eScience:
Grids, Clouds and Parallel Computing

Challenges in eScience Workshop http://dexl.lncc.br/CIS/

Vale Real Hotel - Itaipava - Petrópolis RJ,

Brazil

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eScience:
Grids, Clouds and Parallel Computing

- We analyze the different tradeoffs and goals of Grid, Cloud and parallel (cluster/supercomputer) computing.

- They tradeoff performance, fault tolerance, ease of use (elasticity), cost, interoperability.

- Different application classes (characteristics) fit different architectures and we describe a hybrid model with Grids for data, traditional supercomputers for large scale simulations and clouds for broad based "capacity computing" including many data intensive problems.

- We discuss the impressive features of cloud computing platforms and compare MapReduce and MPI.

- We take most of our examples from the life science area.

- We conclude with a description of FutureGrid -- a TeraGrid system for prototyping new middleware and applications.

Talk Components

- Important Trends

- Clouds and Cloud Technologies

- Data Intensive Science Applications
  - Use of Clouds

- Summary

- FutureGrid

Important Trends

- Data Deluge in all fields of science
- Multicore implies parallel computing important again
  - Performance from extra cores – not extra clock speed
  - GPU enhanced systems can give big power boost
- Clouds – new commercially supported data center model replacing compute grids (and your general purpose computer center)
- Light weight clients: Sensors, Smartphones and tablets accessing and supported by backend services in cloud
- Commercial efforts moving much faster than academia in both innovation and deployment

benefit

years to mainstream adoption

	less than 2 years	2 to 5 years	5 to 10 years	more than 10 years
Transformational		**Cloud Computing** **Cloud Web Platforms** **Media Tablet**	3D Printing Context Delivery Architecture Extreme Transaction Processing	Autonomous Vehicles Human Augmentation Mobile Robots Terahertz Waves
High	Mobile Application Stores Predictive Analytics	Activity Streams E-Book Readers Electronic Paper Interactive TV Internet Micropayment Systems Location-Aware Applications Private Cloud Computing Social Analytics	Augmented Reality Internet TV Virtual Assistants Wireless Power	Mesh Networks: Sensor
Moderate	Consumer-Generated Media Pen-Centric Tablet PCs	3D Flat-Panel TVs and Displays Biometric Authentication Methods Gesture Recognition Idea Management Microblogging Speech Recognition Video Telepresence	4G Standard Public Virtual Worlds Speech-to-Speech Translation Video Search	Computer-Brain Interface
Low				Tangible User Interfaces

As of August 2010

Data Centers Clouds & Economies of Scale I

Range in size from "edge" facilities to megascale.

Economies of scale

Approximate costs for a small size center (1K servers) and a larger, 50K server center.

2 Google warehouses of computers on the banks of the Columbia River, in The Dalles, Oregon
Such centers use 20MW-200MW (Future) each with 150 watts per CPU
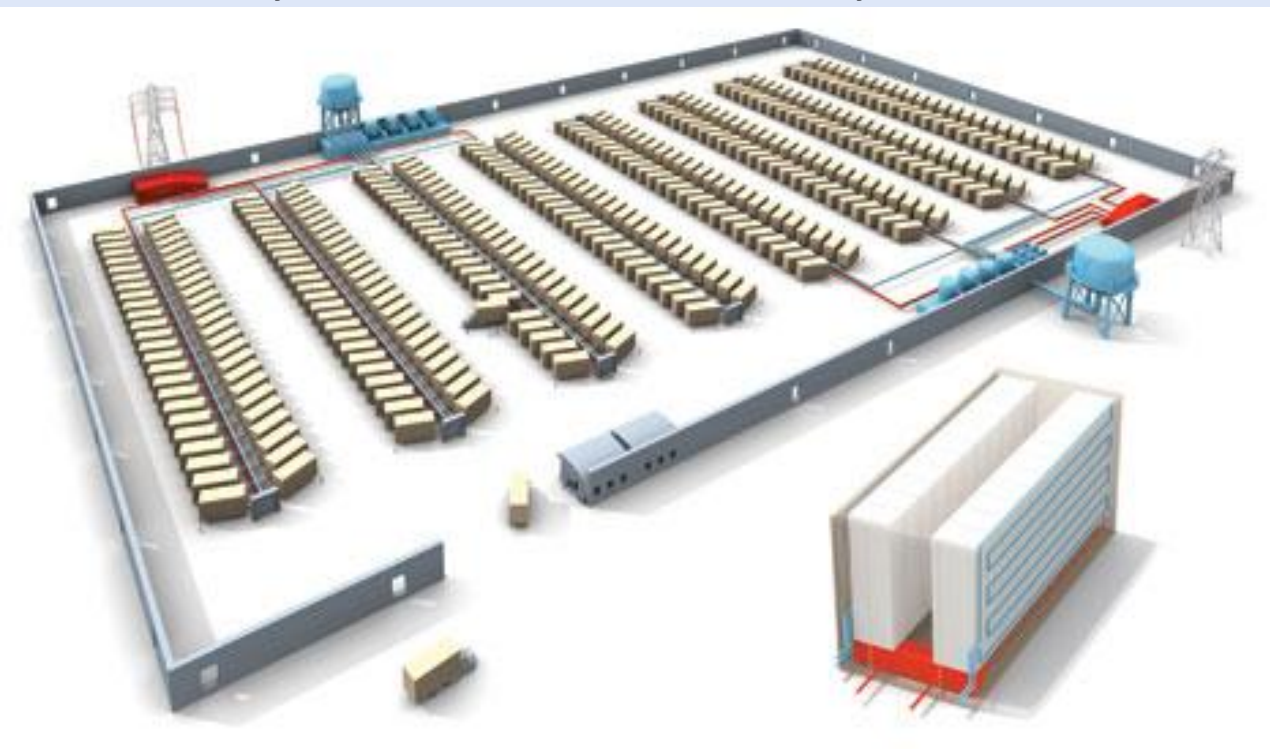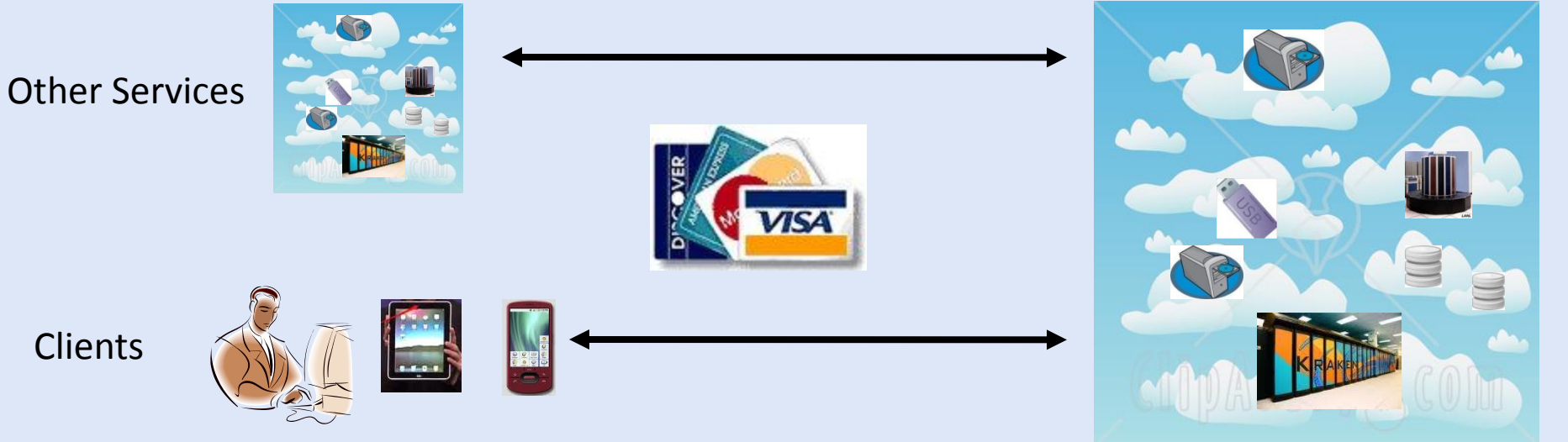Save money from large size, positioning with cheap power and access with Internet

Data Centers, Clouds & Economies of Scale II

- Builds giant data centers with 100,000's of computers; ~ 200-1000 to a shipping container with Internet access

- "Microsoft will cram between 150 and 220 shipping containers filled with data center gear into a new 500,000 square foot Chicago facility. This move marks the most significant, public use of the shipping container systems popularized by the likes of Sun Microsystems and Rackable Systems to date."

X as a Service

- SaaS: Software as a Service imply software capabilities (programs) have a service (messaging) interface
  - Applying systematically reduces system complexity to being linear in number of components
  - Access via messaging rather than by installing in /usr/bin
- IaaS: Infrastructure as a Service or HaaS: Hardware as a Service – get your computer time with a credit card and with a Web interface
- PaaS: Platform as a Service is IaaS plus core software capabilities on which you build SaaS
- Cyberinfrastructure is "Research as a Service"

Other Services

Clients

Philosophy of Clouds and Grids

- **Clouds** are (by definition) commercially supported approach to large scale computing
  - So we should expect Clouds to replace Compute Grids
  - Current Grid technology involves "non-commercial" software solutions which are hard to evolve/sustain
  - Maybe Clouds ~4% IT expenditure 2008 growing to 14% in 2012 (IDC Estimate)
- **Public Clouds** are broadly accessible resources like Amazon and Microsoft Azure – powerful but not easy to customize and perhaps data trust/privacy issues
- **Private Clouds** run similar software and mechanisms but on "your own computers" (not clear if still elastic)
  - Platform features such as Queues, Tables, Databases currently limited
- **Services** still are correct architecture with either REST (Web 2.0) or Web Services
- **Clusters** are still critical concept for MPI or Cloud software

