Massive Multithreading Applied to National Infrastructure and Informatics

LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

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Problem

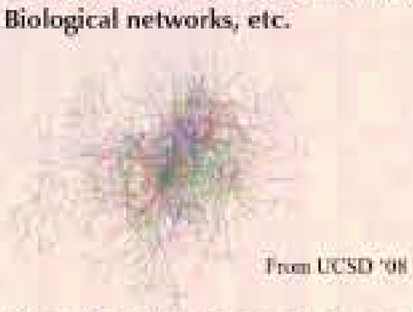
Informatics applications are memory bound. Datasets are huge. Fast CPUs are prohibitively wasteful of power. Can we use special data-driven architectures to address national informatics needs?

Informatics Datasets Are Different

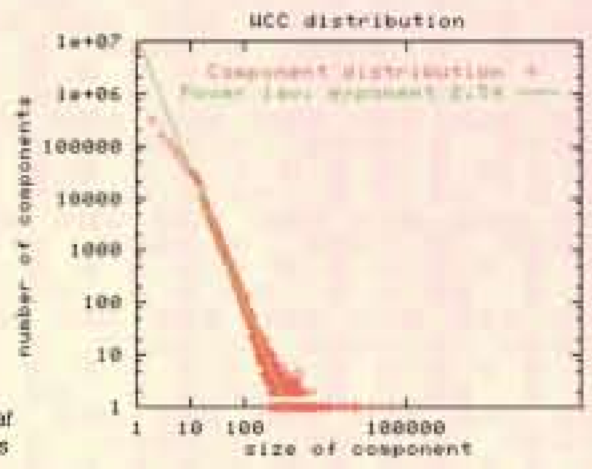
Informatics: The analysis of datasets arising from "information" sources such as the WWW (not physical simulation)

Motivating Applications:

- Homeland security
- Computer security (DOE emphasis)
- Biological networks, etc.



From UCSD '08



Broder, et al. '00

"One of the interesting ramifications of the fact that the PageRank calculation converges rapidly is that the web is an expander-like graph"
Page, Brin, Motwani,Winograd, 1999

Primary HPC Implication: Any partitioning is "bad"

Informatics Problems Demand New Architectures

Distributed Memory Architectures	Massively Multithreaded Architectures	Key Issues
Fast CPU (~3GHz)	Slow CPU (~200-500MHz)	Power, concurrency
Elaborate memory hierarchy	Almost no memory hierarchy	Is cache justified?
Memory per-processor, partitioned	Global address space	Can you partition?
Operating system for threading, synchronization	Hardware for threading, synchronization	How fine-grained is your data interaction?
Programming paradigm is standardized (MPI)	Programming paradigm is machine-specific (mta-pe)	Portability, debuggability

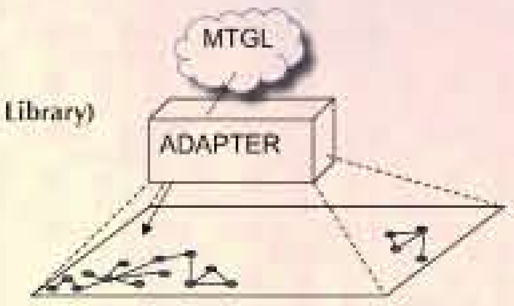
Multithreaded architectures show promise for informatics problems, but more work is necessary…

Approach

Discover and adapt algorithms for massively multithreaded supercomputers, develop a generic software framework for these algorithms, and evaluate them on real data.

We Are Developing the MultiThreaded Graph Library

- Enable multithreaded graph algorithms
- Build upon community standard (Boost Graph Library)
- Adapters abstract data structures and other application specifics
- Hide some shared memory issues
- Preserve good multithreaded performance



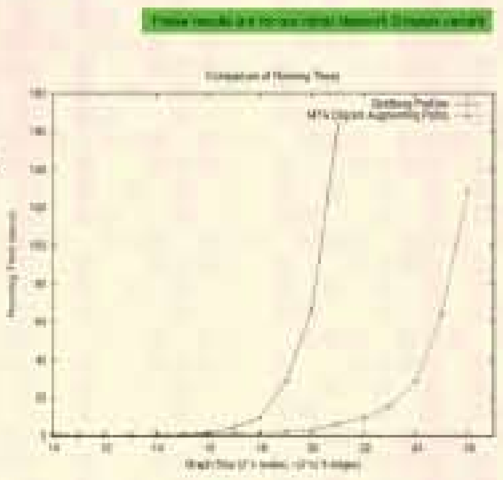
Business model: Open-source code provides a mechanism for Sandia-developed algorithms to be applied to proprietary or sensitive data structures used by customers

Results

Scalable community detection
Scalable detection of short cycles
Scalable maximum flow computation
The MultiThreaded Graph Library (MTGL)

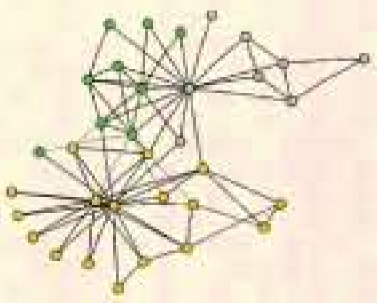
Maximum Flow: Multithreaded Network Simplex Algorithms

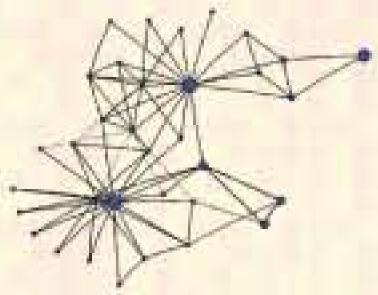
- Flows through networks are a NISAC interest
- Typical runtime O(nm)
- State of the art: Andrew Goldberg's serial methods
- Initial results: we leverage the Cray MTA-2 to extend solvable instance size by 32X



Community Detection: The "Edge Support"

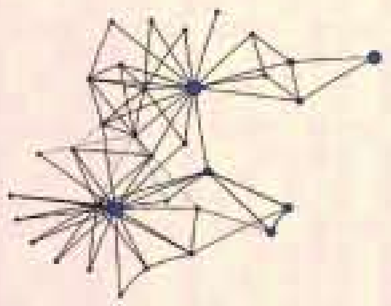
- De Facto state of the art in scalable community detection is the greedy "CNM" heuristic O(n log^2 n)
- Top image shows its solution to the familiar "Zachary's karate club" [Reality: split in two]
- Our facility location based approach suggested a fractional "support" (bottom)
- Darker edges have more "support;" we can now sample an ensemble of solutions





Scalable Community Detection

- Community detection can be modeled as an "Uncapacitated Facility Location Problem" (UFL)
- The UFL has special structure that permits solution in linear time and space
- We have made the kernel of the UFL threadsafe, and demonstrated scalability out to 2560 threads (20 processors) on the Cray MTA-2
- We have a new, untested formulation that is expected to scale farther



Significance

The reputation of the MTGL has led to technical recognition (keynote at 2008 IEEE "MTAAP" workshop) and programmatic impact (new multi-FTE WFO project)

- Copyright/Berkeley open-source license paper work submitted
- Transition to SVN completed
- Nightly testing mechanism introduced
- Preparing for 1.0 release
- Synergies
  - Networks Grand Challenge uses MTGL
  - Large WFO project uses MTGL
  - Proposed "X-Caliber" architecture motivated in part by MTGL apps
  - A few MTGL algorithms are integrated with "qthreads" for SMP/CMP

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