Parallel numerical algorithms: Course overview

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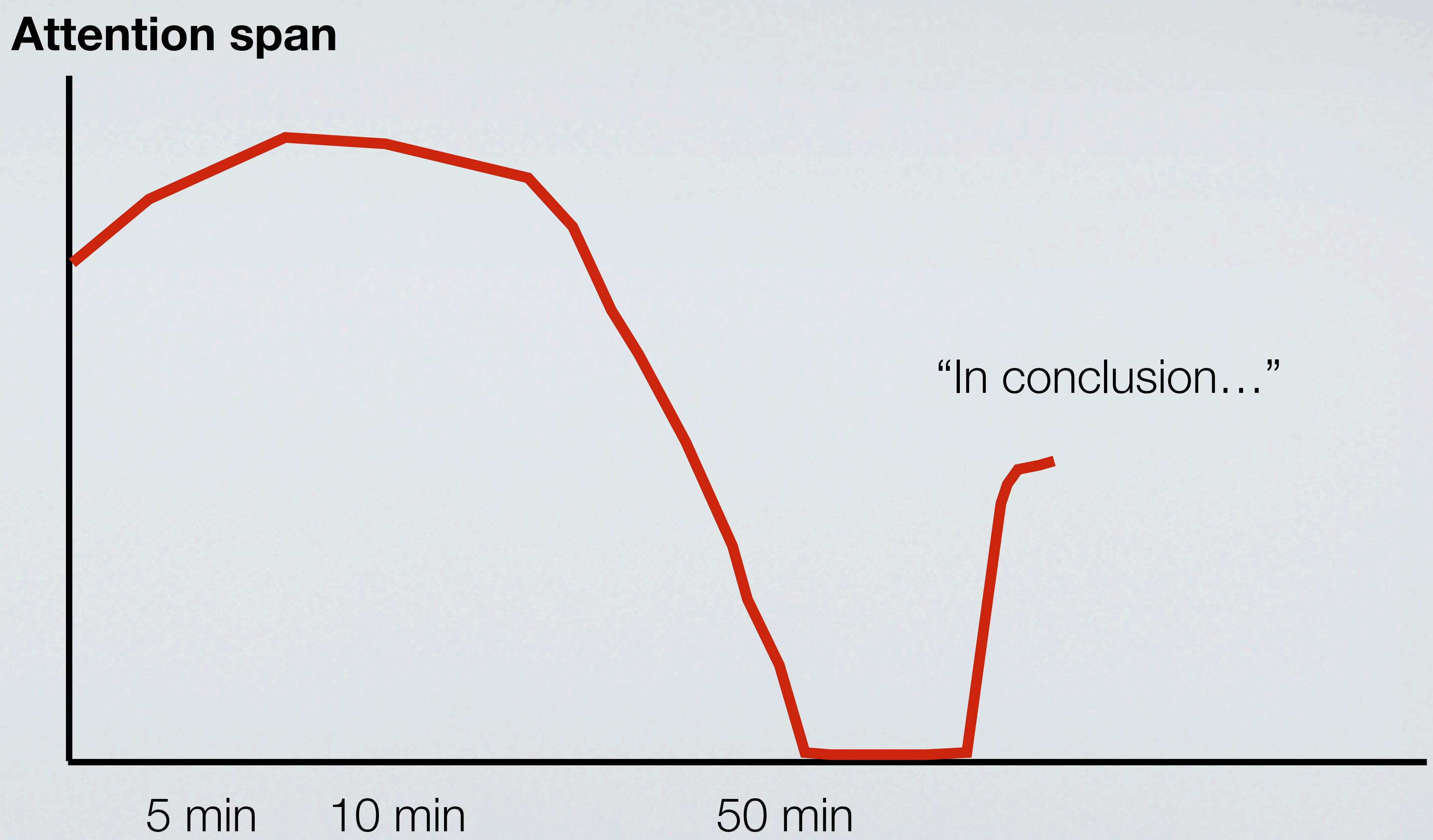
Georgia Institute of Technology

CSE/CS 8803 PNA, Spring 2008

[L.01] Tuesday, January 8, 2008

Sources for today's material

- CS 267 (Yelick @UCB)
- David Keyes
- Williams, *et al*. SC'07 (UCB)
- Higham, *Accuracy and Stability of Numerical Algorithms*



Lecture: Patterson's Law of Attention Span

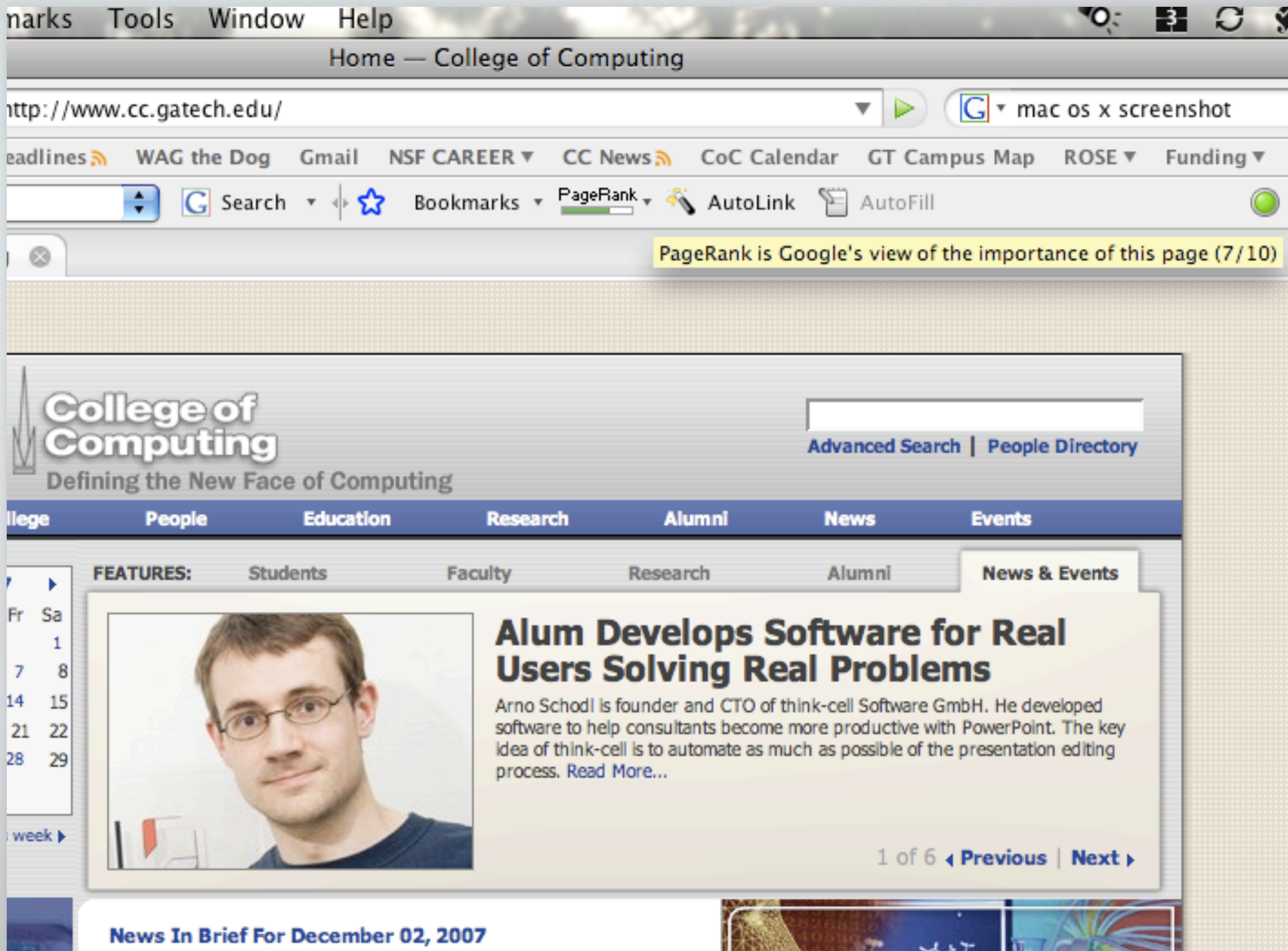
D. Patterson (UC Berkeley)

Why study PNA today?

Why study PNA today?

- Current and **future** apps are numerical, data-intensive
- Parallel hardware widely available
  - *Computing industry betting its future on it!* (next lecture)
- Need to program for parallelism and locality explicitly
- Algorithmic costs changed: “mops” not flops; “accuracy”
- “Winners” unclear

- Interaction of applications, algorithms, and systems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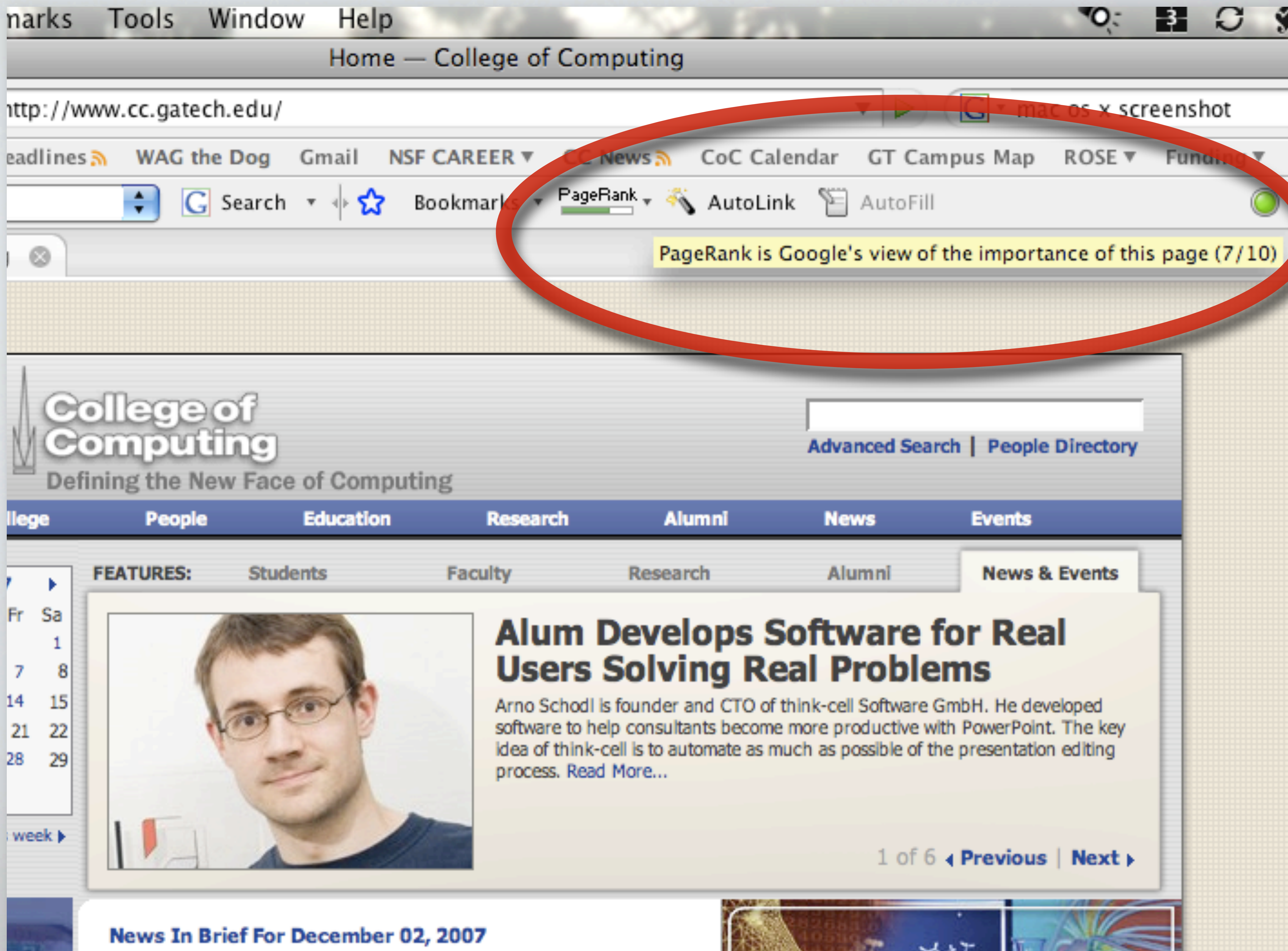
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Application example: Google’s PageRank