Grids MPI and Clouds

- **Grids** are useful for **managing distributed systems**
  - Pioneered service model for Science
  - Developed importance of Workflow
  - Performance issues – communication latency – intrinsic to distributed systems
  - Can never run large differential equation based simulations or datamining
- **Clouds can execute any job class that was good for Grids** plus
  - More attractive due to platform plus **elastic** on-demand model
  - **MapReduce easier to use than MPI for appropriate parallel jobs**
  - Currently have performance limitations due to poor affinity (locality) for compute-compute (MPI) and Compute-data
  - These limitations are not "inevitable" and should gradually improve as in July 13 Amazon Cluster announcement
  - Will probably never be best for most sophisticated parallel differential equation based simulations
- **Classic Supercomputers** (MPI Engines) run **communication demanding differential equation based simulations**
  - **MapReduce and Clouds replaces MPI** for other problems
  - Much more data processed today by MapReduce than MPI (Industry Informational Retrieval ~50 Petabytes per day)

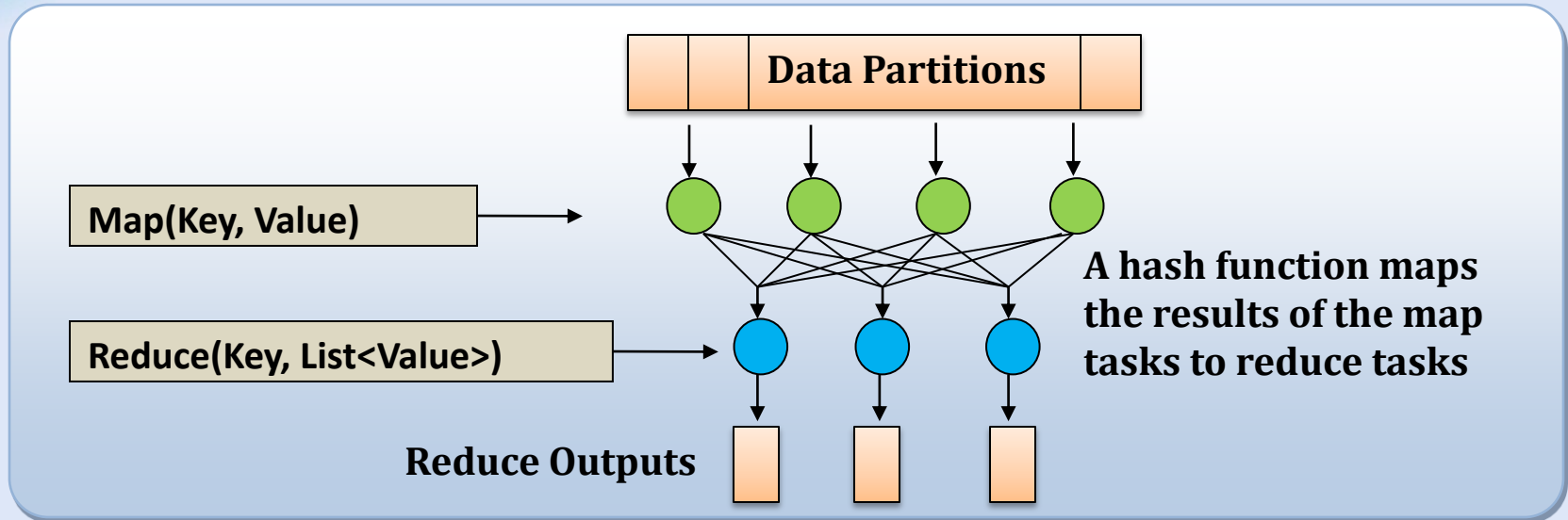# Cloud Computing: Infrastructure and Runtimes

- Cloud infrastructure: outsourcing of servers, computing, data, file space, utility computing, etc.
  - Handled through Web services that control virtual machine lifecycles.
- Cloud runtimes or Platform: tools (for using clouds) to do data-parallel (and other) computations.
  - Apache Hadoop, Google MapReduce, Microsoft Dryad, Bigtable, Chubby and others
  - MapReduce designed for information retrieval but is excellent for a wide range of science data analysis applications
  - Can also do much traditional parallel computing for data-mining if extended to support iterative operations
  - MapReduce not usually on Virtual Machines

Authentication and Authorization: Provide single sign in to both FutureGrid and Commercial Clouds linked by workflow
Workflow: Support workflows that link job components between FutureGrid and Commercial Clouds. Trident from Microsoft Research is initial candidate
Data Transport: Transport data between job components on FutureGrid and Commercial Clouds respecting custom storage patterns
Program Library: Store Images and other Program material (basic FutureGrid facility)
Blob: Basic storage concept similar to Azure Blob or Amazon S3
DPFS Data Parallel File System: Support of file systems like Google (MapReduce), HDFS (Hadoop) or Cosmos (dryad) with compute-data affinity optimized for data processing
Table: Support of Table Data structures modeled on Apache Hbase/CouchDB or Amazon SimpleDB/Azure Table. There is "Big" and "Little" tables – generally NOSQL
SQL: Relational Database
Queues: Publish Subscribe based queuing system
Worker Role: This concept is implicitly used in both Amazon and TeraGrid but was first introduced as a high level construct by Azure
MapReduce: Support MapReduce Programming model including Hadoop on Linux, Dryad on Windows HPCS and Twister on Windows and Linux
Software as a Service: This concept is shared between Clouds and Grids and can be supported without special attention
Web Role: This is used in Azure to describe important link to user and can be supported in FutureGrid with a Portal framework

MapReduce

Data Partitions

Map(Key, Value)

Reduce(Key, List<Value>)

A hash function maps the results of the map tasks to reduce tasks

Reduce Outputs

- Implementations (Hadoop – Java; Dryad – Windows) support:
  - Splitting of data
  - Passing the output of map functions to reduce functions
  - Sorting the inputs to the reduce function based on the intermediate keys
  - Quality of service
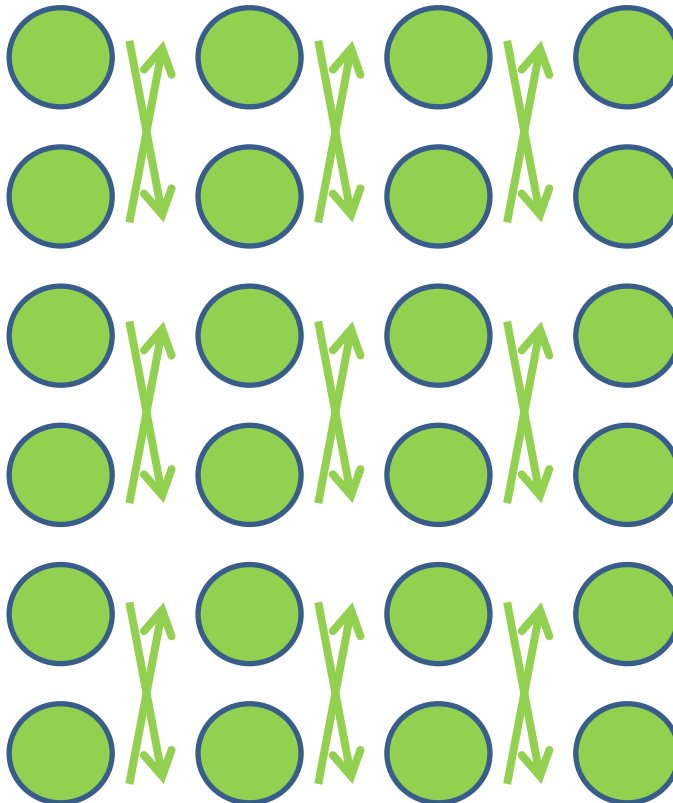
MapReduce "File/Data Repository" Parallelism

Map = (data parallel) computation reading and writing data

Reduce = Collective/Consolidation phase e.g. forming multiple global sums as in histogram

Instruments

Disks

Iterative MapReduce

Map   Map   Map   Map

Reduce   Reduce   Reduce

Reduce

Portals/Users

High Energy Physics Data Analysis

An application analyzing data from Large Hadron Collider
(1TB but 100 Petabytes eventually)

Reduce Phase of Particle Physics "Find the Higgs" using Dryad

- Combine Histograms produced by separate Root "Maps" (of event data to partial histograms) into a single Histogram delivered to Client
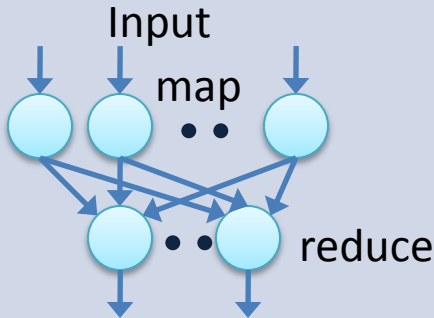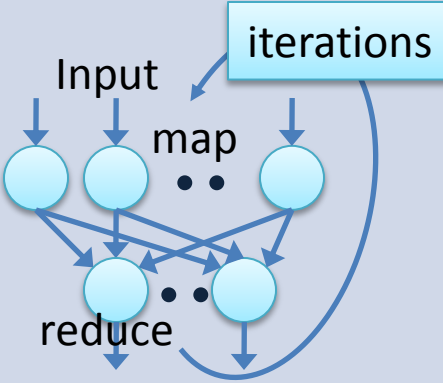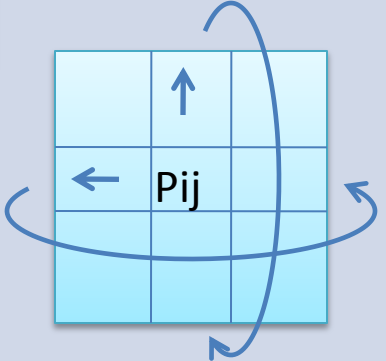
Application Classes

Old classification of Parallel software/hardware in terms of 5 (becoming 6) "Application architecture" Structures)

1	Synchronous	Lockstep Operation as in SIMD architectures	**SIMD**
2	Loosely Synchronous	Iterative Compute-Communication stages with independent compute (map) operations for each CPU. Heart of most MPI jobs	**MPP**
3	Asynchronous	Computer Chess; Combinatorial Search often supported by dynamic threads	**MPP**
4	**Pleasingly Parallel**	Each component independent – in 1988, Fox estimated at 20% of total number of applications	**Grids**
5	**Metaproblems**	Coarse grain (asynchronous) combinations of classes 1)-4). The preserve of workflow.	**Grids**
6	**MapReduce++**	It describes file(database) to file(database) operations which has subcategories including. 1) Pleasingly Parallel Map Only 2) Map followed by reductions 3) Iterative "Map followed by reductions" – Extension of Current Technologies that supports much linear algebra and datamining	**Clouds** **Hadoop/ Dryad** **Twister**

