Big Iron for Big Data: An Unnatural Alliance?

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Sandia National Labs

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Big data analytics (BD) versus scientific simulations (SS)

- **Programming model**:
  - SS: polish same code for years, tune its performance
  - BD: quick & dirty or agile, morph tools for data
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- **Data usage & ownership**:
  - SS: big data is an output, not an input
  - BD: big data is an input, maybe an output
  - BD: data may be sensitive or proprietary
  - BD: compute where data is, "own" the data

I/O needs for big data computing

Olympic metric for **price**: gold, silver, bronze

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Gold-plated solution:

- top-10 machine (petascale, ORNL Jaguar)
- **$100M**, 224K cores
- custom Spider parallel file system (Lustre)
  - not NFS, tuned for big-chunk read/writes
  - 10 Pbytes, 13K disks
  - 240 GB/sec, IOPs = $\sim$1M
- data itself not valuable (regenerate by simulation)
- code & CPU time to create it is valuable

I/O needs for big data computing

Olympic metric for **price**: gold, aluminum, bronze

Aluminum-plated solution:

- top-500 machine (bioinformatics cluster at Columbia U)
- **$2.5M**, 4000 cores using data 24/7
- clustered commercial NAS (Isilon, Panasas, ...)
  - NFS, scalable capacity, 1B small files
  - 1 Pbyte, 1000 disks
  - 20 Gb/sec, 500K IOPs
- data generated externally ($>$ Moore's and Kryder's laws)
- data is highly valuable, must be easy to manage/backup

I/O needs for big data computing

Olympic metric for **price**: gold, aluminum, plywood

Plywood-plated solution:

- Google, Facebook, Twitter = racks of cheap cores and disks
- **minimal $$**, could not care less about top-500 and LINPACK
- 1+ disk/core:
  - scalable capacity
  - 100 Pbytes, 100K disks (made this up)
  - 10 TB/sec, 20M IOPs
- my summer vacation photos may be valuable
- much of data is not valuable (continually refreshed)

Bottom line

Medal:	$/PByte	TB/core	PB/Pflop	IOPs/PB
Gold:	$10M	0.044	5	∼100K
Aluminum:	$2.5M	0.25	40	500K
Plywood:	$0.3M	1+	100+	∼200K

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- Big data computing done on aluminum and plywood
- No one wants to pay **gold prices** to do big data computing
- Don't want to pay for compute speed & interconnect
- Do want to pay for storage capacity and I/O capability

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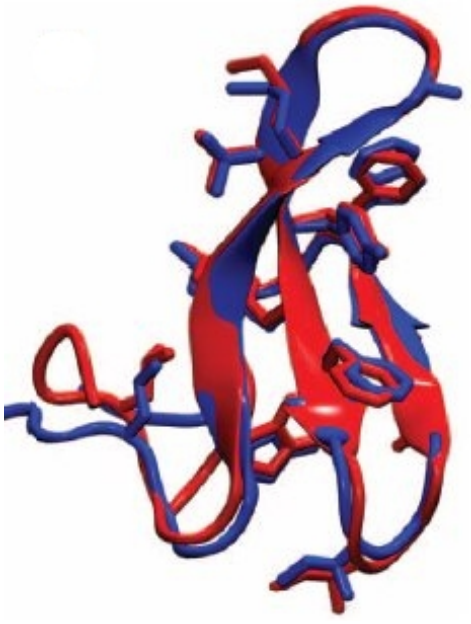
- **Additional issues**:
  - run where data is produced & stored (local vs center)
  - data accessibility (add, delete, backup)

MapReduce for scientific data

Tiankai Tu, et al (DE Shaw), *Scalable Parallel Framework for Analyzing Terascale MD Trajectories*, SC 2008.