Google’s web search procedure

- Step 1: Rank all web pages, given the web
  - Update every once in a while
- Step 2: Return list of matching pages in order by rank, given query
  - At “query-time”

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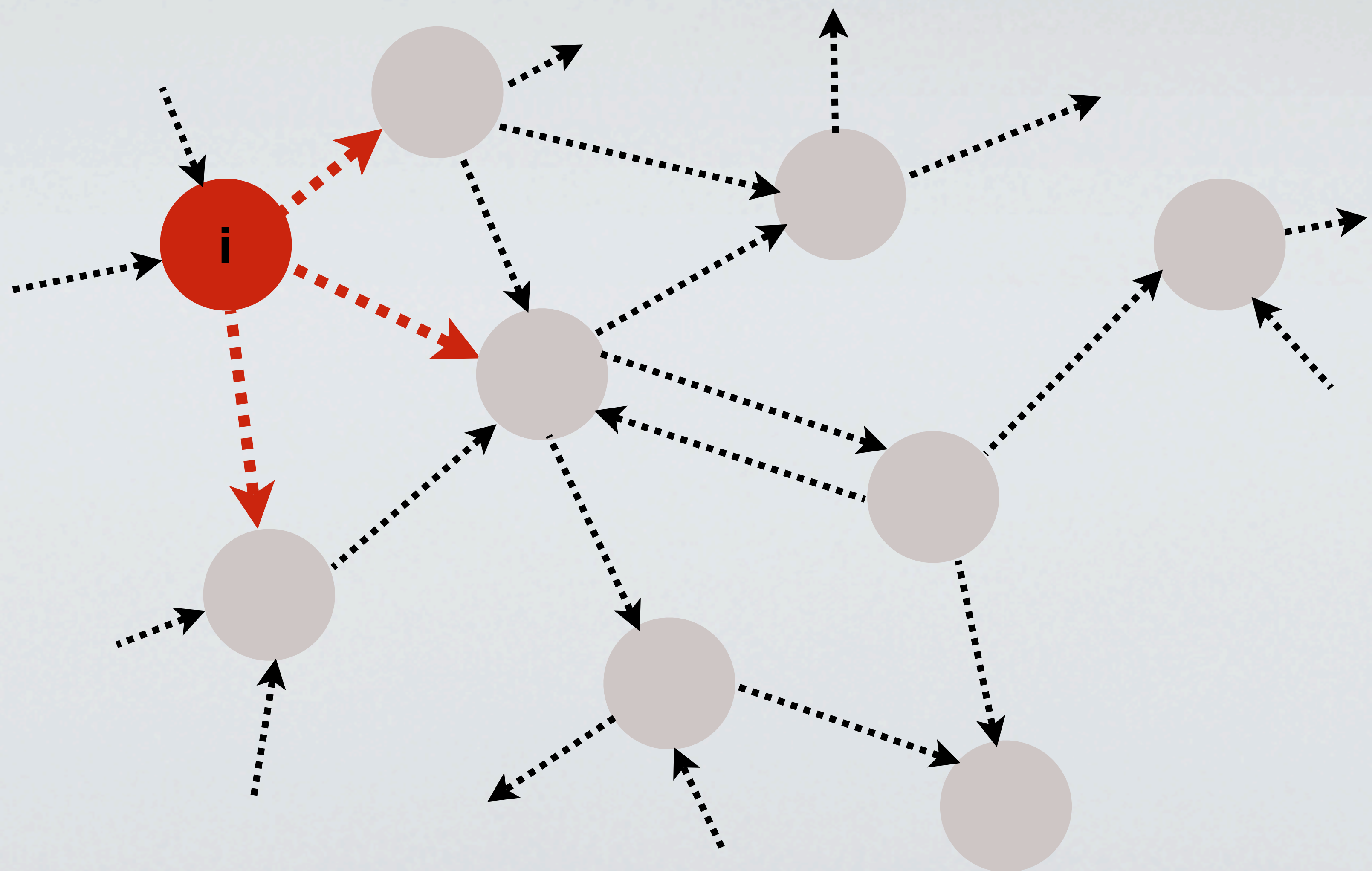
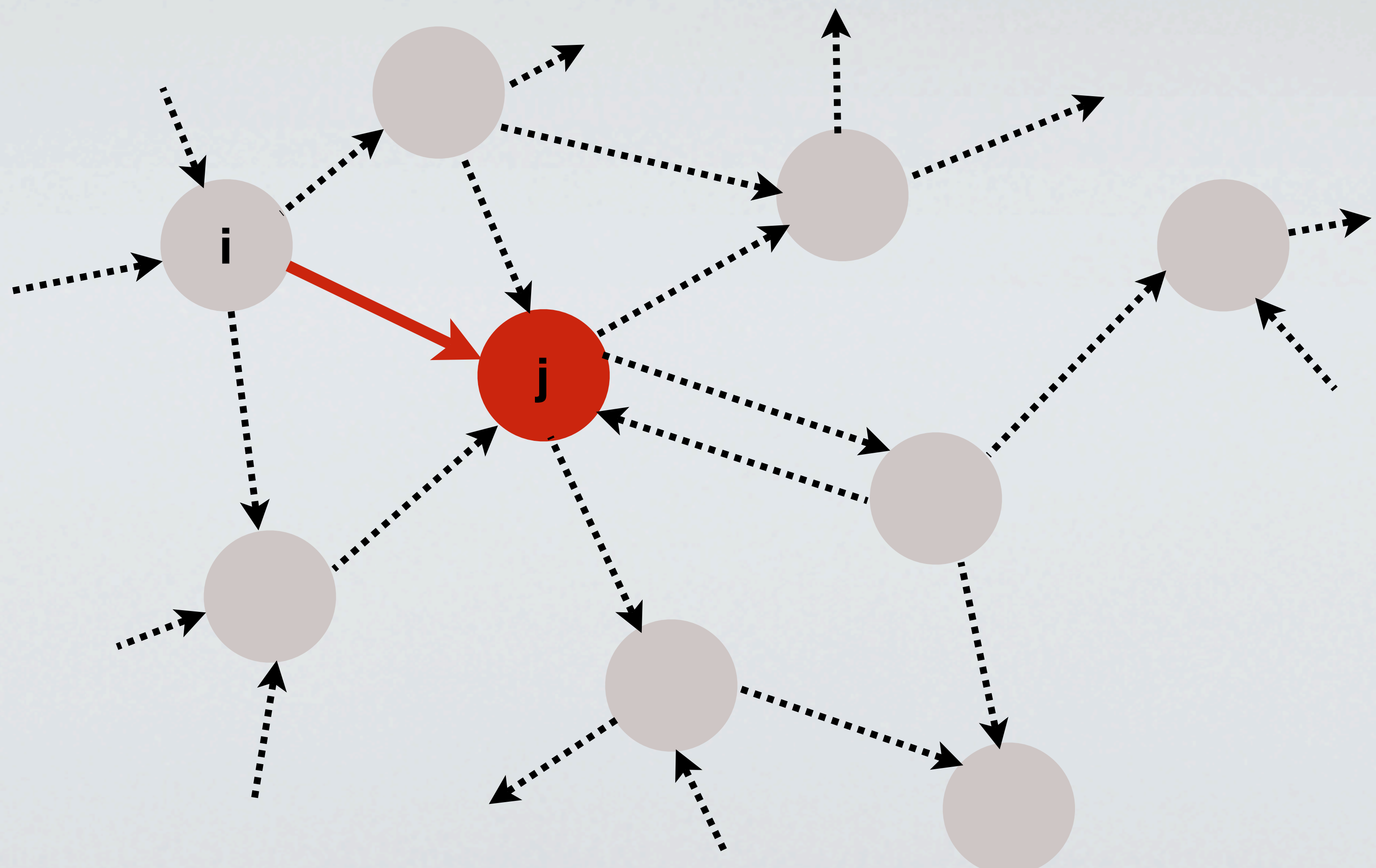
- Step 2: Return list of matching pages in order by rank, given query
  - At “query-time”
- **Compute ranking using a “random surfer” model**



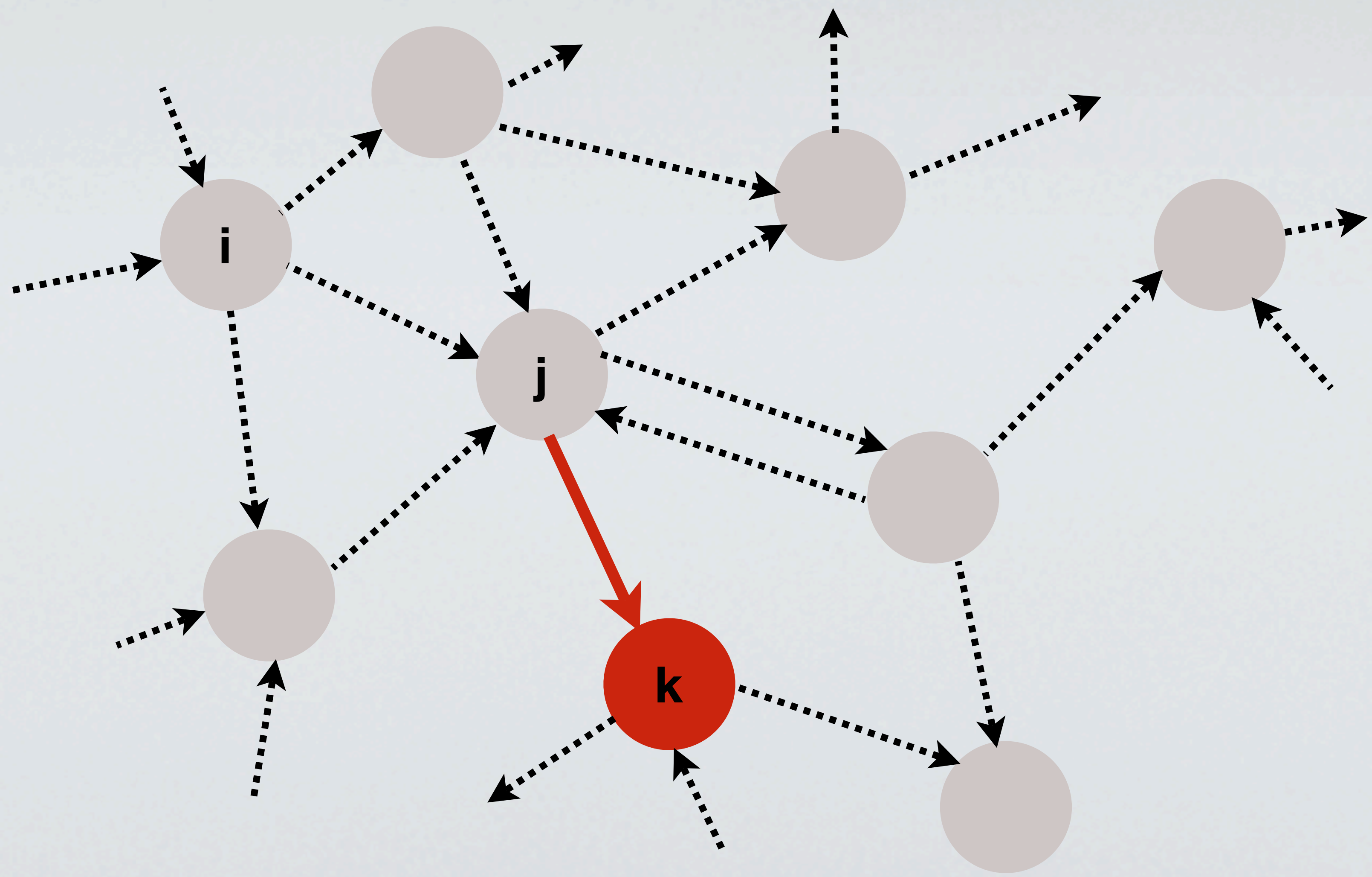
Start on page *i*.