Applications & Different Interconnection Patterns

Map Only	Classic MapReduce	Iterative Reductions MapReduce++	Loosely Synchronous
Input → map → Output	Input → map → reduce	Input → map → reduce (iterations)	Pij
CAP3 Analysis Document conversion (PDF -> HTML) Brute force searches in cryptography Parametric sweeps	High Energy Physics (**HEP**) Histograms **SWG** gene alignment Distributed search Distributed sorting Information retrieval	Expectation maximization algorithms Clustering Linear Algebra	Many MPI scientific applications utilizing wide variety of communication constructs including local interactions
- CAP3 Gene Assembly - PolarGrid Matlab data analysis	- Information Retrieval - HEP Data Analysis - Calculation of Pairwise Distances for ALU Sequences	- Kmeans - **Deterministic Annealing Clustering** - Multidimensional Scaling **MDS**	- Solving Differential Equations and - particle dynamics with short range forces

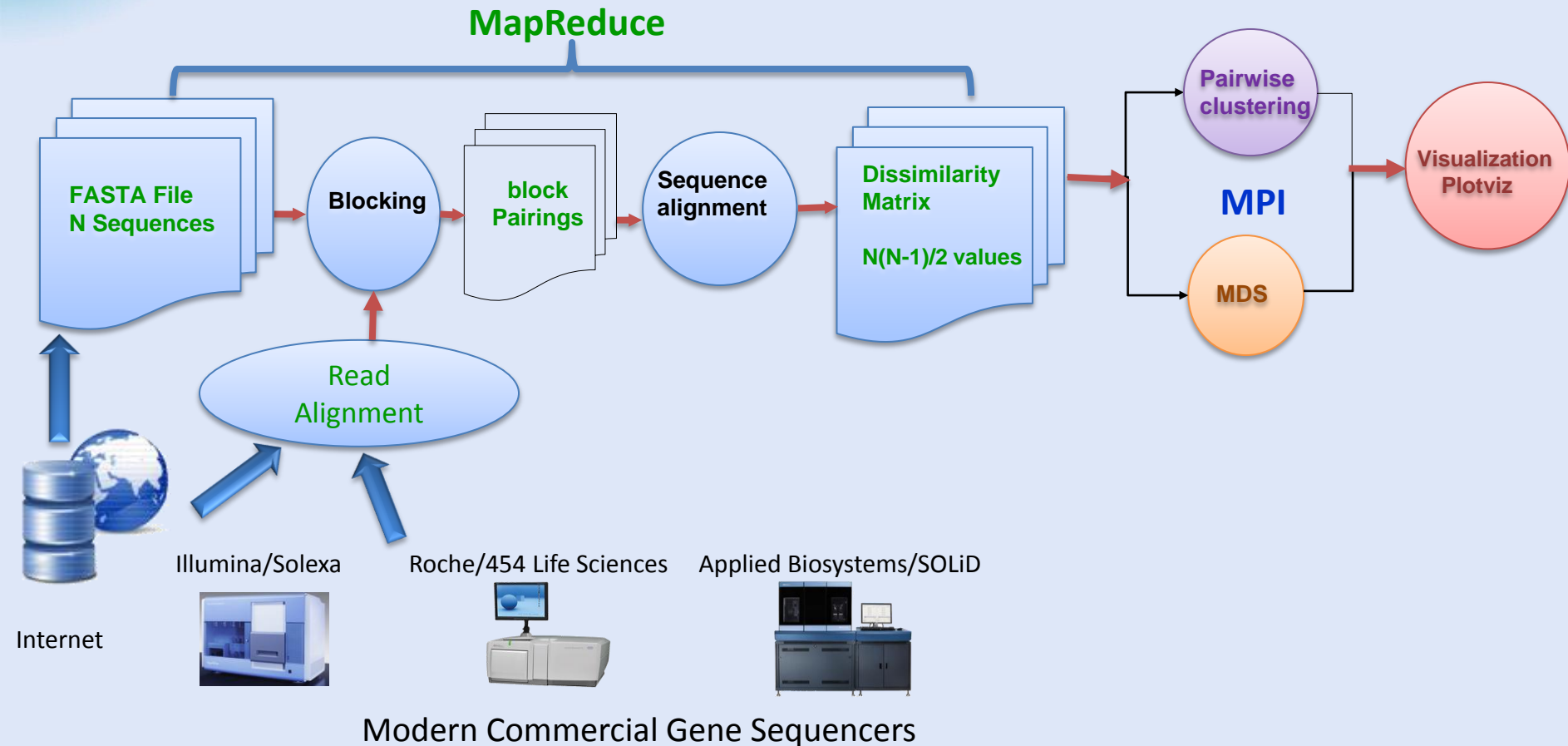← Domain of MapReduce and Iterative Extensions →   MPI

Fault Tolerance and MapReduce

- MPI does "maps" followed by "communication" including "reduce" but does this iteratively
- There must (for most communication patterns of interest) be a strict synchronization at end of each communication phase
  - Thus if a process fails then everything grinds to a halt
- In MapReduce, all Map processes and all reduce processes are independent and stateless and read and write to disks
  - As 1 or 2 (reduce+map) iterations, no difficult synchronization issues
- Thus failures can easily be recovered by rerunning process without other jobs hanging around waiting
- Re-examine MPI fault tolerance in light of MapReduce
  - Twister will interpolate between MPI and MapReduce

DNA Sequencing Pipeline

Modern Commercial Gene Sequencers

- This chart illustrate our research of a pipeline mode to provide services on demand (Software as a Service SaaS)
- User submit their jobs to the pipeline. The components are services and so is the whole pipeline.
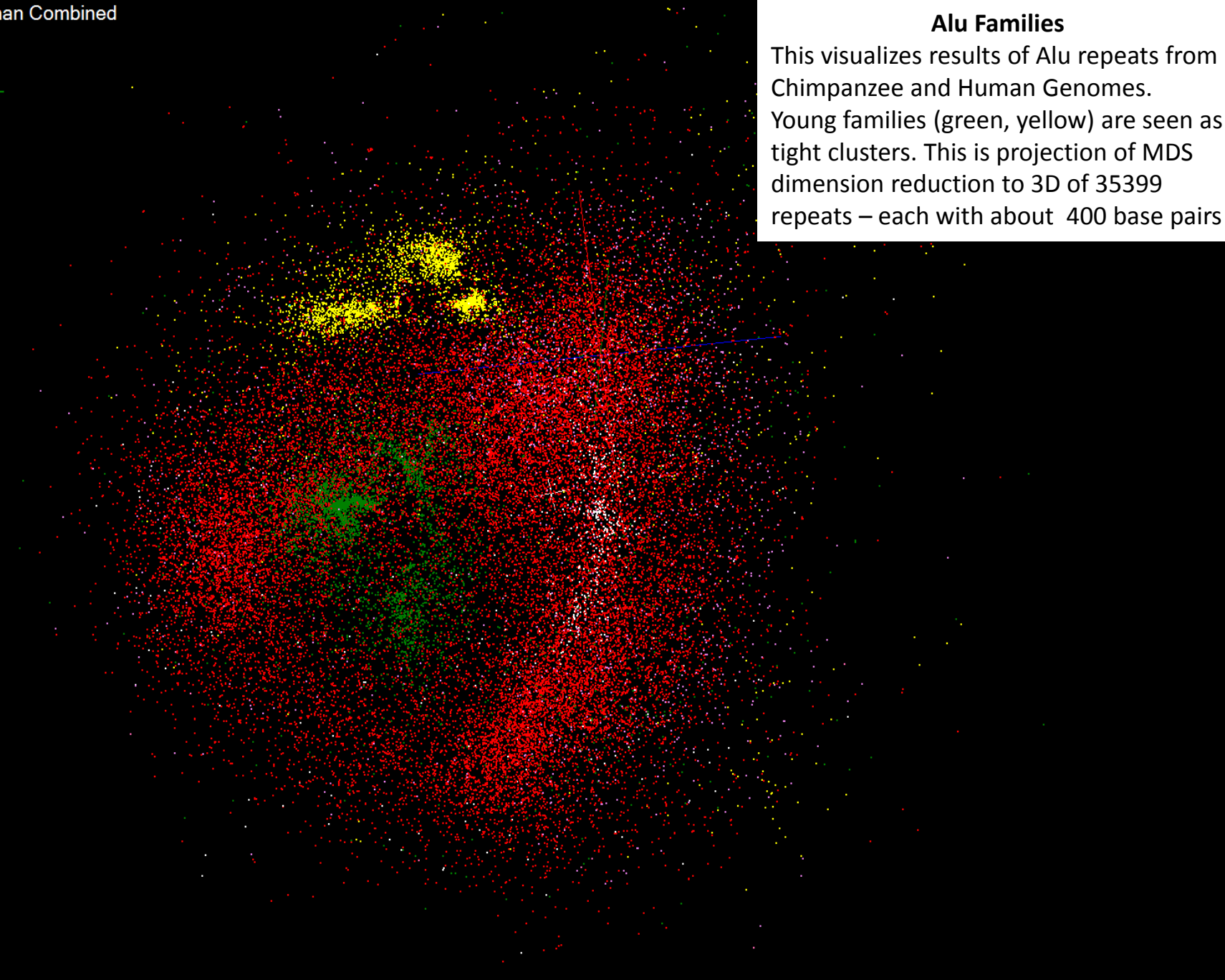
Alu and Metagenomics Workflow
All Pairs

- Data is a collection of N sequences. Need to calculate N^2 dissimilarities (distances) between sequences.
  - These cannot be thought of as vectors because there are missing characters
- Step 1: Calculate N^2 dissimilarities (distances) between sequences
- Step 2: Find families by clustering (using much better methods than Kmeans). As no vectors, use vector free $O(N^2)$ methods
- Step 3: Map to 3D for visualization using Multidimensional Scaling (MDS) – also $O(N^2)$
- Note N = 50,000 runs in 10 hours (the complete pipeline above) on 768 cores
- Need to address millions of sequences; develop new $O(NlogN)$ algorithms
- Currently using a mix of MapReduce (step 1) and MPI as steps 2,3 use classic matrix algorithms
- Twister could do all steps as MDS, Clustering just need MPI Broadcast/Reduce