- 1M atoms, 100M snapshots $\Rightarrow$ **3 Pbytes**
- Stats on where each atom traveled
  - near-approach to docking site
  - membrane crossings



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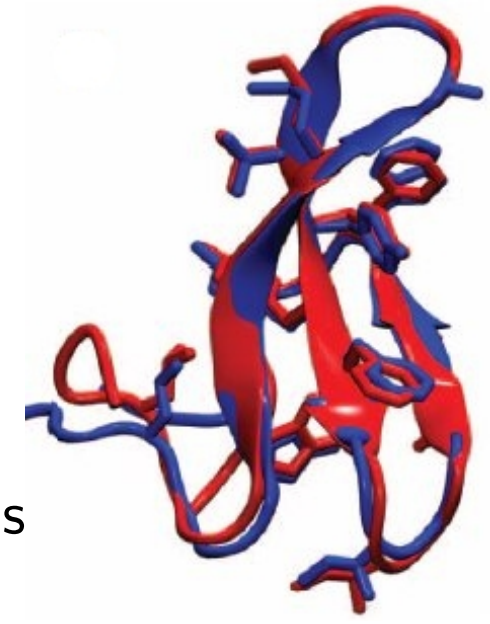

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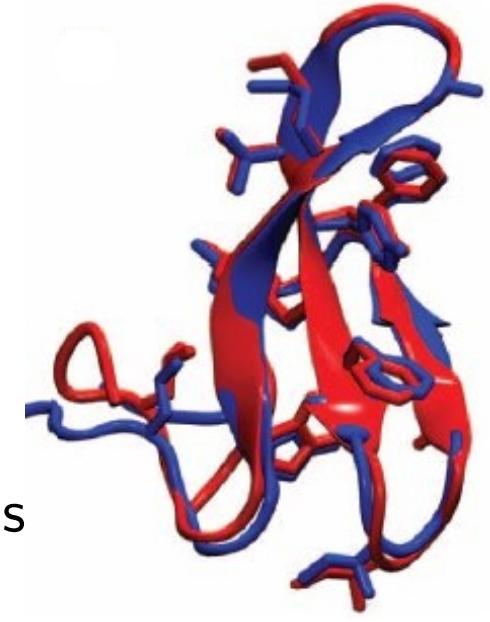

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- **Key point**: extremely parallel comp + MPI_All2all comm

Why is MapReduce attractive?

- **Plus**:
  - write only the code that only you can write
  - write zero parallel code (no parallel debugging)
  - out-of-core for free
- **Plus/minus** (features!):
  - ignore data locality
  - load balance thru random distribution
    - key hashing = slow global address space
  - maximize communication (all2all)
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Matches big data programming model:
minimal human effort, not maximal performance

MapReduce software

- Hadoop:
  - HDFS, fault tolerance
  - extra big-data goodies (BigTable, etc)
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  - extra big-data goodies (BigTable, etc)
  - no one runs it on gold-plated platforms
- MR-MPI: **http://mapreduce.sandia.gov**
  - MapReduce on top of MPI
  - Lightweight, portable, C++ library with C API
  - Out-of-core on big iron if each proc can write scratch files
  - No HDFS (parallel file system with data redundancy)
  - No fault-tolerance (blame it on MPI)

What could you do with MapReduce at Petascale?

- Post-simulation analysis of big data output
- Graph algorithms:
  - vertex ranking via **PageRank** (460)
  - connected components (250)
  - triangle enumeration (260)
  - single-source shortest path (240)
  - **sub-graph isomorphism** (430)