A “random surfer” model.



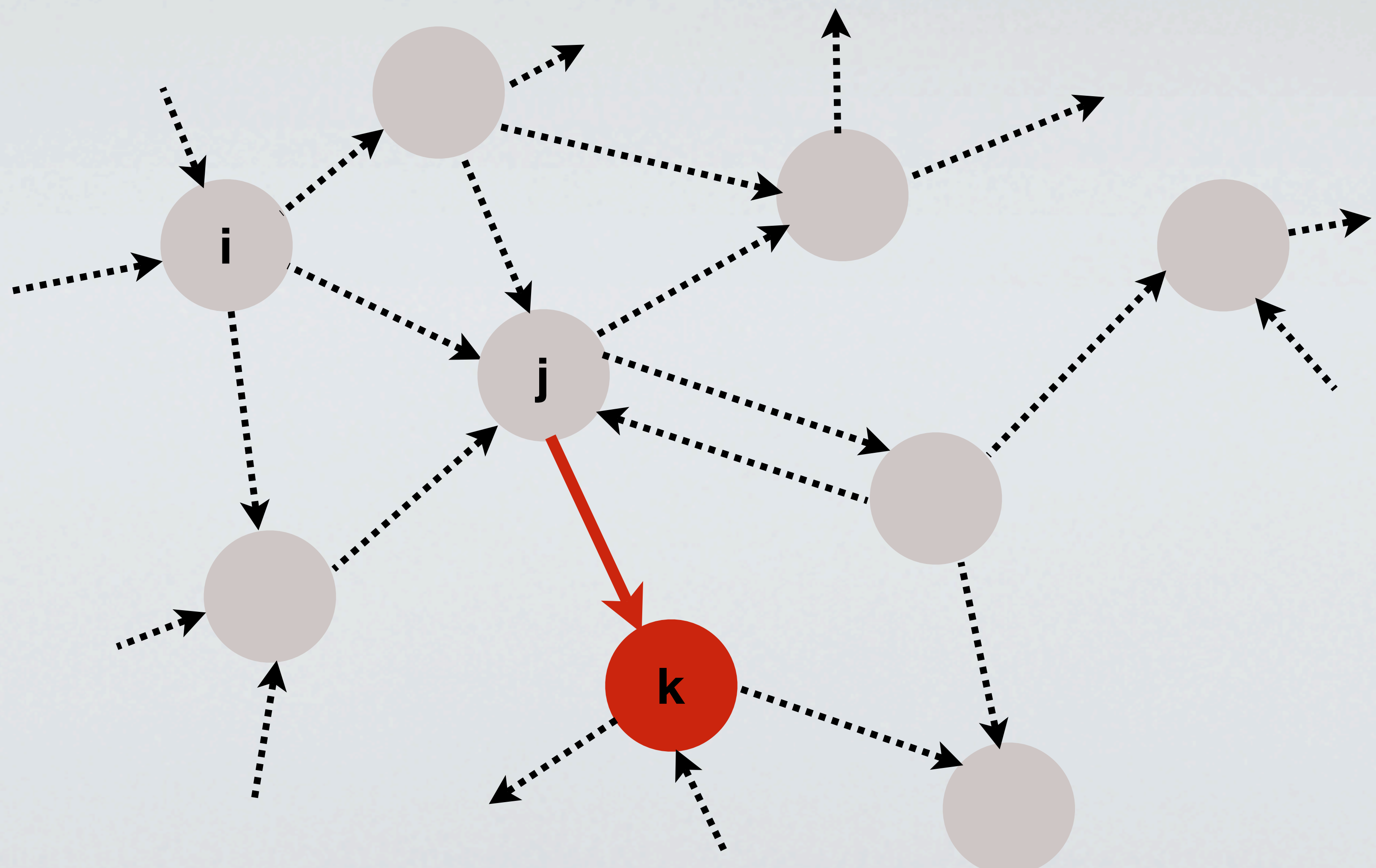
Jump to *j* with some probability.

A “random surfer” model.



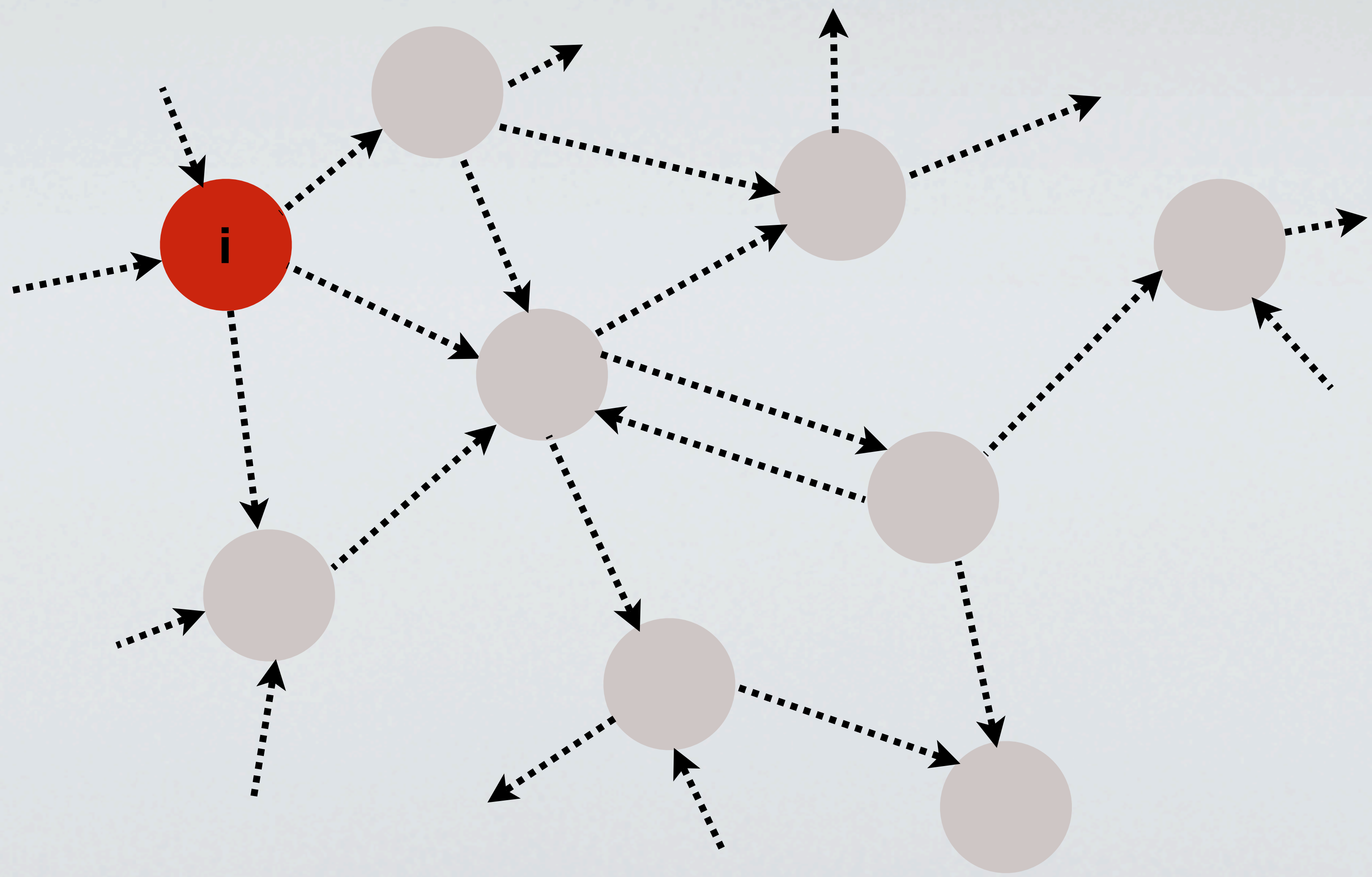
Repeat.

A “random surfer” model.



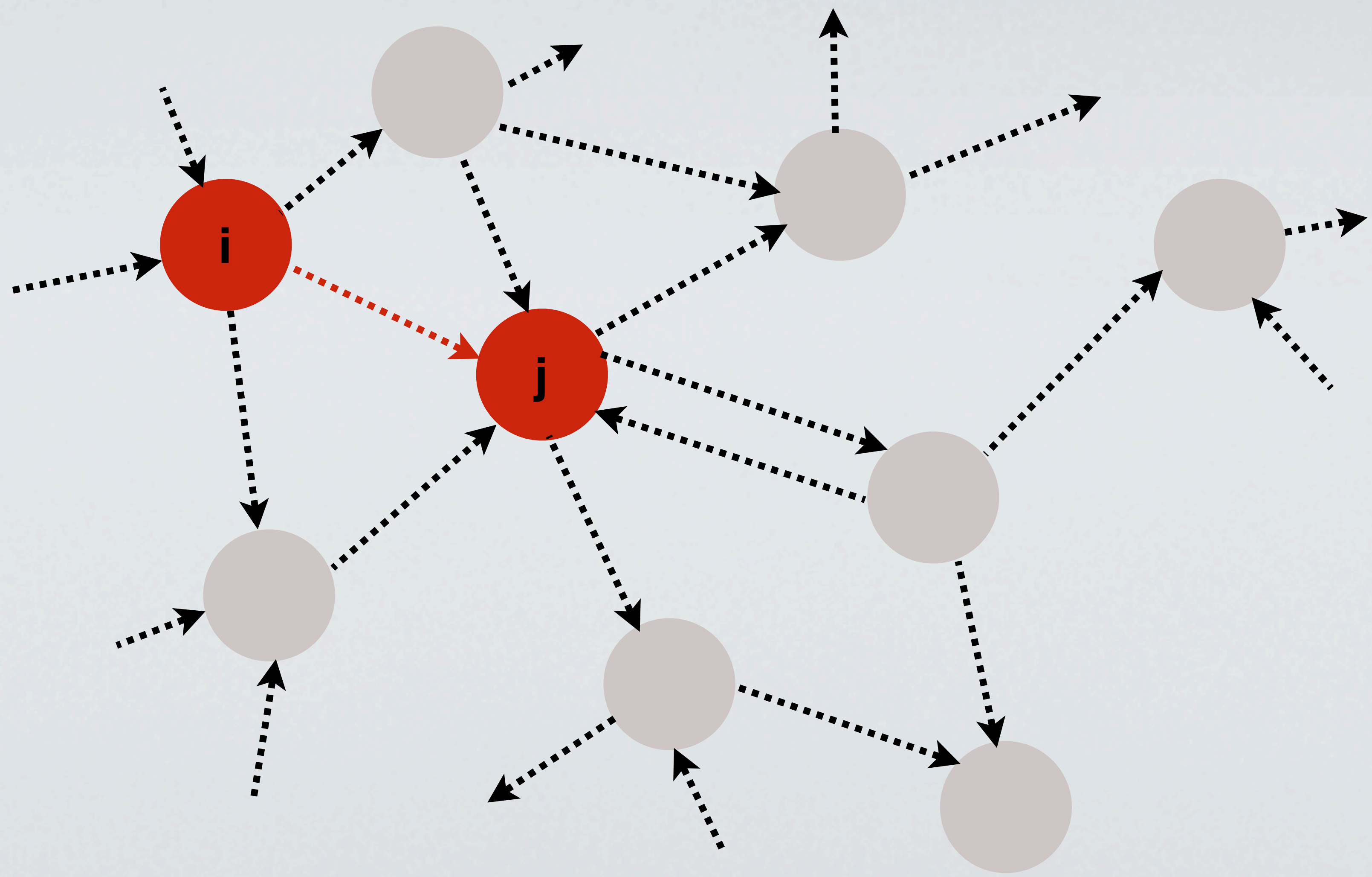
Where will the surfer end up?