Chimp and Human Combined

AluY 25522
AluYa5 - 4191-
AluYa8 - 105
AluYb - 7
AluYb8 - 2765
AluYb9 - 493
AluYc3 - 3
AluYc5 - 2
AluYd8 - 1477
AluYg - 5
AluYg6 - 676
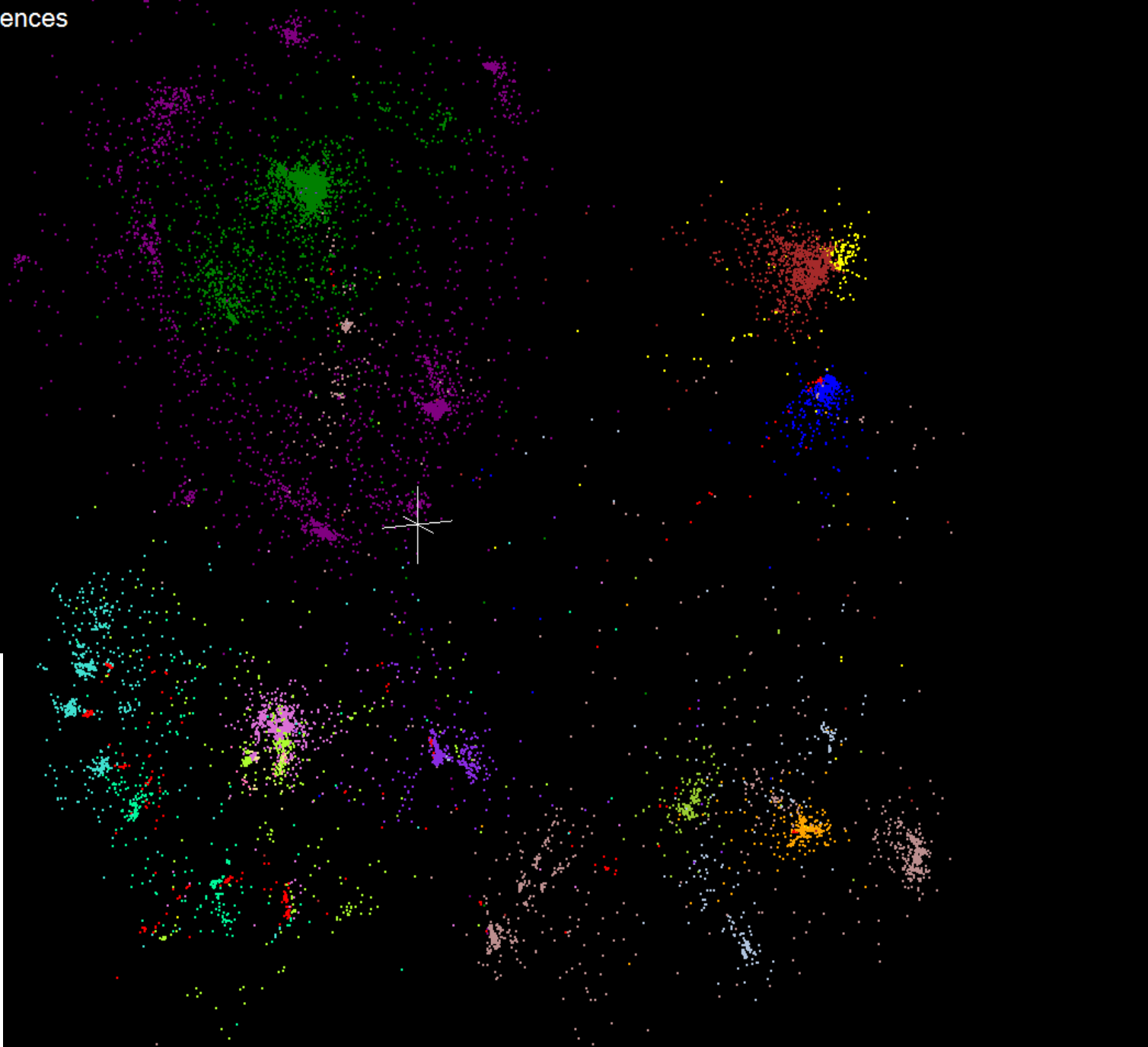AluYh - 2
AluYh9 - 89
AluYc - 2

Alu Families

This visualizes results of Alu repeats from Chimpanzee and Human Genomes. Young families (green, yellow) are seen as tight clusters. This is projection of MDS dimension reduction to 3D of 35399 repeats – each with about 400 base pairs

Metagenomics 30,000 sequences
Clustered into 17

- 415
- 4917
- 4087
- 1466
- 4875
- 1168
- 2133
- 147
- 1012
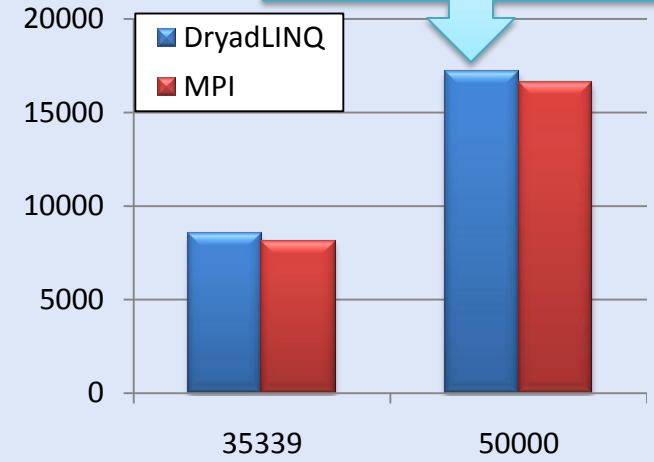- 1016
- 455
- 447
- 135
- 433
- 1422
- 2776

Metagenomics
This visualizes results of
dimension reduction to
3D of 30000 gene
sequences from an
environmental sample.
The many different
genes are classified by
clustering algorithm and
visualized by MDS
dimension reduction

All-Pairs Using DryadLINQ

Calculate Pairwise Distances (Smith Waterman Gotoh)
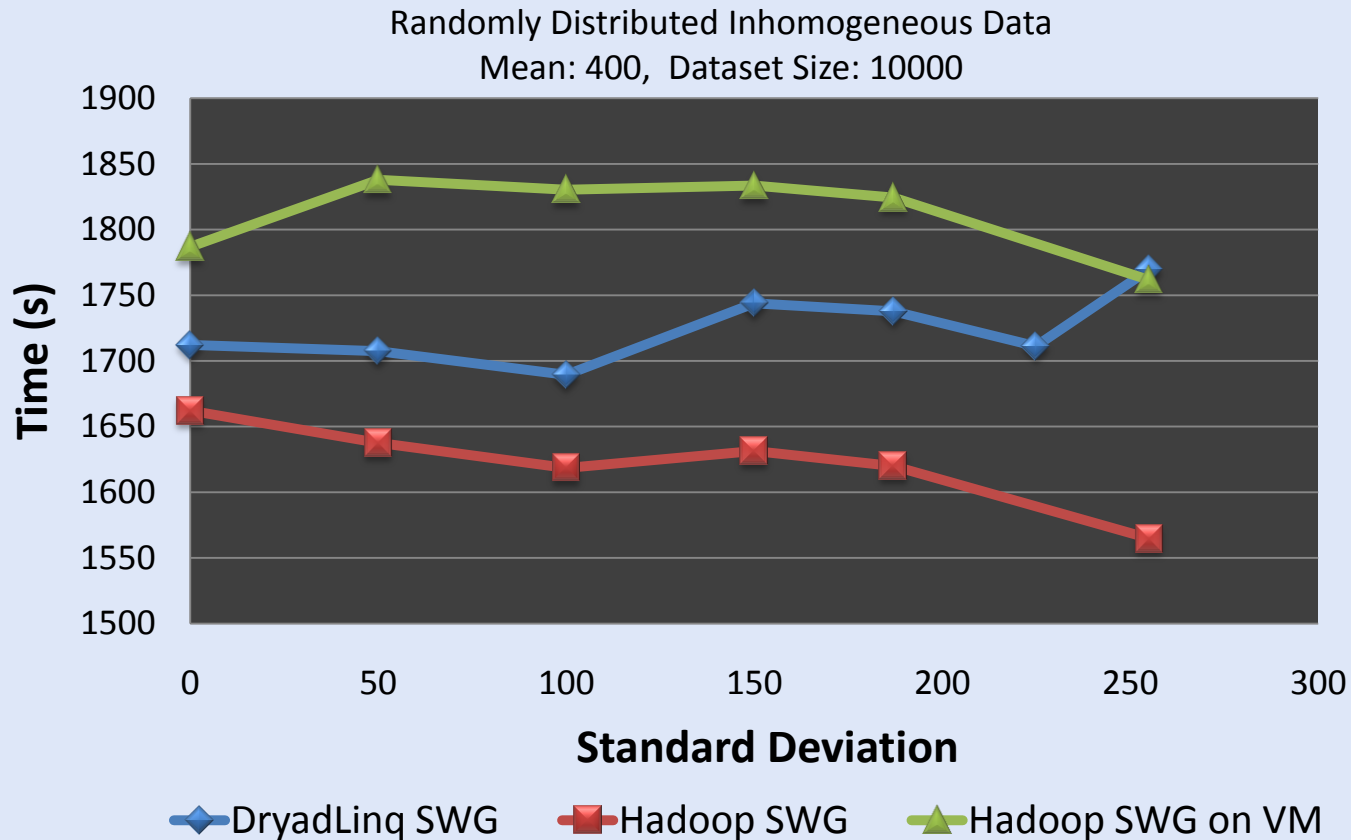
125 million distances
4 hours & 46 minutes

- Calculate pairwise distances for a collection of genes (used for clustering, MDS)
- Fine grained tasks in MPI
- Coarse grained tasks in DryadLINQ
- Performed on 768 cores (Tempest Cluster)

Moretti, C., Bui, H., Hollingsworth, K., Rich, B., Flynn, P., & Thain, D. (2009). All-Pairs: An Abstraction for Data Intensive Computing on Campus Grids. *IEEE Transactions on Parallel and Distributed Systems* , 21, 21-36.