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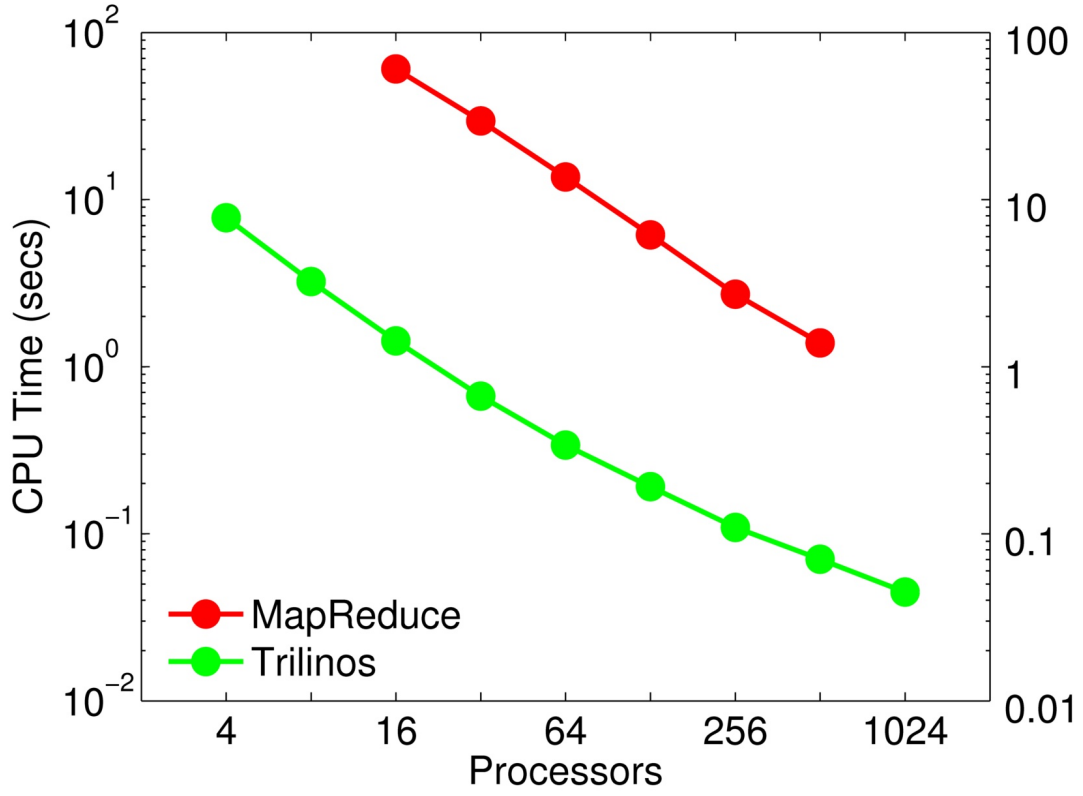
  - **sub-graph isomorphism** (430)
- Matrix operations:
  - matrix-vector multiply (PageRank kernel)
  - tall-skinny QR (D Gleich, P Constantine)
    - simulation data $\Rightarrow$ cheaper surrogate model
    - 500M x 100 dense matrix $\Rightarrow$ 30 min on 256 plywood cores
- Machine learning: classification, clustering, ...
- Win the TeraSort benchmark

No free lunch: PageRank (matvec) performance

Cray XT3 (gold), 1/4 billion edge highly sparse, irregular matrix



- MapReduce communicates matrix elements
- But recall: load-balance, out-of-core for free

Sub-graph isomorphism for data mining

- Data mining, **needle-in-haystack** anomaly search
- Huge graph with **colored vertices, edges** (labels)
- **SGI** = find all occurrences of small target graph

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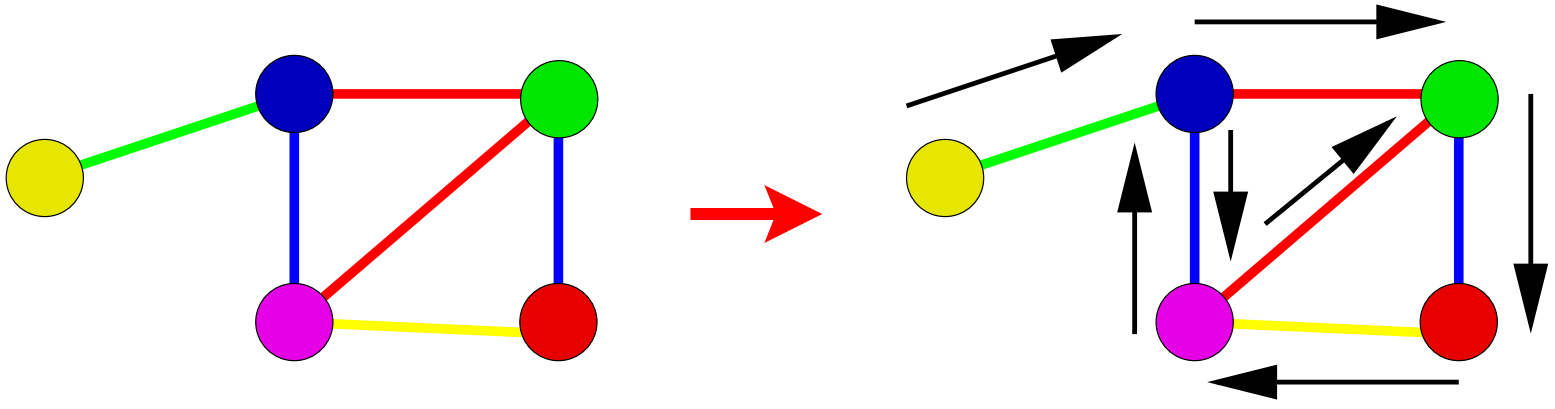

