar to previous, but non-unit edge weights

Let s be given, and set $d(s) = 0$
Set $d(v) = \infty$ for all other nodes v
for $|E|-1$ *times* **do**
  for *all edges* $e = (u,v)$ **do**
    Relax: **if** $d(u) + w_{uv} < d(v)$ **then**
      Set $d(v) \leftarrow d(u) + w_{uv}$

$$y^t = x^t G \equiv \forall_i \colon y_j = \min\bigl\{x_j, \min_{i \colon G_{ij} \neq 0} \{x_i + g_{ij}\}\bigr\},$$

All-pairs shortest path

$$\Delta_{k+1}(u,v) = \min\left\{\Delta_k(u,v), \Delta_k(u,k) + \Delta_k(k,v)\right\}. \tag{1}$$

Algebraically:

for k *from zero to* $|V|$ **do**
$\quad D \leftarrow D._{\min}\left[D(:,k) \min\cdot_+ D(k,:)\right]$

Similarity to Gaussian elimination

Pagerank

T stochastic: all rowsums are 1.

Prove $x^te = 1 \Rightarrow x^tT = 1$

Pagerank is essentially a power method: $x^t, x^tT, x^tT^2, \ldots$ modeling page transitions.

Prevent getting stuck with random jump:

$$x^t \leftarrow sx^tT + (1-s)e^t$$

Solution of linear system:

$$x^t(I - sT) = (1-s)e^t$$

Observe

$$(I - sT)^{-1} = I + sT + s^2T^2 + \cdots$$

‘Real world’ graphs

- Graphs imply sparse matrix vector product
- . . . but the graphs are unlike PDE graphs
- differences:
  - low diameter
  - high degree
  - power law
- treat as random sparse: use dense techniques
- 2D matrix partitioning: each block non-null, but sparse

Parallel treatment

- Intuitive approach: partitioning of nodes
- equivalent to 1D matrix distribution
- not scalable $\Rightarrow$ 2D distribution
- equivalent to distribution of edges
- unlike with PDE graphs, random placement may actually be good