Hadoop/Dryad Comparison
Inhomogeneous Data I

Randomly Distributed Inhomogeneous Data
Mean: 400, Dataset Size: 10000

Inhomogeneity of data does not have a significant effect when the sequence lengths are randomly distributed

Dryad with Windows HPCS compared to Hadoop with Linux RHEL on Idataplex (32 nodes)
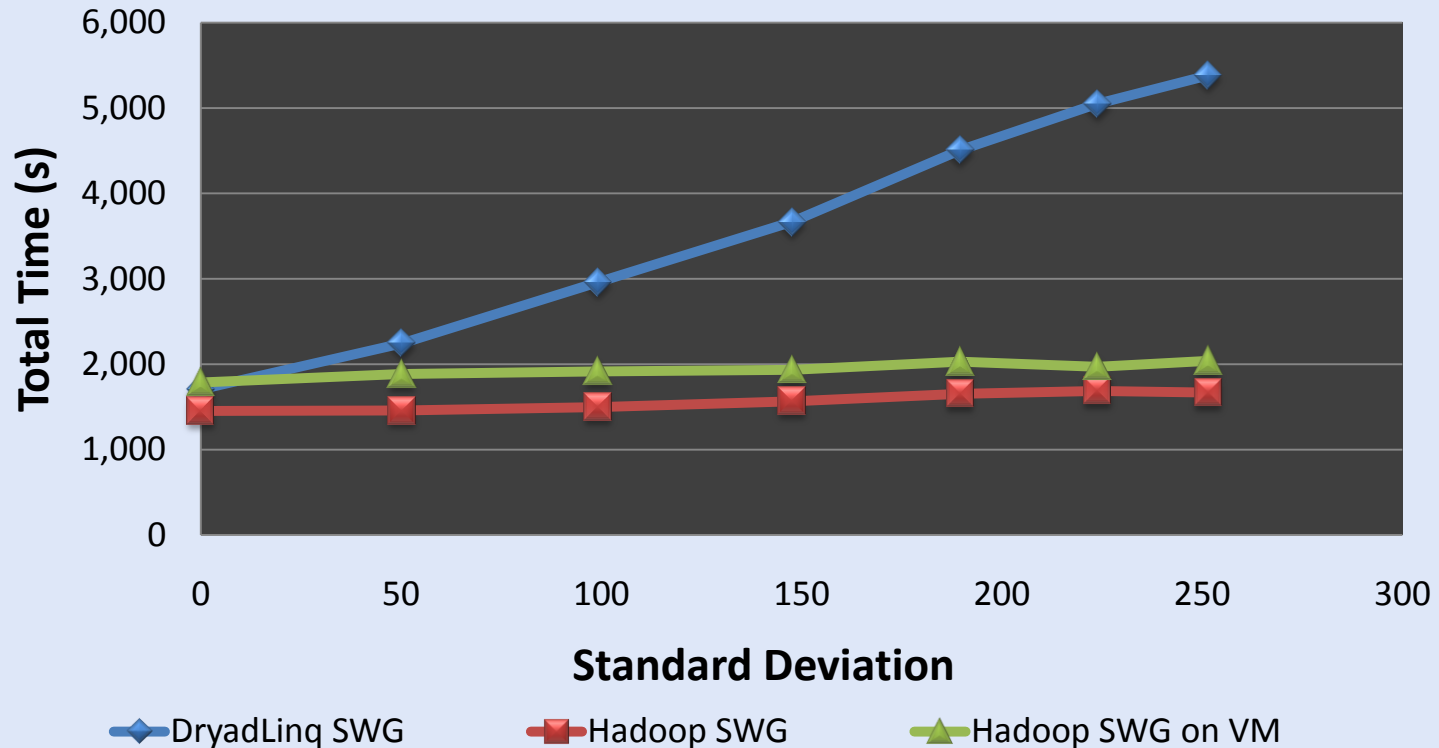
Hadoop/Dryad Comparison
Inhomogeneous Data II

Skewed Distributed Inhomogeneous data
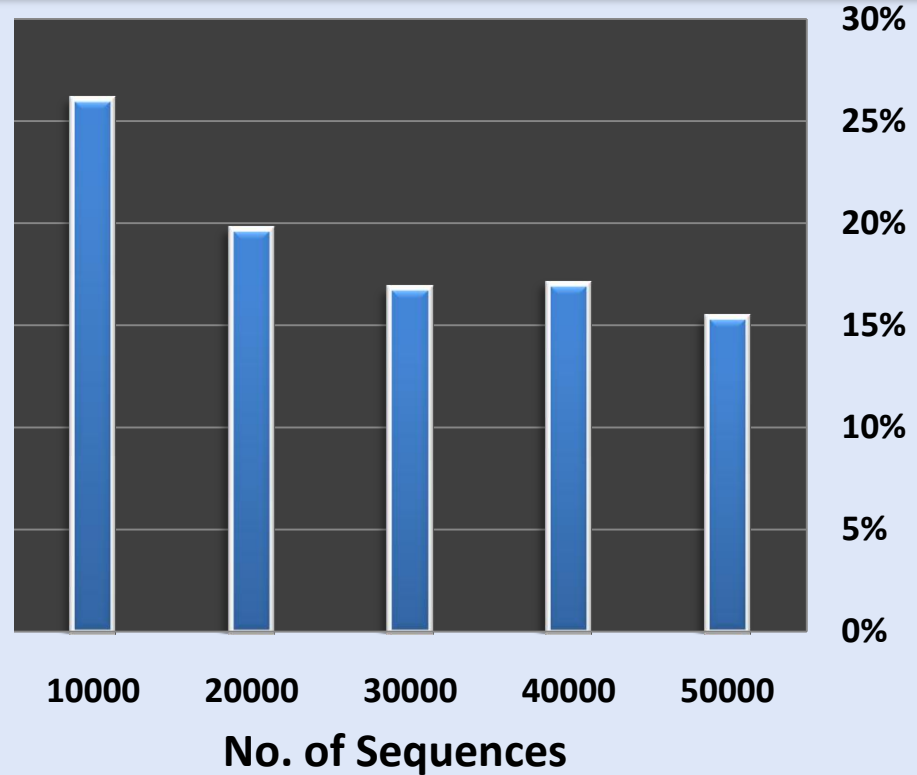Mean: 400, Dataset Size: 10000

This shows the natural load balancing of Hadoop MR dynamic task assignment using a global pipe line in contrast to the DryadLinq static assignment

Dryad with Windows HPCS compared to Hadoop with Linux RHEL on Idataplex (32 nodes)

Hadoop VM Performance Degradation

$$\text{Perf. Degradation} = (T_{vm} - T_{baremetal})/T_{baremetal}$$

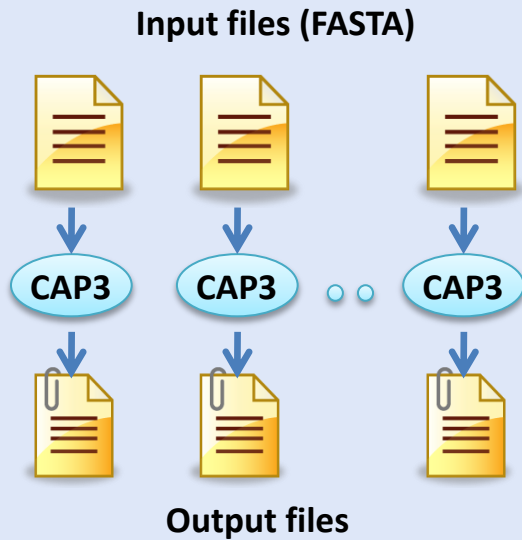Perf. Degradation On VM (Hadoop)

15.3% Degradation at largest data set size

Applications using Dryad & DryadLINQ
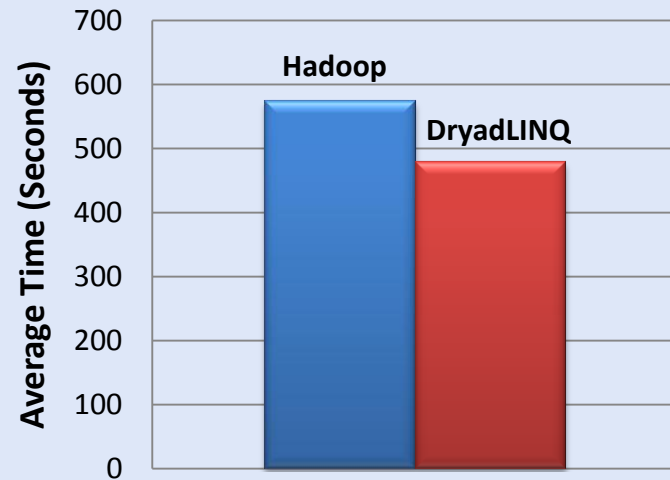
CAP3 - **Expressed Sequence Tag assembly to re-construct full-length mRNA**

Input files (FASTA)

CAP3 → CAP3 → ∘ ∘ → CAP3

Output files

Time to process 1280 files each with ~375 sequences
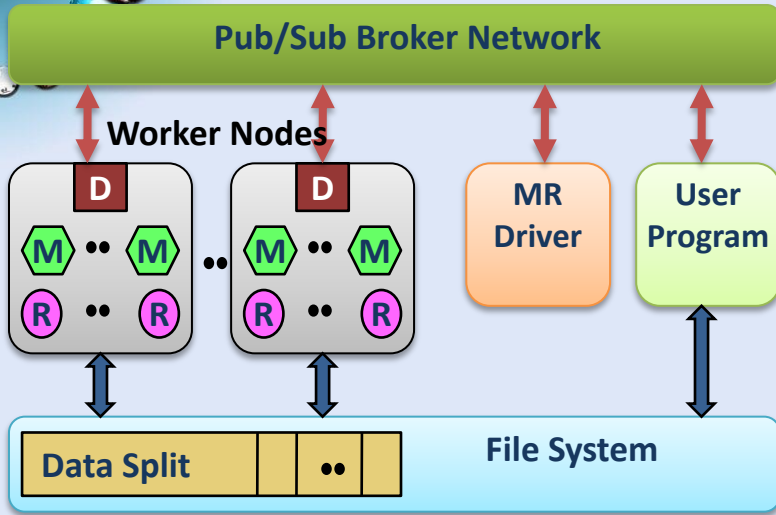