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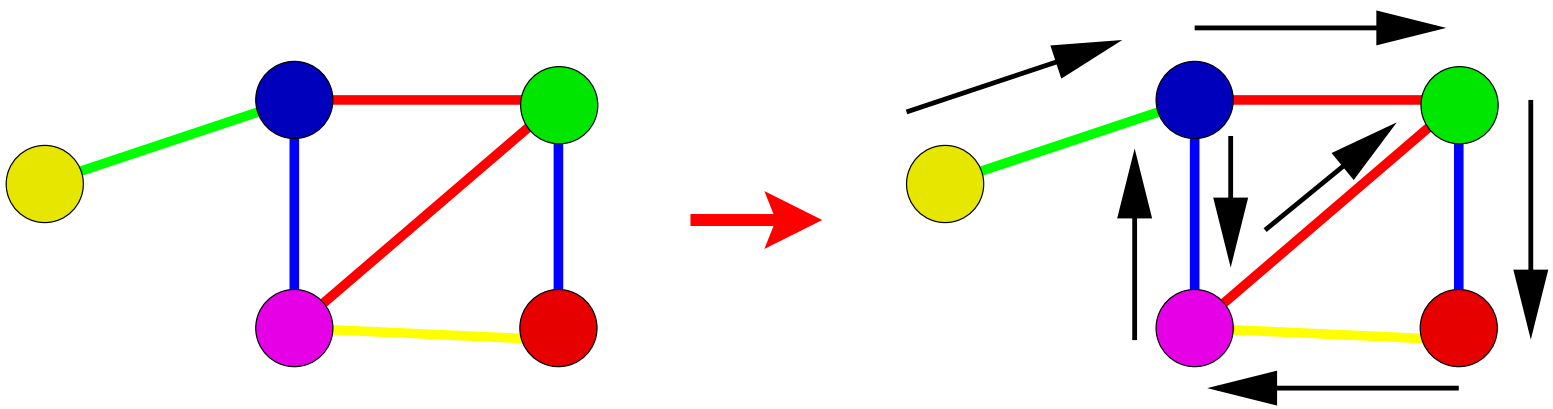

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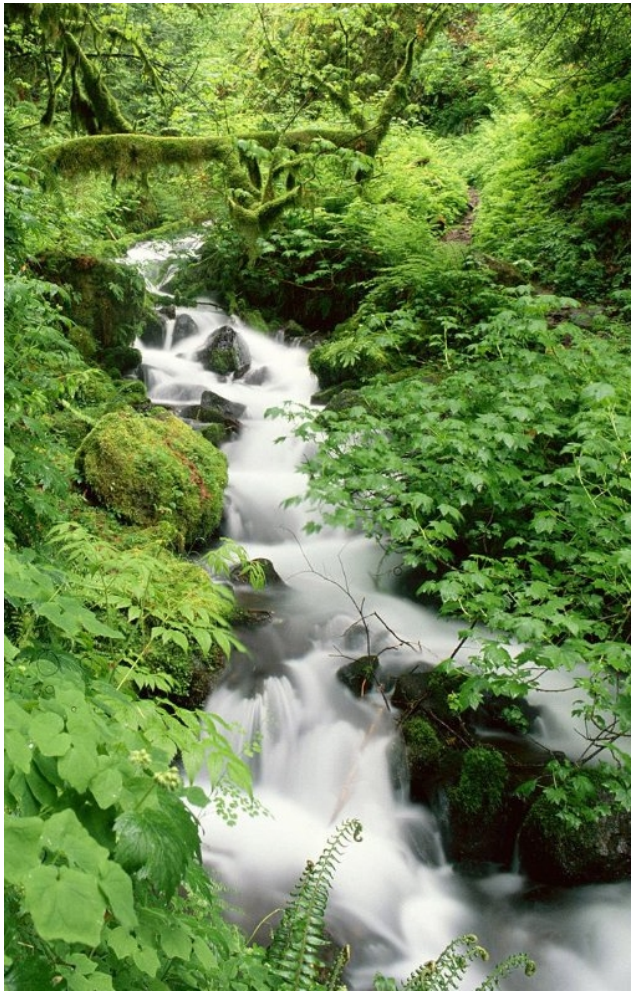
Example: 18 Tbytes ⇒ 107 B edges ⇒ 573 K matches
in 55 minutes on 256 **plywood** cores