A “random surfer” model.



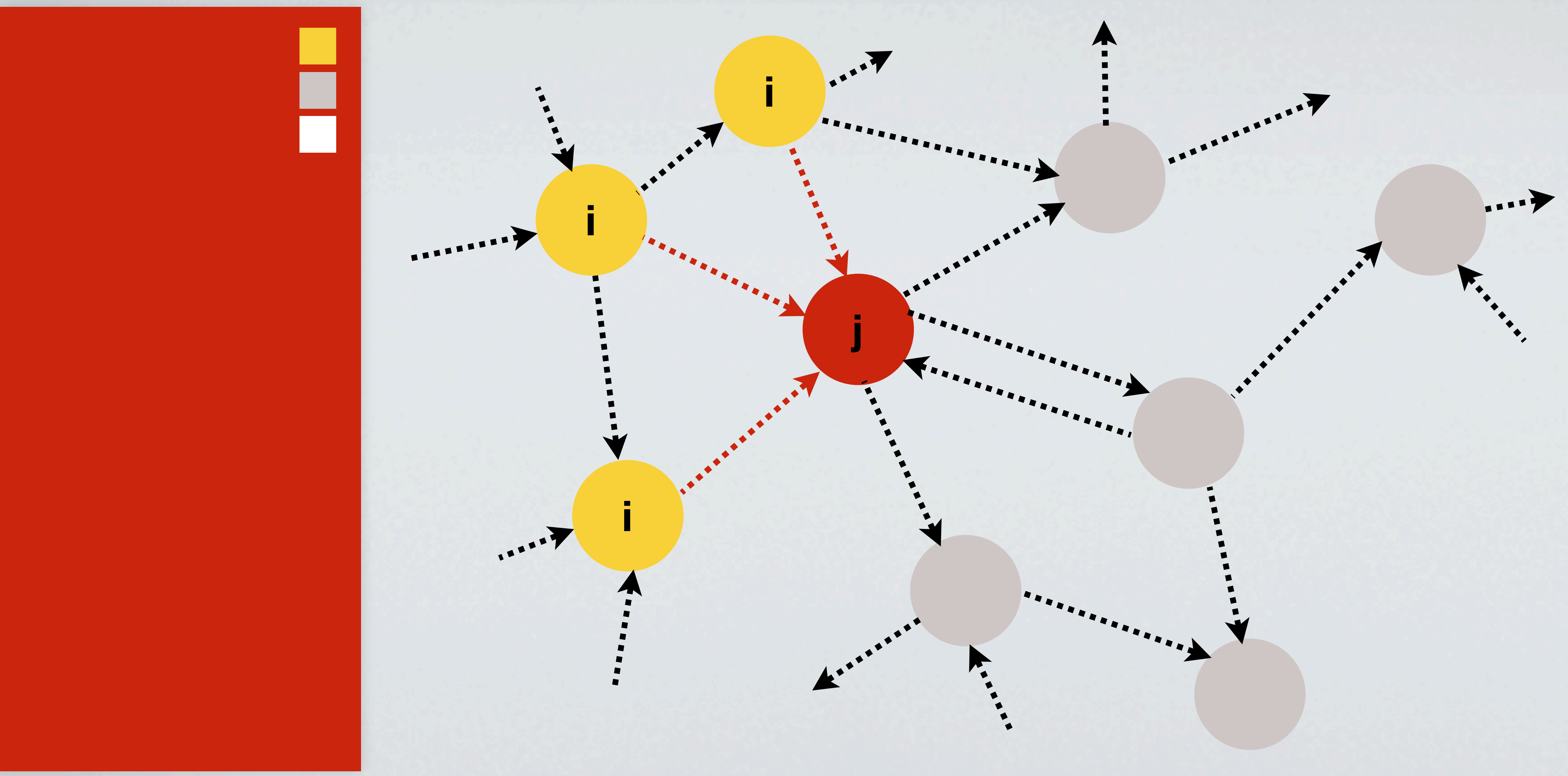
$$x_t(i)$$

Probability of being on page *i* at time *t*.



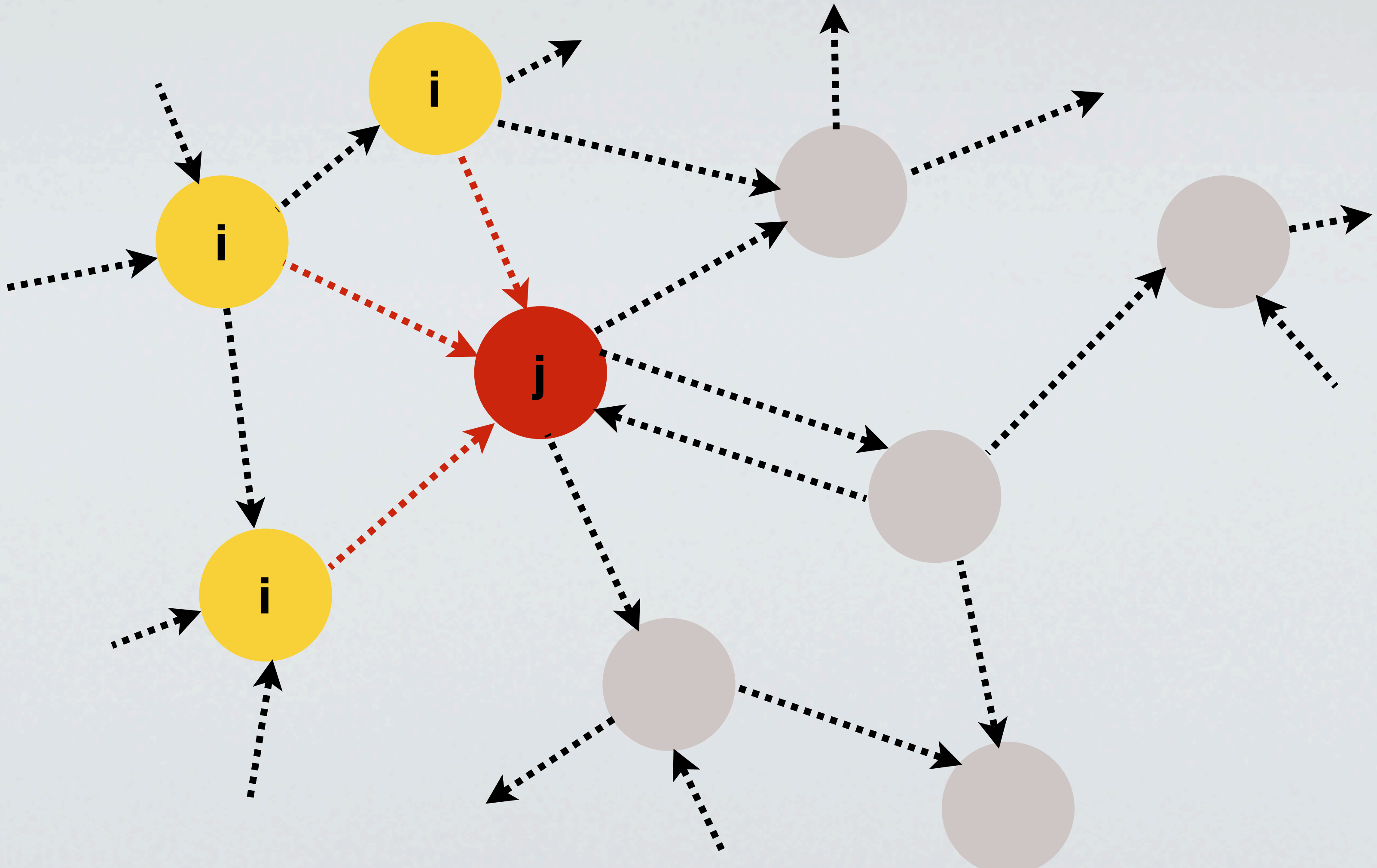
$$W(i, j)$$

Transition probability (=0 if no link).



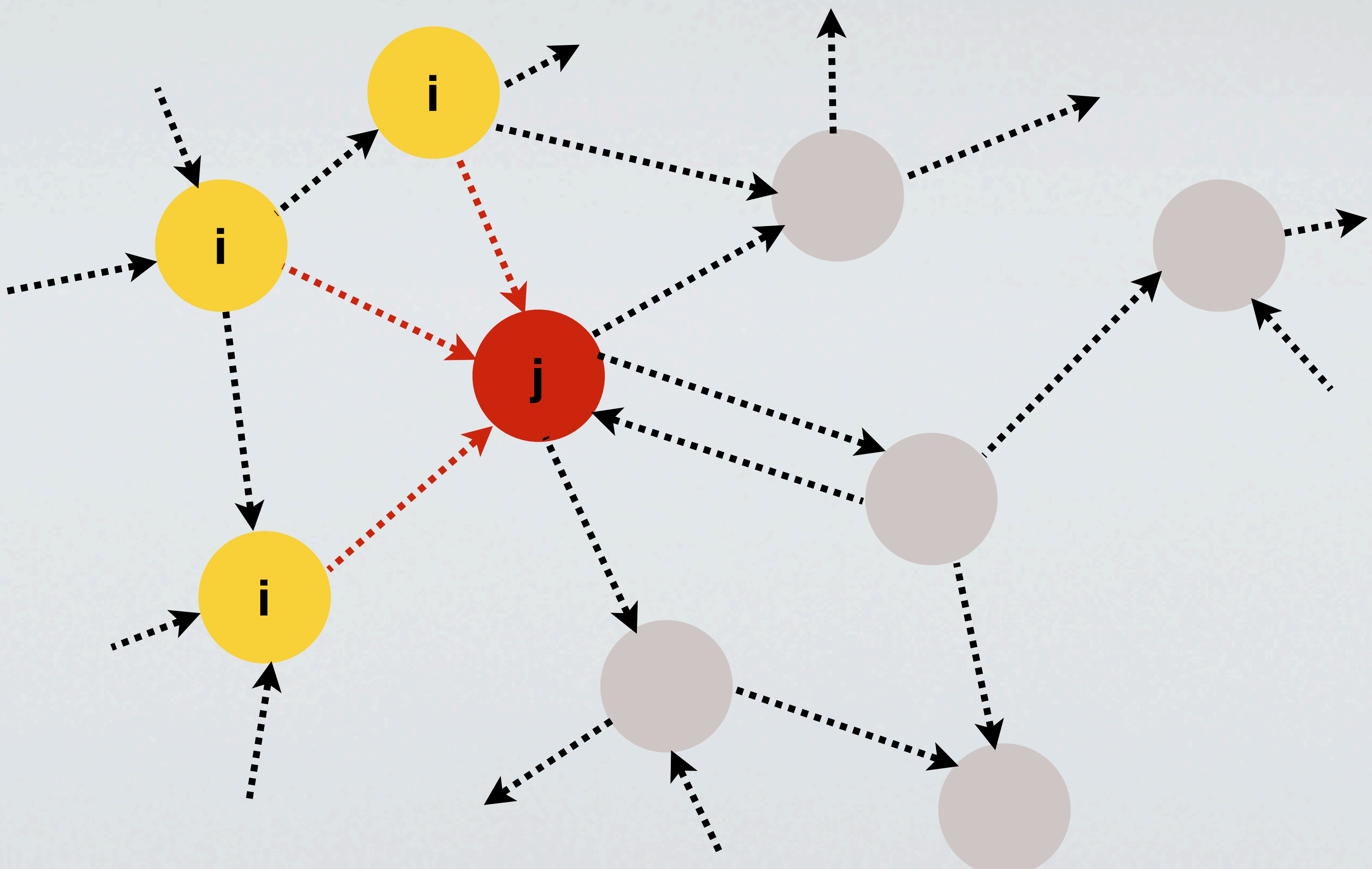
$$x_{t+1}(j) = \sum_{i=1}^{n} x_t(i) \cdot W(i,j)$$