Hadoop

DryadLINQ

Average Time (Seconds)

- Perform using DryadLINQ and Apache Hadoop implementations
- Single "Select" operation in DryadLINQ
- "Map only" operation in Hadoop

X. Huang, A. Madan, "CAP3: A DNA Sequence Assembly Program," Genome Research, vol. 9, no. 9, pp. 868-877, 1999.
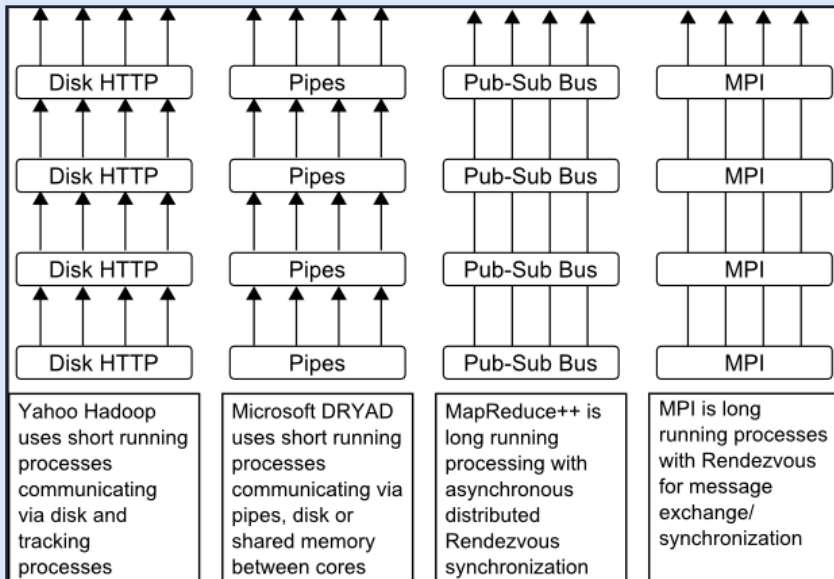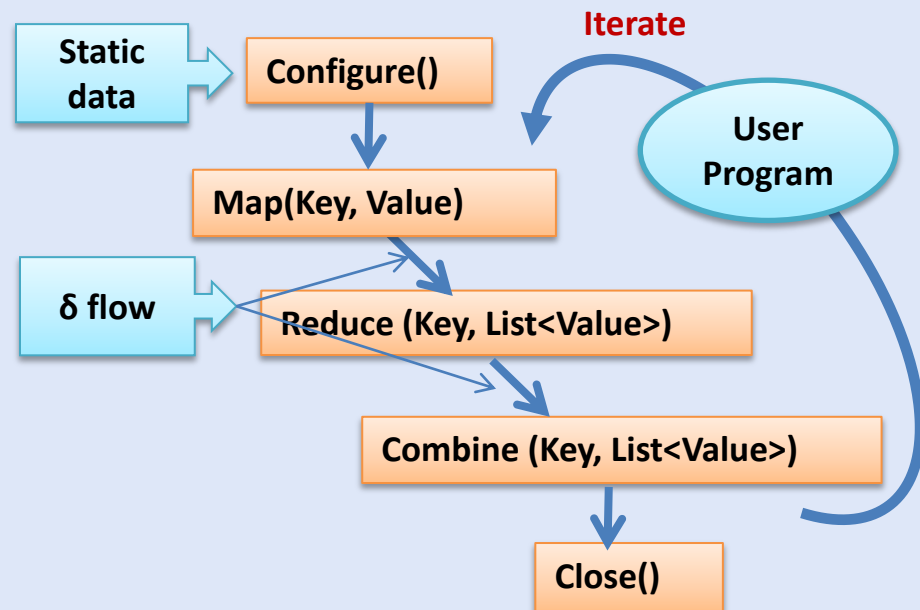
Twister

Pub/Sub Broker Network

Worker Nodes

D M •• M	**D** M •• M
R •• R	R •• R

MR Driver

User Program

Data Split •• **File System**

- **M** Map Worker
- **R** Reduce Worker
- **D** MRDeamon
- ↕ Data Read/Write
- ↕ Communication

- Streaming based communication
- Intermediate results are directly transferred from the map tasks to the reduce tasks – **eliminates local files**
- Cacheable map/reduce tasks
  - Static data remains in memory
- Combine phase to combine reductions
- User Program is the **composer** of MapReduce computations
- **Extends** the MapReduce model to iterative computations

Disk HTTP	Pipes	Pub-Sub Bus	MPI
Disk HTTP	Pipes	Pub-Sub Bus	MPI
Disk HTTP	Pipes	Pub-Sub Bus	MPI
Disk HTTP	Pipes	Pub-Sub Bus	MPI
Yahoo Hadoop uses short running processes communicating via disk and tracking processes	Microsoft DRYAD uses short running processes communicating via pipes, disk or shared memory between cores	MapReduce++ is long running processing with asynchronous distributed Rendezvous synchronization	MPI is long running processes with Rendezvous for message exchange/ synchronization

Different synchronization and intercommunication mechanisms used by the parallel runtimes

Iterate

Static data → **Configure()**

User Program

Map(Key, Value)

δ flow → **Reduce (Key, List<Value>)**

Combine (Key, List<Value>)

Close()

Iterative and non-Iterative Computations

K-means

Data split - 2D data points

map()   map()

Compute the distance to each data point from each cluster center and assign points to the cluster centers

reduce()

Compute the new cluster centers

User Program

Compute the error and decide whether to continue iteration

Smith Waterman is a non iterative case and of course runs fine

Performance of K-Means

Average time for 16 iterations (Seconds) Log Scale — Number of 2D Data Points

Run using 256 CPU cores

Hadoop
DryadLINQ
Twister
MPI

DryadLINQ
Hadoop
Twister

Total Running Time (Seconds) — Number of SW-G calculations (in millions)
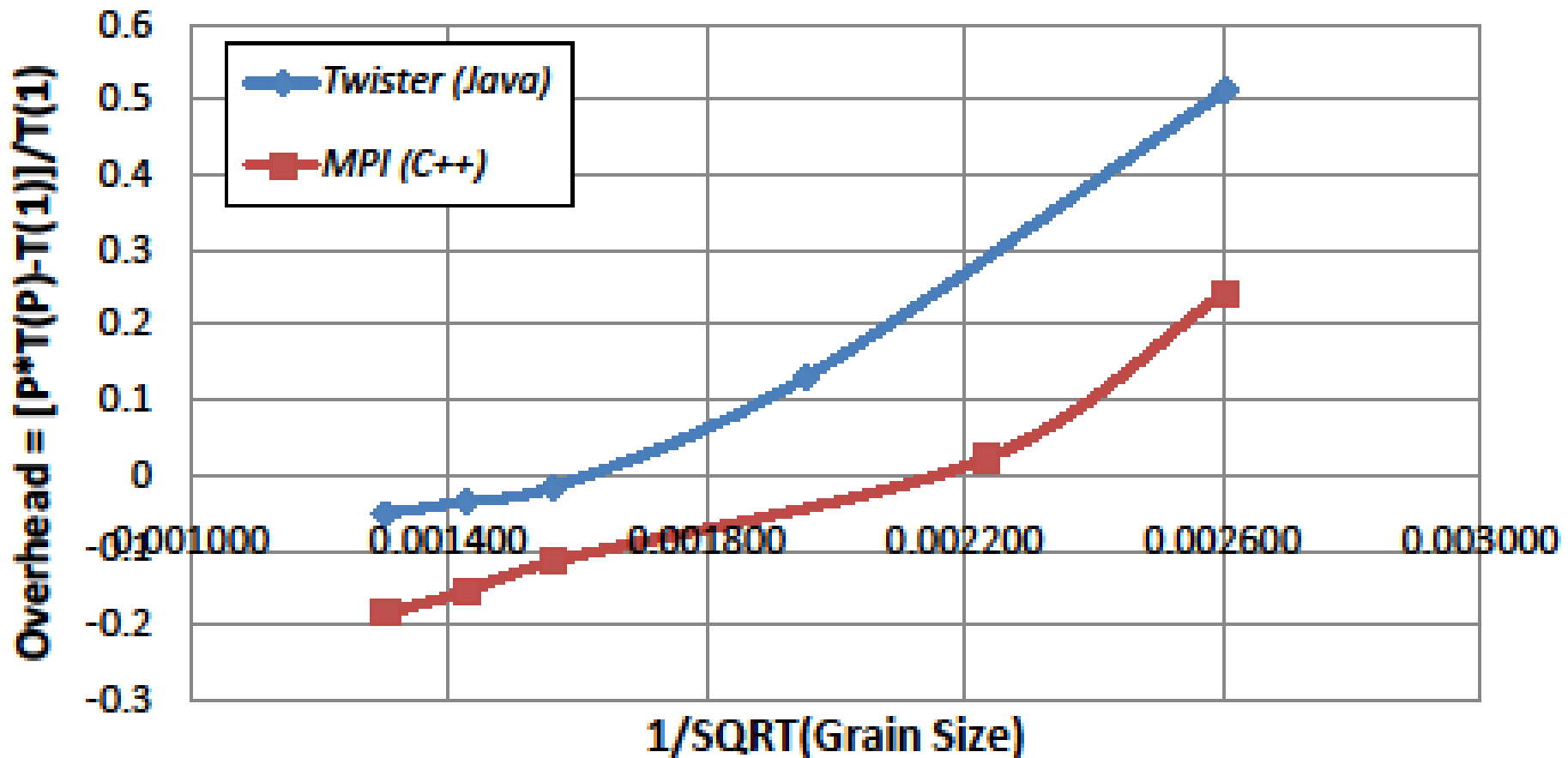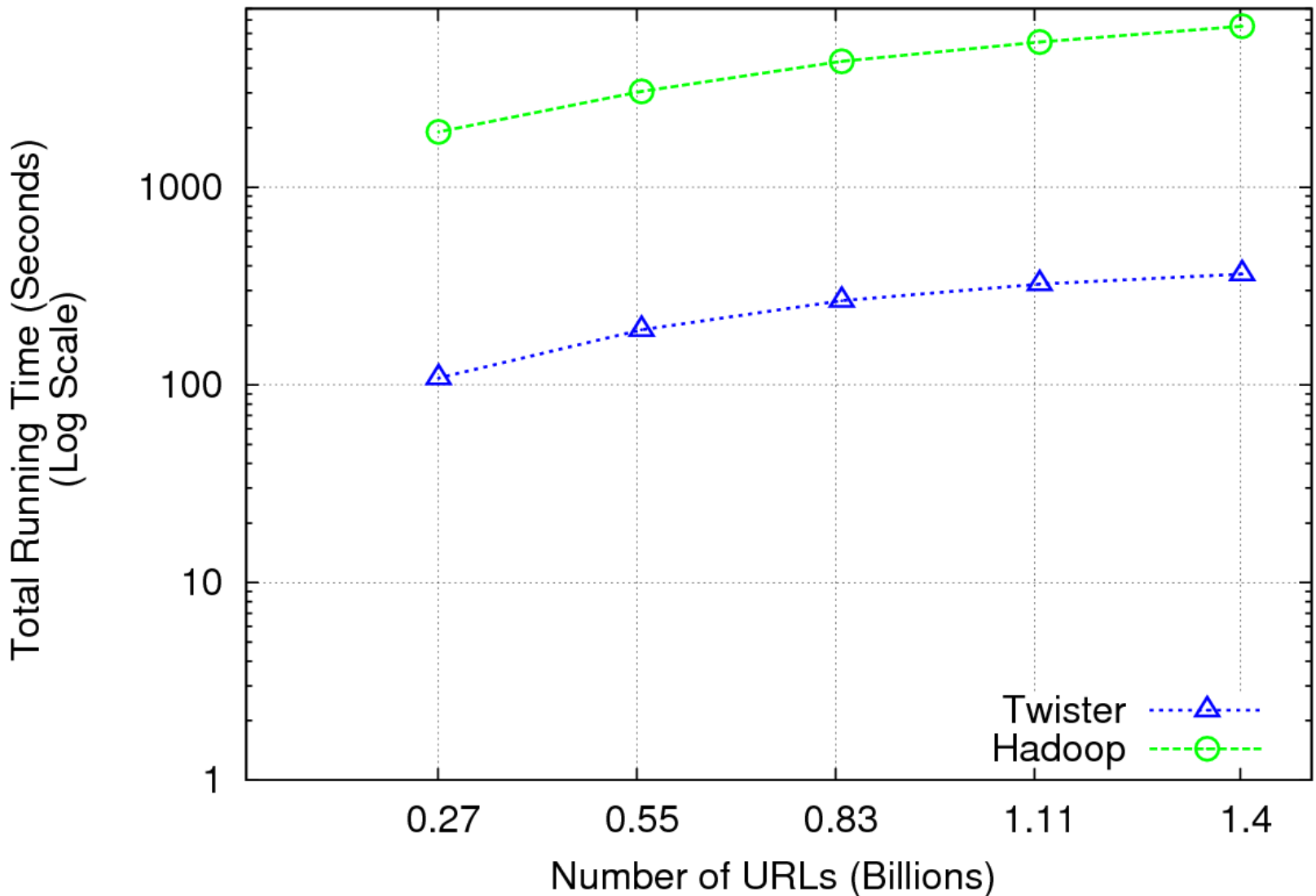
Matrix Multiplication
64 cores