Streaming data

- Continuous, real-time I/O
- Stream = small datums at high rate
- **Resource-constrained processing**:
  - only see datums once
  - compute/datum $<$ stream rate
  - only store state that fits in memory
  - age/expire data
- Pipeline model is attractive:
  - datums flow thru compute kernels
  - hook kernels together to perform analysis
  - split stream to enable shared or distributed-memory parallelism



Streaming software

- IBM InfoSphere (commercial)
- Twitter Storm (open-source)
- PHISH: **http://www.sandia.gov/~sjplimp/phish.html**
  - Parallel Harness for Informatic Stream Hashing
  - phish swim in a stream
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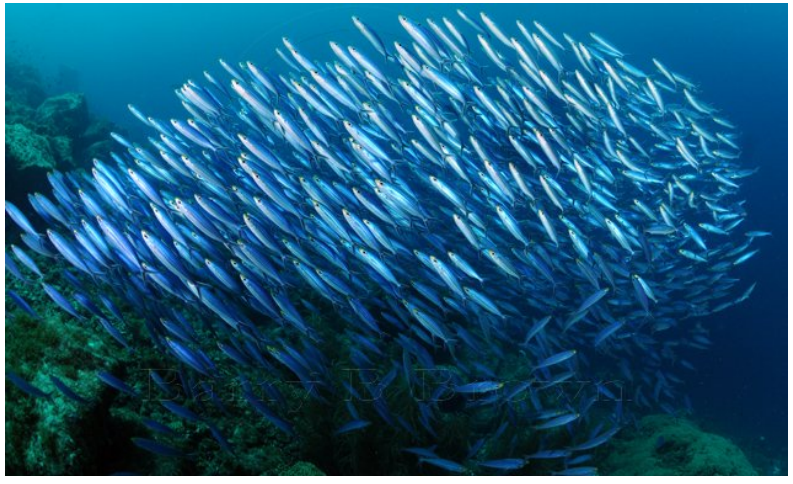