Probability of being on page *j* at time *t+1*, with transition probability *W(i,j)*.



$$x_{t+1} = W^T \cdot x_t$$

Repeat **matrix-vector multiply** until convergence.



$$
\begin{aligned}
x_{t+1} &= W^T \cdot x_t = (W^T)^2 \cdot x_{t-1} = \cdots \\
&= (W^T)^{t+1} \cdot x_0
\end{aligned}
$$

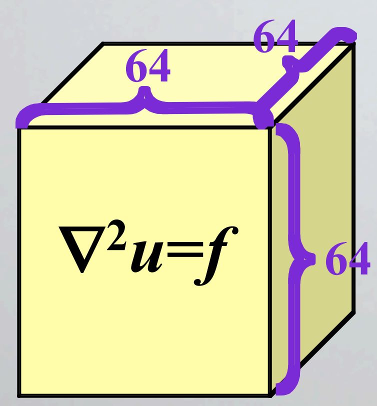
“Power method” for computing the principal eigenvector of W^T.

Applications and architectures

Units of measurement

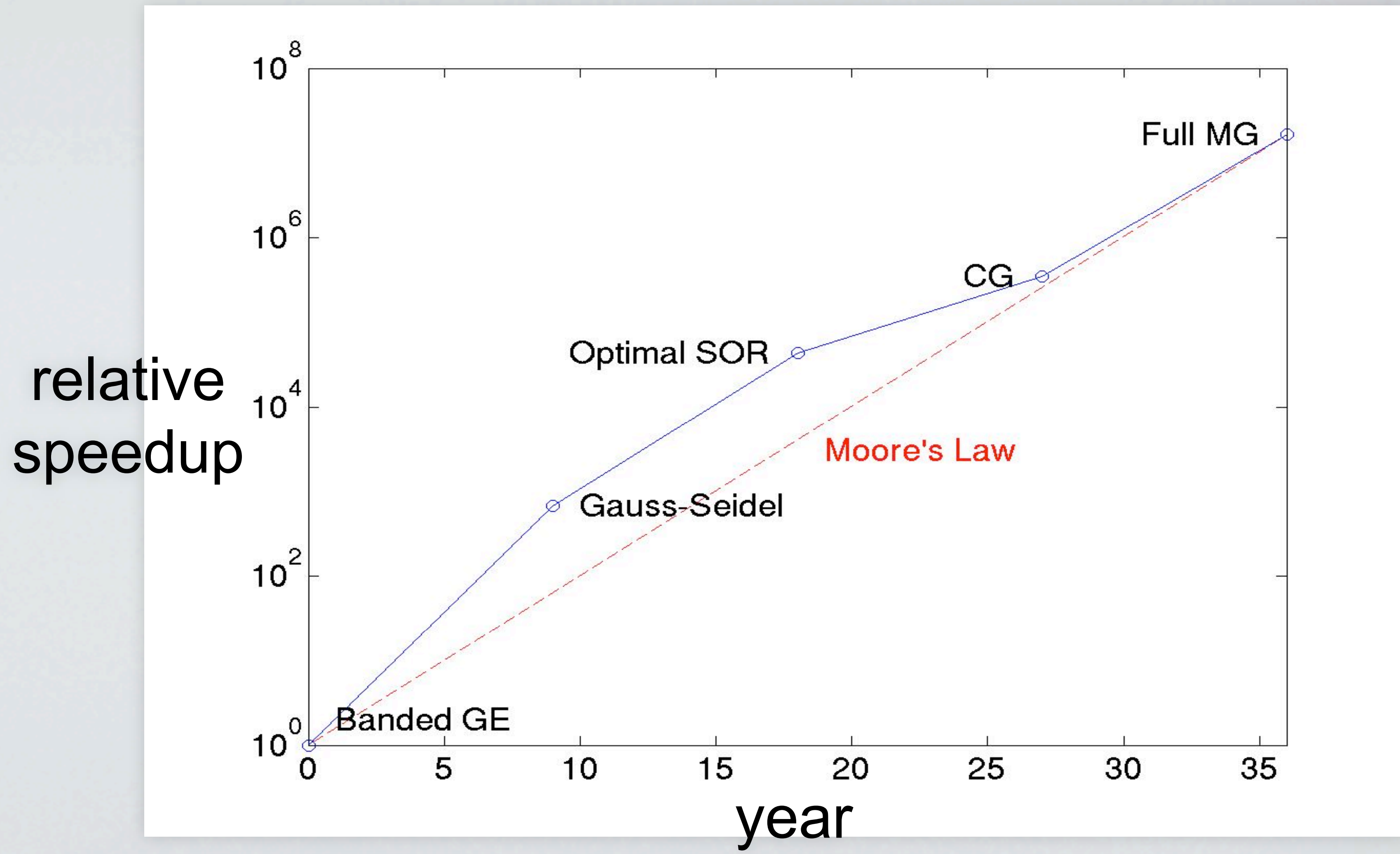
- “Flop”: Floating-point operation
- “Flop/s”: Flops per second
- “Bytes”: Size of data (double-precision float is 8 bytes)
- Today’s peak speeds
  - Single processor core ~5 Gflop/s
  - STI-Cell (8-core) ~15 Gflop/s
  - NVIDIA Tesla (128-core) ~500 Gflop/s
- Note: Achievable speeds often < 10% of peak

Year	Method	Reference	Storage	Flops
1947	Gaussian Elimination	Von Neumann & Goldstine	n^5	n^7
1950	Optimal SOR	Young	n^3	$n^4 \log n$
1971	Conj. grad.	Reid	n^3	$n^{3.5} \log n$
1984	Full multigrid	Brandt	n^3	n^3



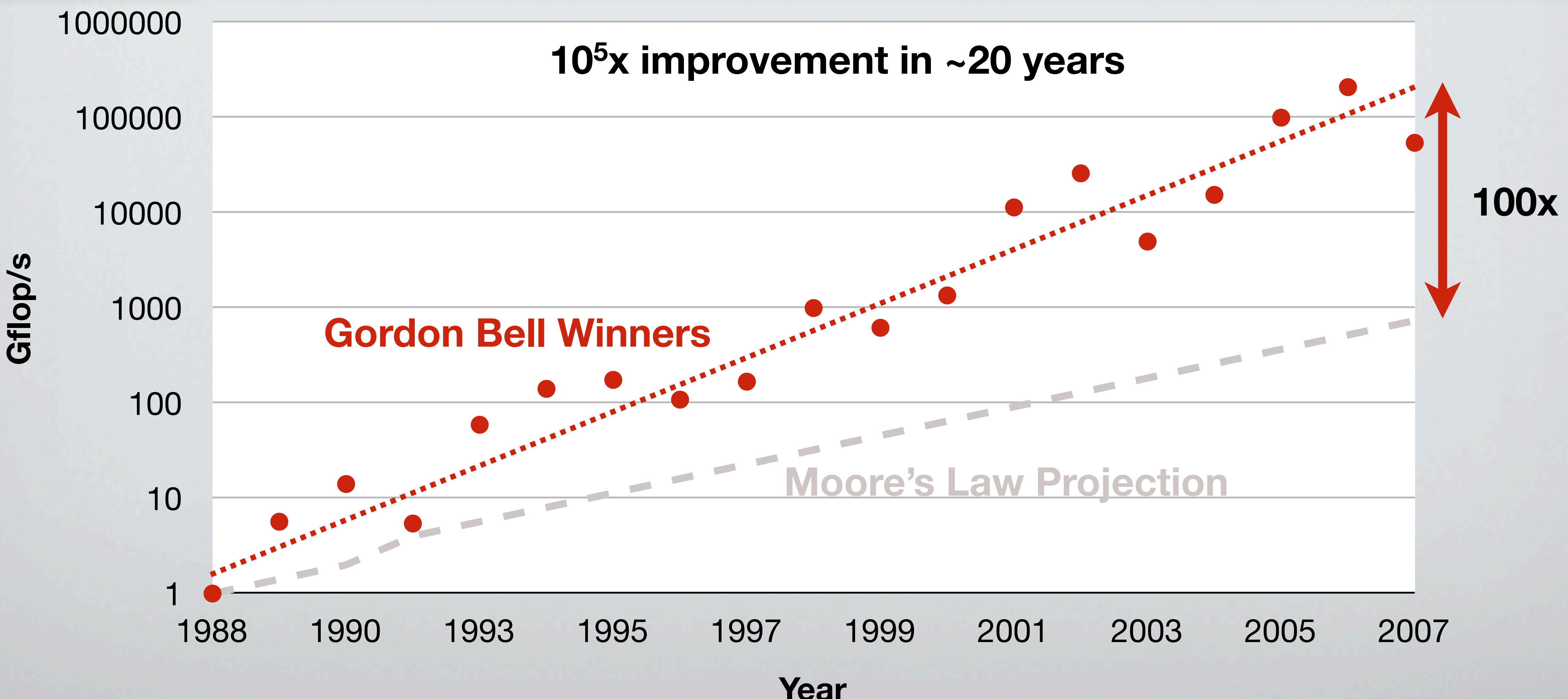
Algorithmic efficiency rivals architectural advances in scale.