Overhead OpenMPI v Twister negative overhead due to cache

Overhead of Matrix Multiplication (256 CPU cores)

Performance of Pagerank using ClueWeb Data (Time for 20 iterations)
using 32 nodes (256 CPU cores) of Crevasse

TwisterMPIReduce

PairwiseClustering MPI	Multi Dimensional Scaling MPI	Generative Topographic Mapping MPI	Other …

TwisterMPIReduce

Azure Twister (C# C++) | **Java Twister**

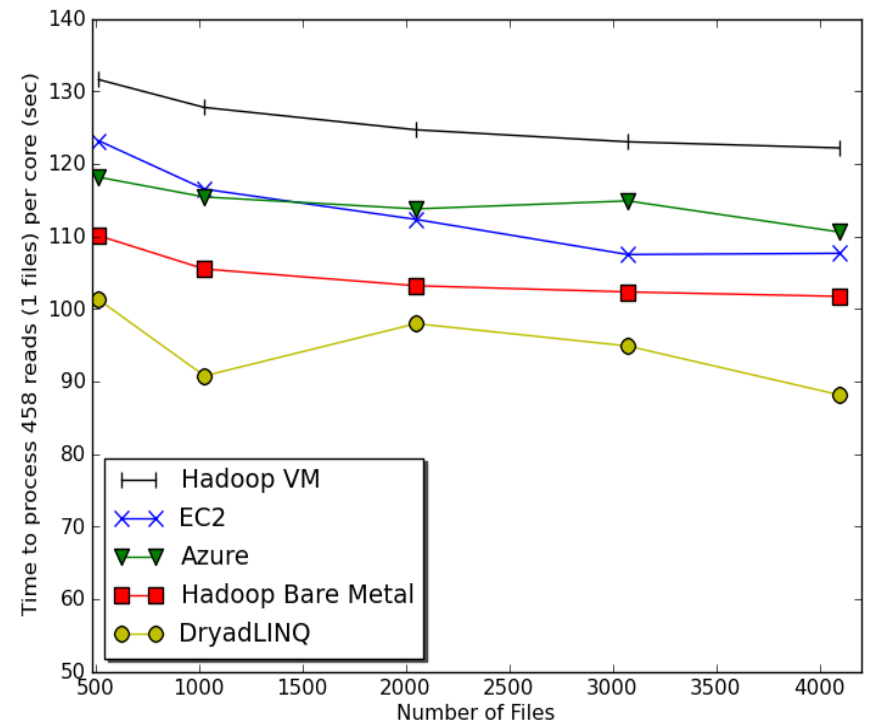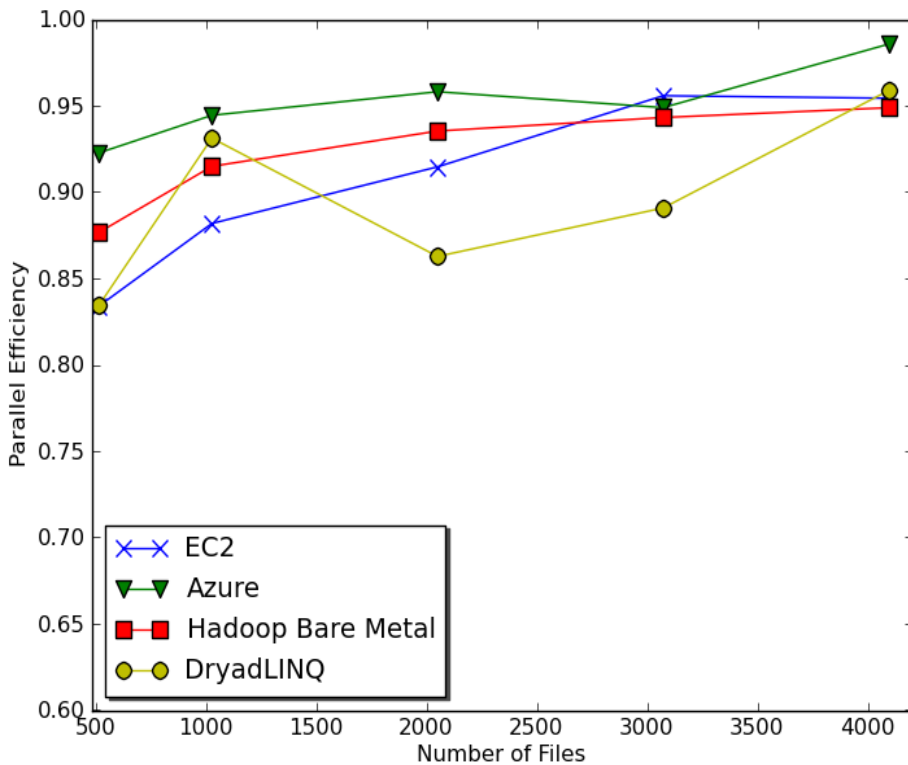**Microsoft Azure** | **FutureGrid** | **Local Cluster** | **Amazon EC2**