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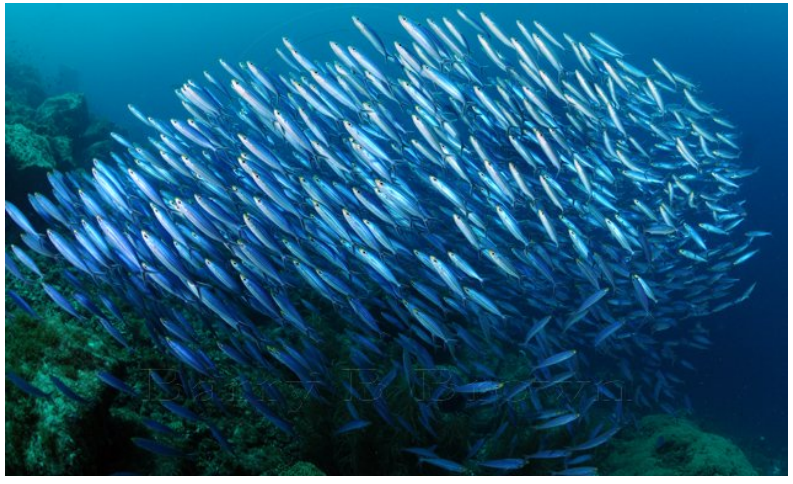
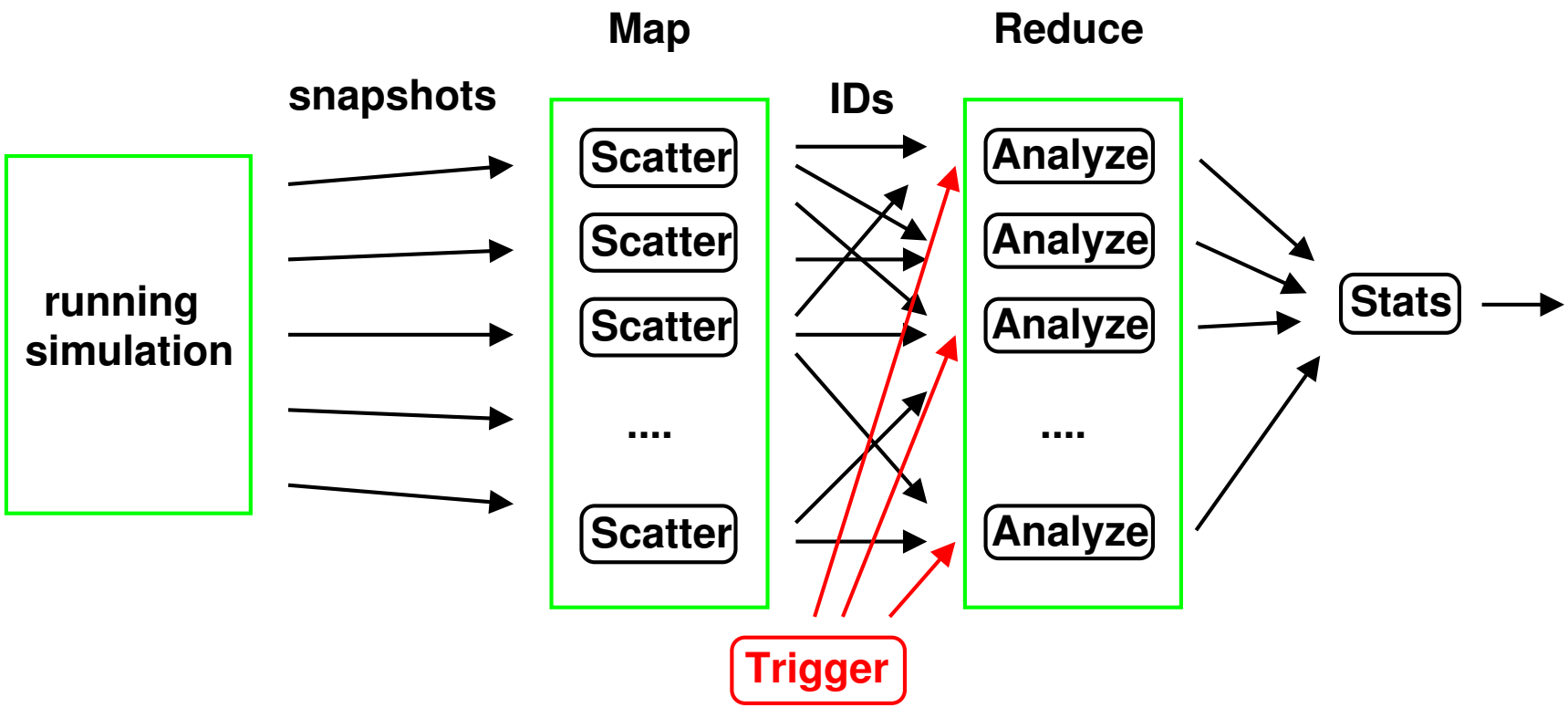


- Key point: **zillions of small messages** flowing thru processes

PHISH net for real-time simulation data analysis

- Gold vs aluminum vs plywood:
  - Most streaming is high data rate, low computation
  - Mismatch: continuous streaming versus batch jobs
  - Could couple to simulation for **"steering"**



Big Iron and Big Data: An Unnatural Alliance?

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It is not done well; but you are surprised to find it done at all.

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Unnatural MPI:

- ignoring data locality
- all2all (MapReduce)
- tiny messages (streaming)
- lots of I/O

If you want that dog to walk at Petascale ...

Data analytics for informatics problems (e.g. MapReduce):

- fast all2all for data movement (bisection bandwidth)
- fast I/O rate to parallel disks for out-of-core

Streaming algorithms for informatics problems:

- high throughput (zillions of small messages)
- also low latency

Both need:

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- hi-speed access to external world (source of data)

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Caveat: have ignored **fault tolerance**

- Hadoop and Twitter Storm have it
- MPI does not

Thanks & links

Sandia **collaborators**:

- Karen Devine (MR-MPI)
- Tim Shead (PHISH)
- Todd Plantenga, Jon Berry, Cindy Phillips (graph algorithms)

Open-source packages (BSD license):

- **http://mapreduce.sandia.gov** (MapReduce-MPI)
- **http://www.sandia.gov/~sjplimp/phish.html** (PHISH)

Papers:

- Plimpton & Devine, *"MapReduce in MPI for large-scale graph algorithms"*, Parallel Computing, 37, 610 (2011).
- Plantenga, *"Inexact subgraph isomorphism in MapReduce"*, submitted to JPDC (2011).
- Plimpton & Shead, *"PHISH tales"*, in progress (2012).