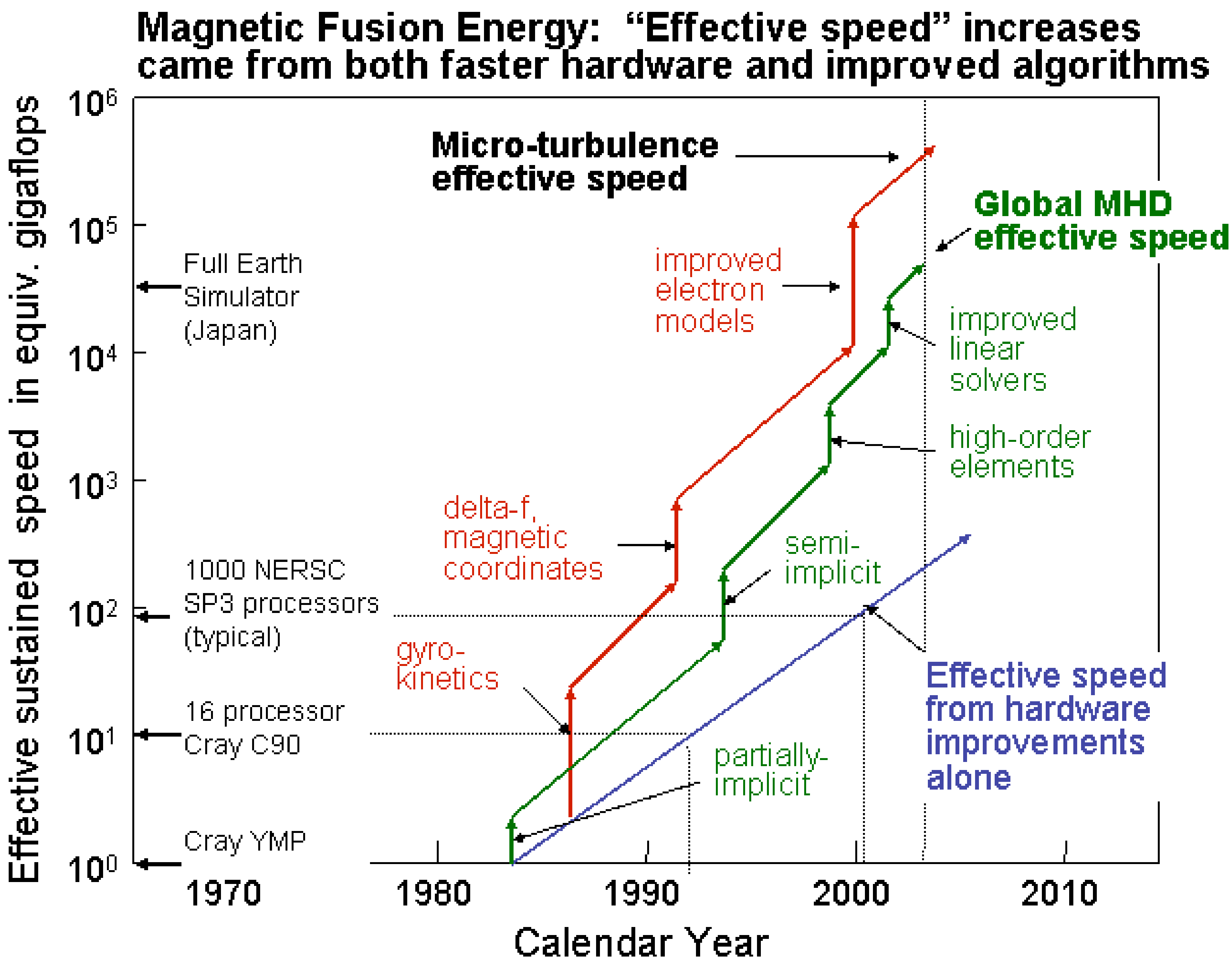
If n=64, flops reduced by ~16 M [6 mo. to 1 sec.]; Source: Keyes (2004)



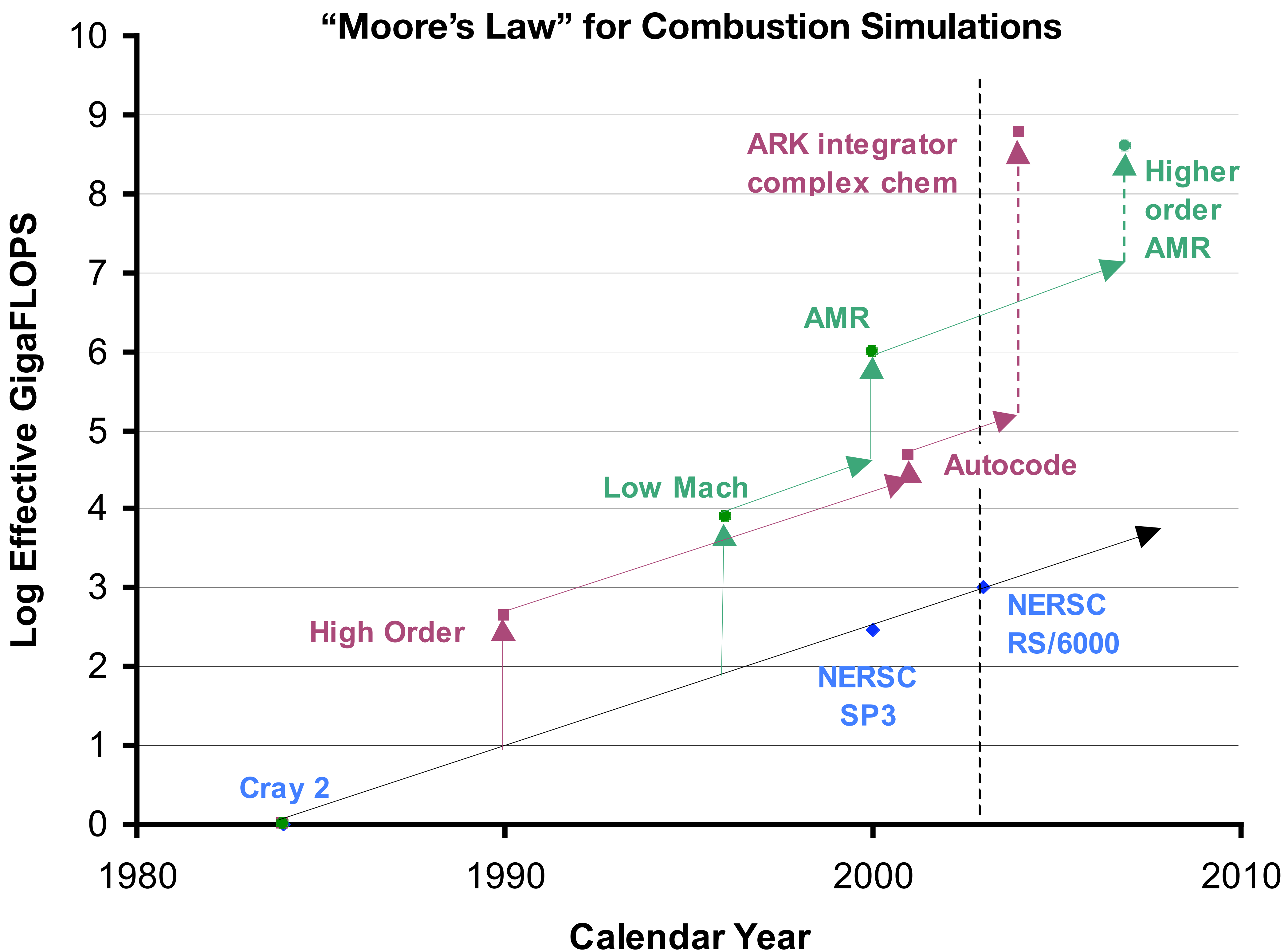
Algorithmic and architectural improvements go hand-in-hand.

Parallelism and algorithmic innovation outpace Moore's Law





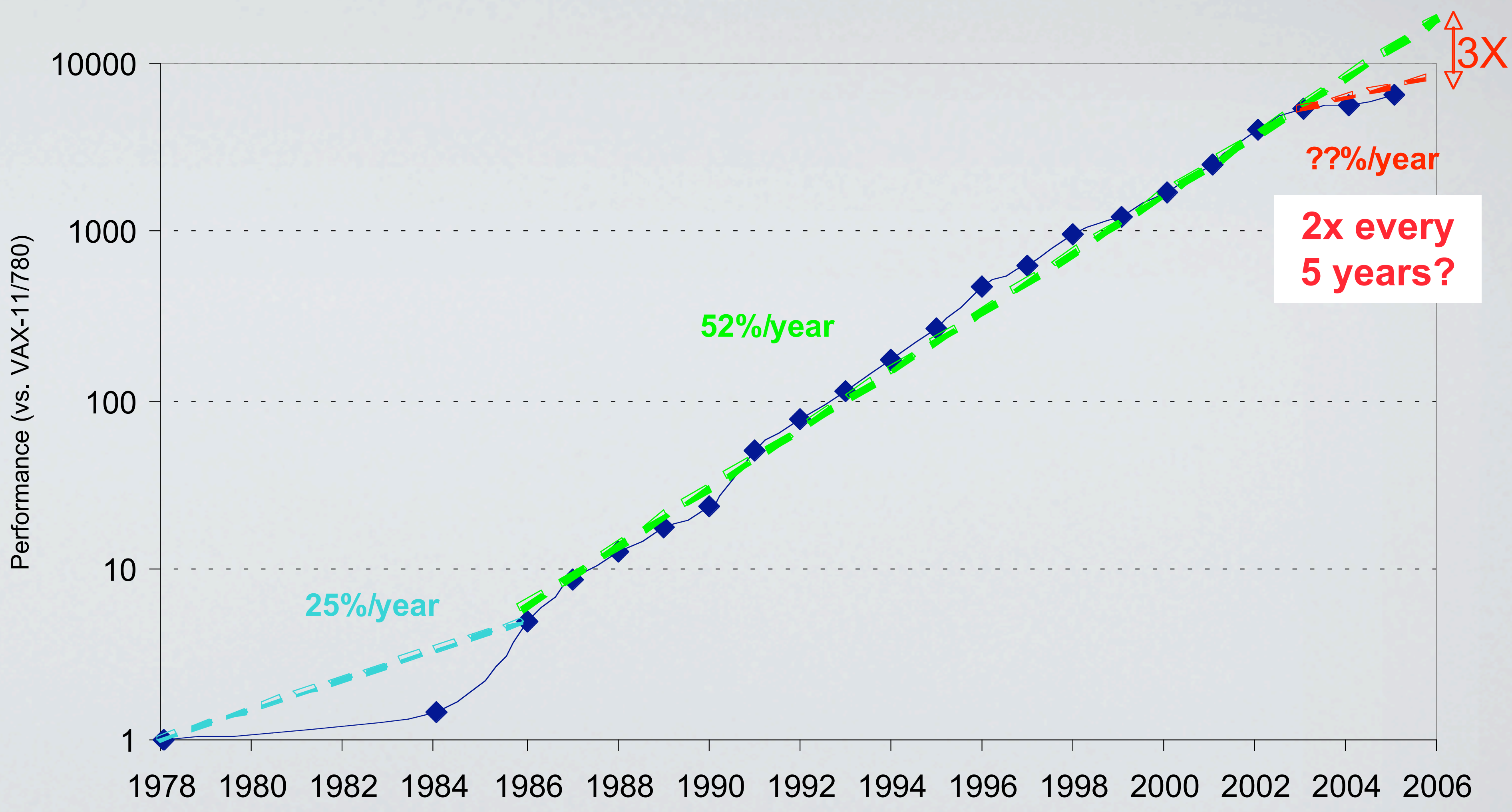
Source: SCaLeS report 2 (2004), *via* D. Keyes. http://pnl.gov/scales



Source: SCaLeS report 2 (2004), *via* D. Keyes. http://pnl.gov/scales

Intel, on their hardware strategy:

"We are dedicating all of our future product development to multicore designs. … This is a sea change in computing." (2005)



Uniprocessor performance not keeping up with Moore's law.

Source: Hennessey and Patterson, CA:AQA (4th edition), 2006

What’s so hard about parallel programming?

On p processors with fraction s serial work:

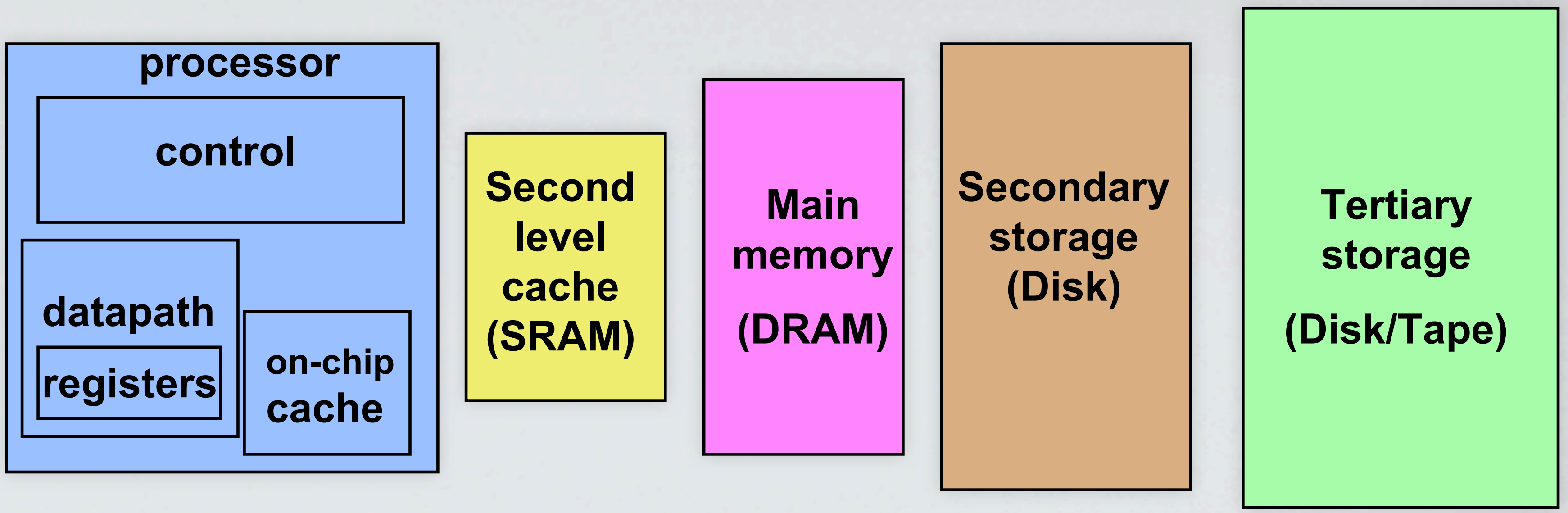
$$\begin{aligned}\text{Speedup}(p) &= \frac{\text{Time}(1)}{\text{Time}(p)} \\ &\leq \frac{1}{s + \frac{1-s}{p}} \\ &\leq \frac{1}{s}\end{aligned}$$

Finding enough parallelism.

Amdahl's Law: Maximum speedup limited by sequential part.

Parallelism incurs overheads.

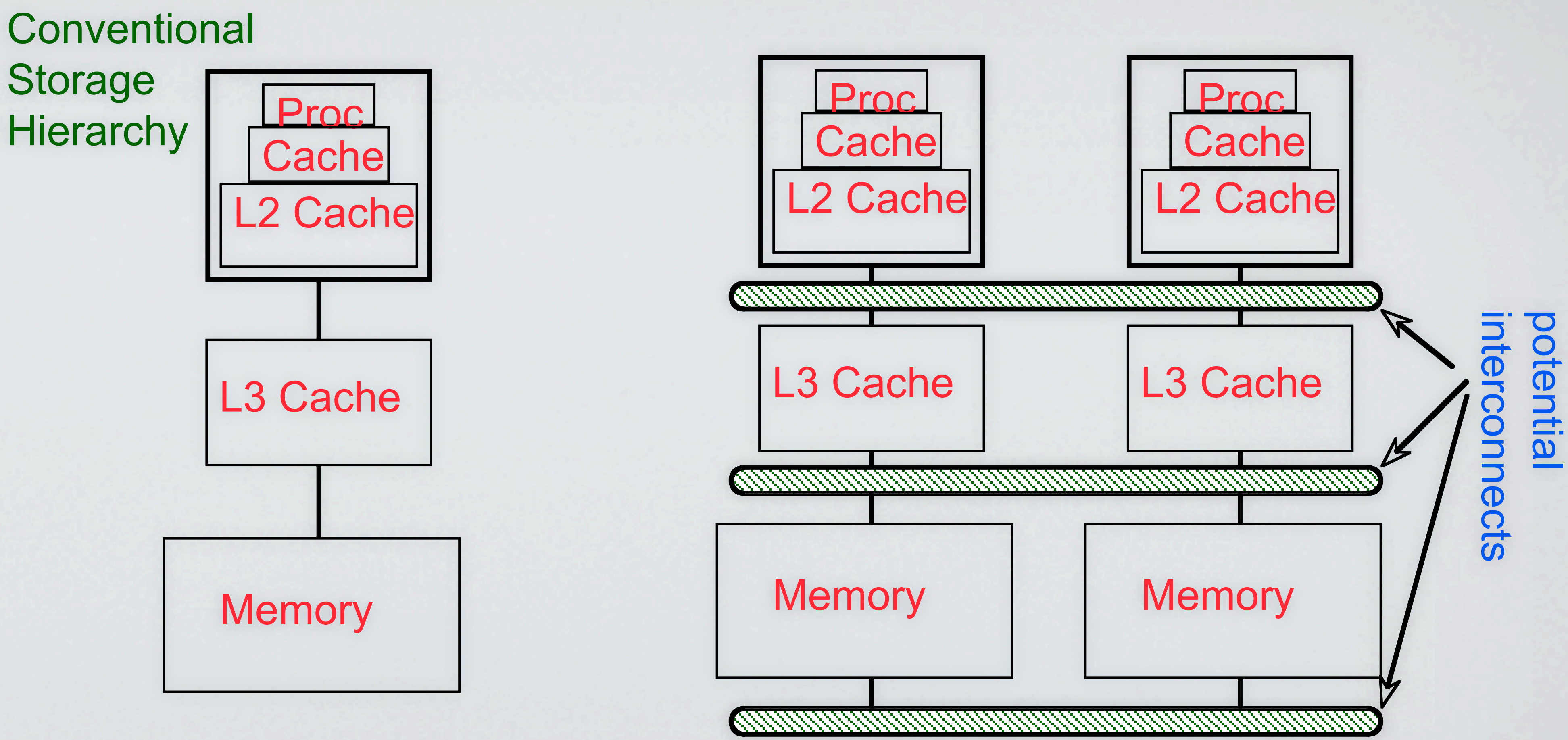
- Examples of overheads:
  - Cost of starting a thread or process
  - Cost of communicating shared data
  - Cost of synchronization
  - Cost of extra (redundant) computation
- Costs may be milliseconds, which is millions of flops
- Tradeoff: Granularity of task vs. amount of parallelism



Cost	1ns	10ns	100ns	10ms	10sec
Size	B	KB	MB	GB	TB

Memory hierarchies: Non-uniform memory access cost.

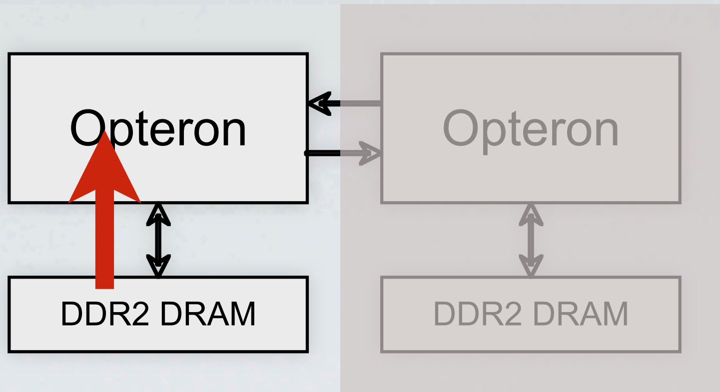
Better algorithms and implementations exploit locality.



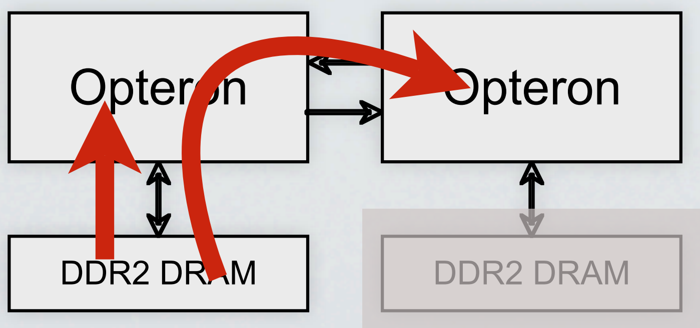
NUMA in the parallel setting.

Processors should minimize communication (remote data access).

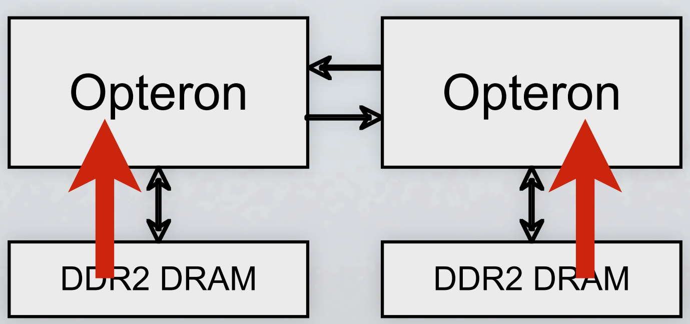
NUMA ⇒ Explicit data placement.



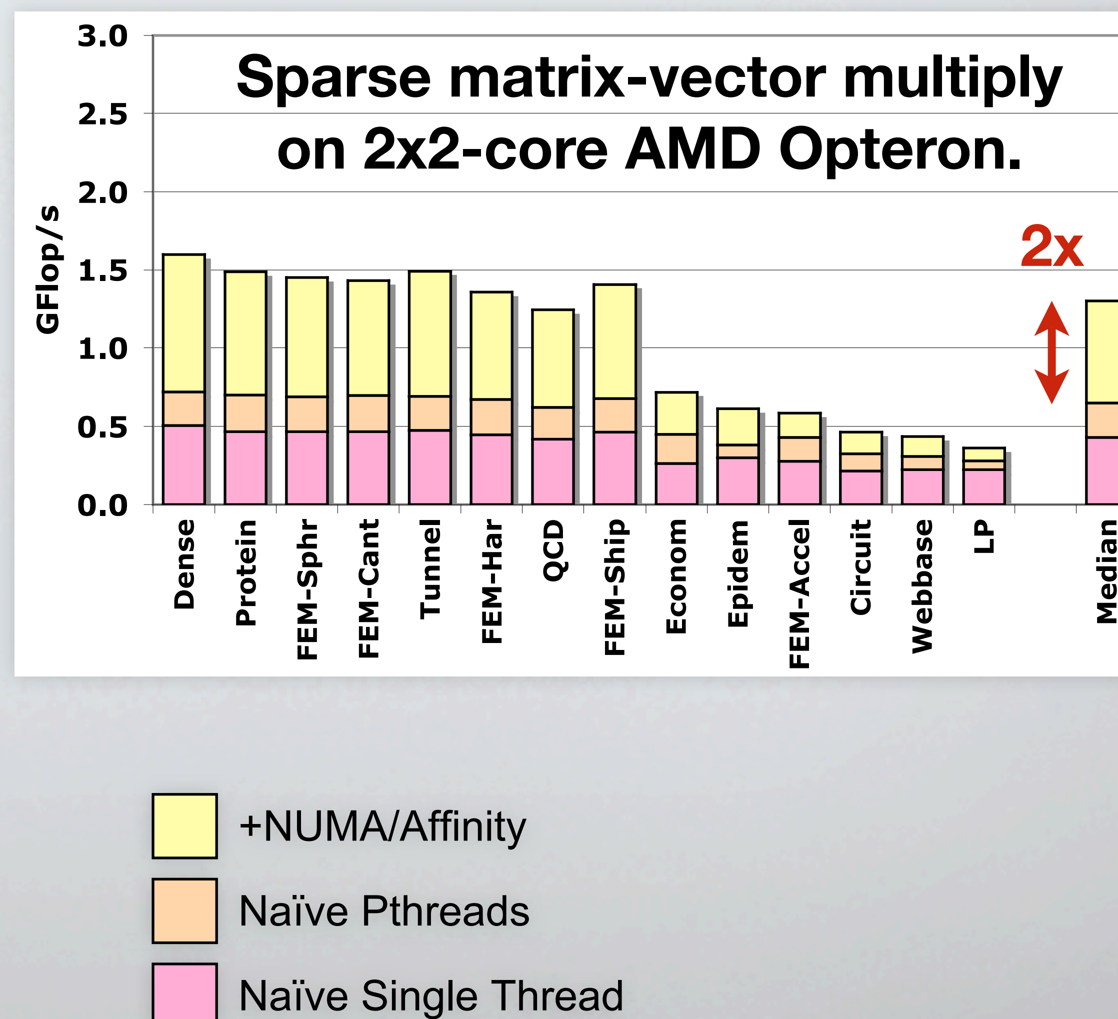
Single Thread



Multiple Threads,
One memory controller



Multiple Threads,
Both memory controllers



$$y = AA^T x$$

$$\begin{aligned} t &\leftarrow A^T x \\ y &\leftarrow A t \end{aligned}$$

For large *A*, "reads" *A* twice.

NUMA ⇒ Seek **algorithmic** reuse.

$$AA^T x = (a_1 \cdots a_n) \begin{pmatrix} a_1^T \\ \vdots \\ a_n^T \end{pmatrix} x = \sum_{i=1}^{n} a_i \left(a_i^T x\right)$$

Reorganize to improve reuse.

Algorithms and implementations must guard against load imbalance.

- Load imbalance: Subset of processors becomes idle
  - Insufficient parallelism
  - Unequally sized tasks
- Sources of imbalance
  - Local adaptation (adaptive mesh refinement)
  - Tree-structured computations
  - Fundamentally unstructured problem

Large-scale parallelism may raise numerical accuracy issues.

- Finite-ness of precision matters more for larger problems
  - Ill-conditioning
  - Round-off
- Example: Compute variance of data set using "two-pass" algorithm (right)
  - In single prec. ($\epsilon \sim 10^{-7}$), all digits lost when $n \sim 10$ million

$$
\begin{aligned}
\bar{x} &= \frac{1}{n}\sum_{i=1}^{n} x_i \\
\sigma(x) &= \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2
\end{aligned}
$$

$$
\begin{aligned}
\text{Let } \hat{\sigma}(x) &= \textit{computed } \sigma(x), \\
\text{and } \epsilon &= \text{machine precision.} \\
\text{then:} &
\end{aligned}
$$

$$
\frac{\hat{\sigma}(x) - \sigma(x)}{\sigma(x)} \leq (n+3)\epsilon + O\left(\epsilon^2\right)
$$

Course organization

Student make-up of course?

- Mostly CS students, so will emphasize algorithm-to-machine mapping more than new-algorithm-development
- Work in teams of two and three; be interdisciplinary where possible!

Workload and grading

- Grading
  - 10% - Class participation and “scribe notes”
  - 24% - Two homework/programming assignments
  - 6% - Attend SIAM PP and write-up what you learned
  - **60% - Course project**
- All homework during first 8 weeks; last 8 weeks for your project!
- Collaboration encouraged, but don’t “cheat.”
- No textbook, but will supplement lectures with readings

Schedule of topics (approximate)

- Week 1: Overview and hardware trends
- Week 2: Sources of parallelism & locality; performance modeling
- Week 3: Basics of parallel programming [HW 1]
- Week 4: Structured grids; dense linear algebra
- Week 5-6: Dense and sparse linear algebra
- Week 7: FFT ; floating-point issues
- Week 8: Single-processor performance tuning [HW 2; project proposals]
  - Guest lecture by Hyesoon Kim on General-purpose GPU programming

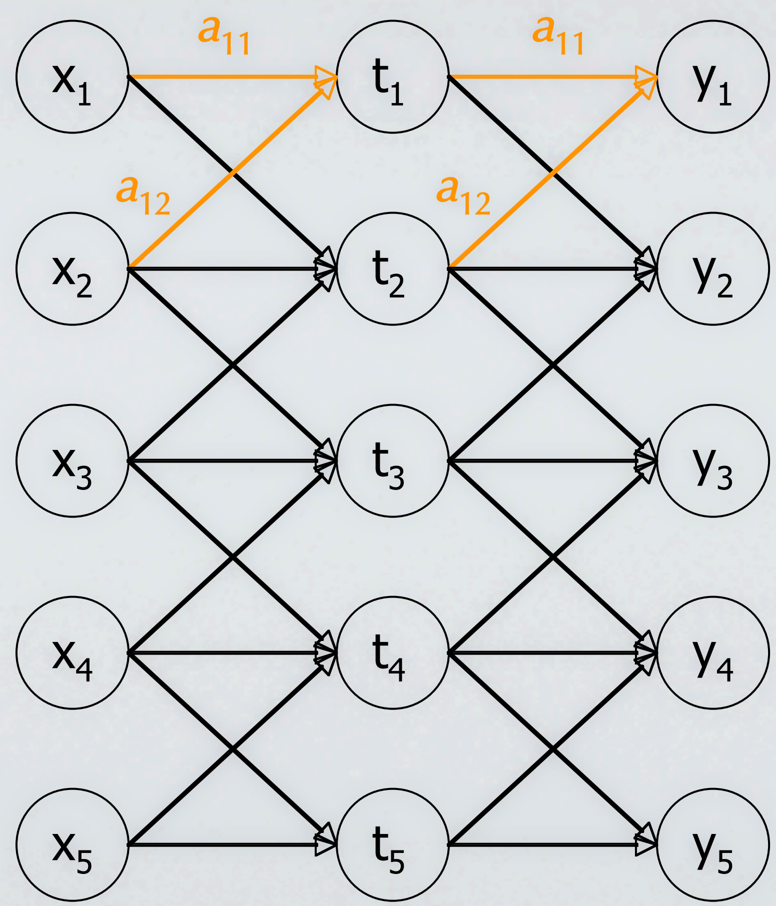
Schedule of topics (2)

- Week 9: Automatic performance tuning (autotuning)
- Week 10: Load balancing; SIAM PP
- Week 11-12: Particle methods; graph partitioning [Project checkpoint]
- Week 13: PDEs
- Week 14: Event-driven methods
- Week 15: Volunteer computing ; parallel languages research
- Week 16: Project presentations
- Project write-up due on “final exam” day

Homework #0: Complete course survey

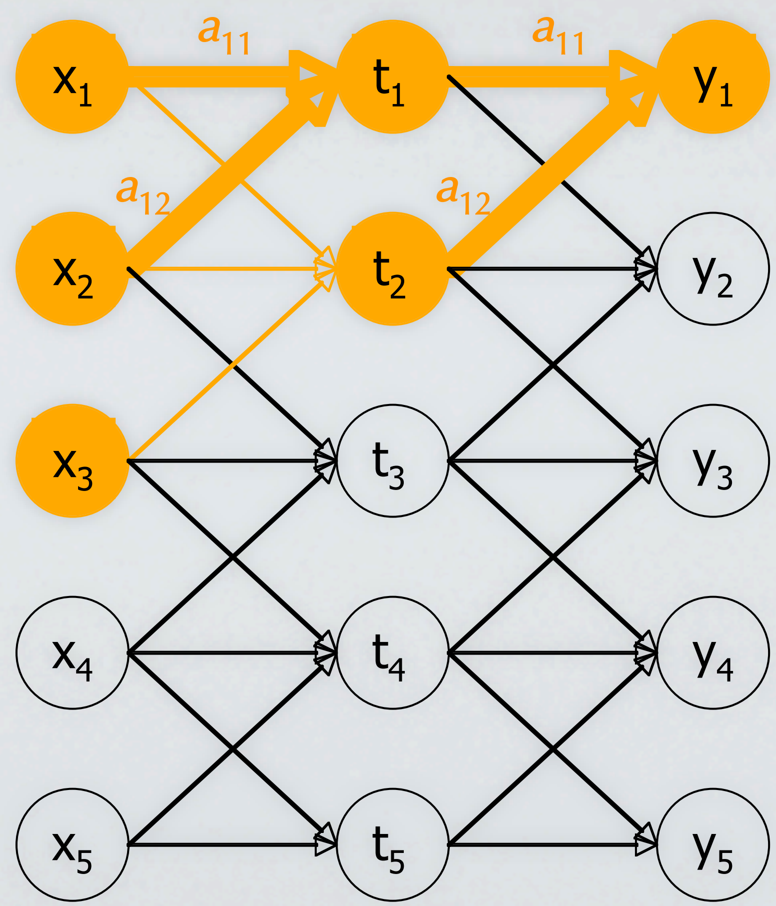
- I will post all materials at GT T-Square site for “CSE-8803-PNA”
  - Go to: http://t-square.gatech.edu
  - Note: Cross-listed with CS-8803-PNA / CS-4803-PNA, but ignore these
- Fill out survey questions under “Poll” tab
- When you “submit” the assignment, briefly describe what you hope to get out of this course
- Also: Use “Forum” to introduce yourselves

“In conclusion…”



Need for locality and parallelism drives new algorithms.

Example: $y = A^2 * x$



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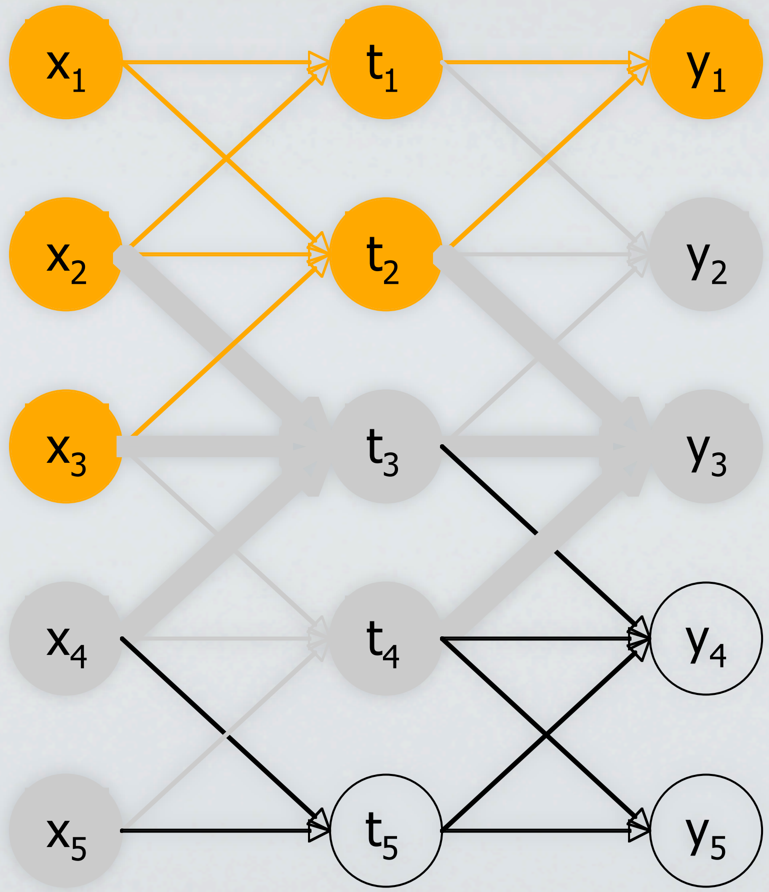

Need for locality and parallelism drives new algorithms.

Example: $y = A^{2*}x$. A new kernel implies a new algorithm… ?

Some questions raised by this example.

- This algorithm has locality, but what about parallelism?
  - What is the relationship between locality and parallelism?
- The “inner loop” of a solver based on this kernel is now A^{k}*x, not just A*x. How does this change the “outer loops?”

Technical challenges of PNA

- Precision, memory, and processing are finite resources
- Curse of dimensionality: 3D space + time eats up Moore's Law
- Hardware changes quickly
- Huge amount of *relevant* domain-knowledge exists: Collaborate!
- Parallel programming is hard