- Runtime package supporting subset of MPI mapped to Twister

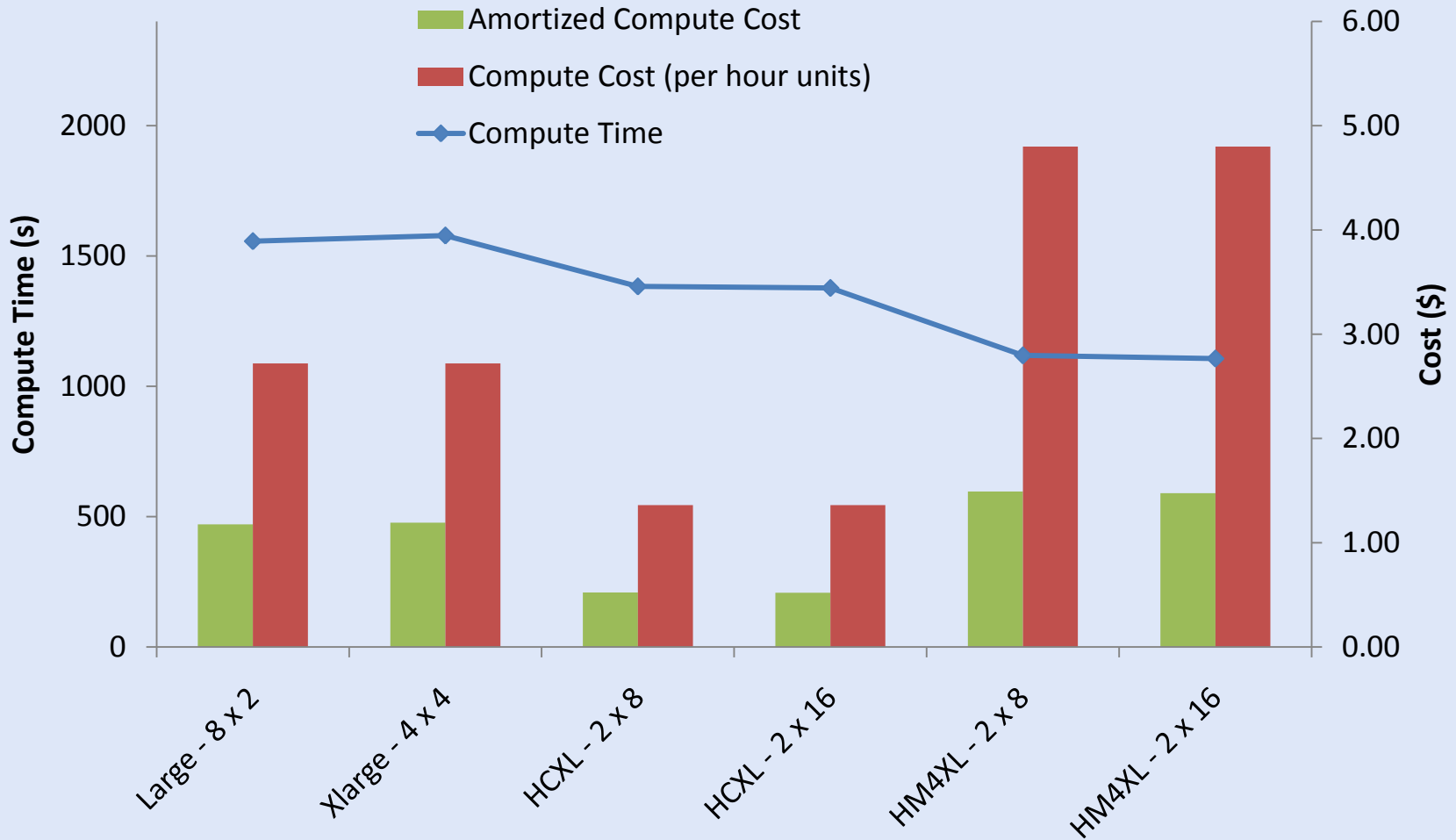- Set-up, Barrier, Broadcast, Reduce

Sequence Assembly in the Clouds

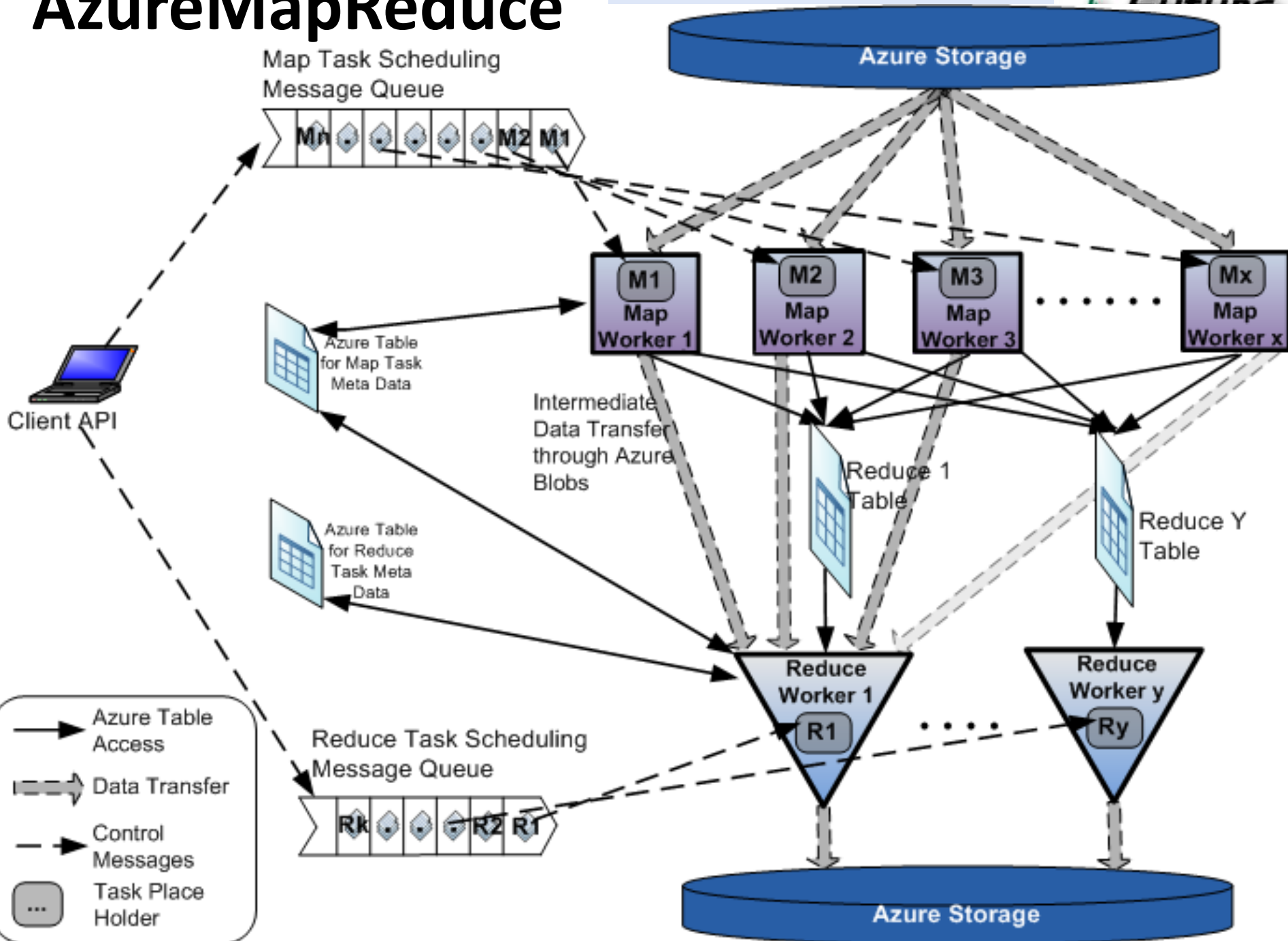**Cap3** Parallel **Efficiency**

Cap3 – **Time** Per core per file (458 reads in each file) to process sequences

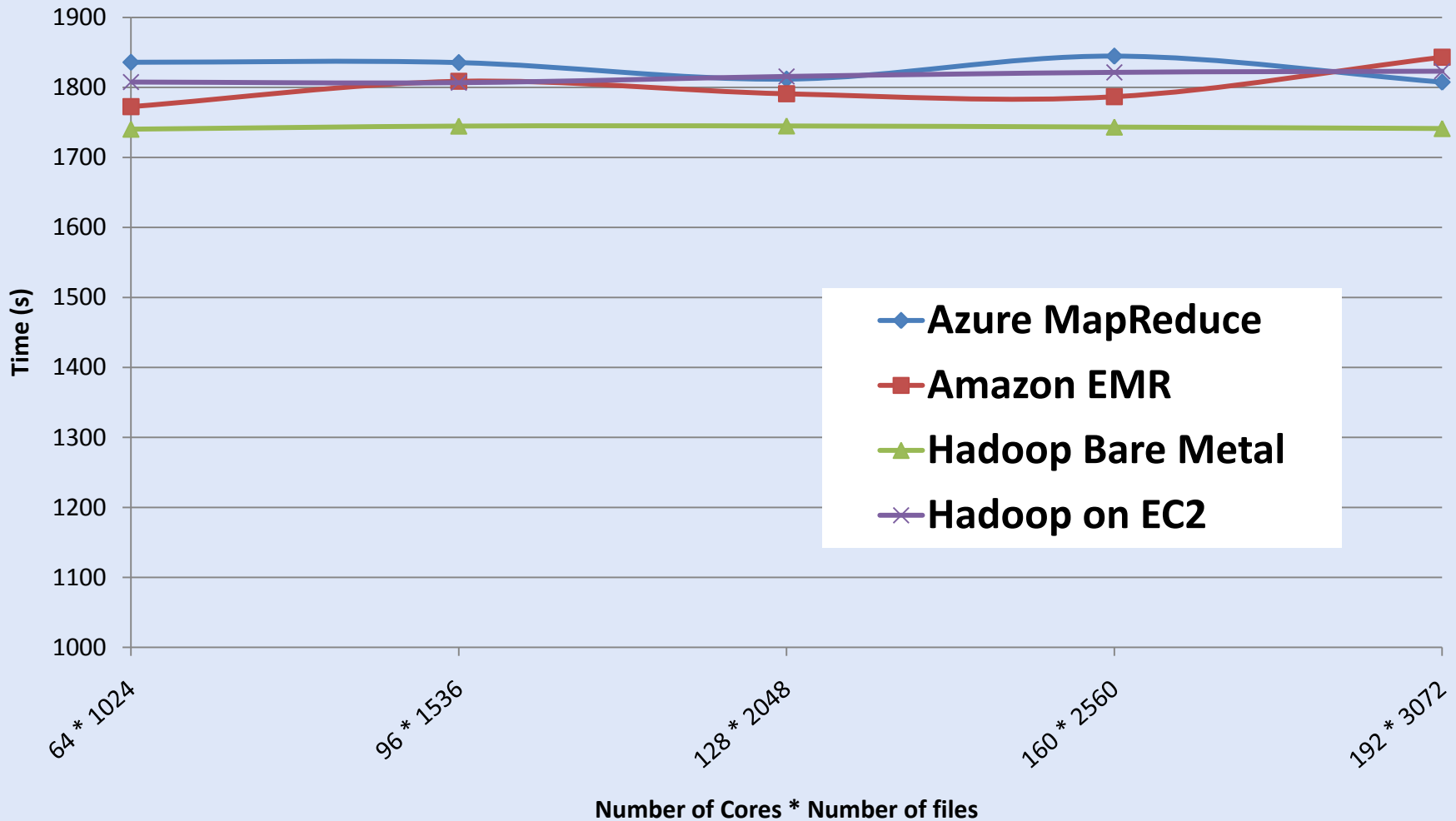# Cap3 Performance with Different EC2 Instance Types

AzureMapReduce

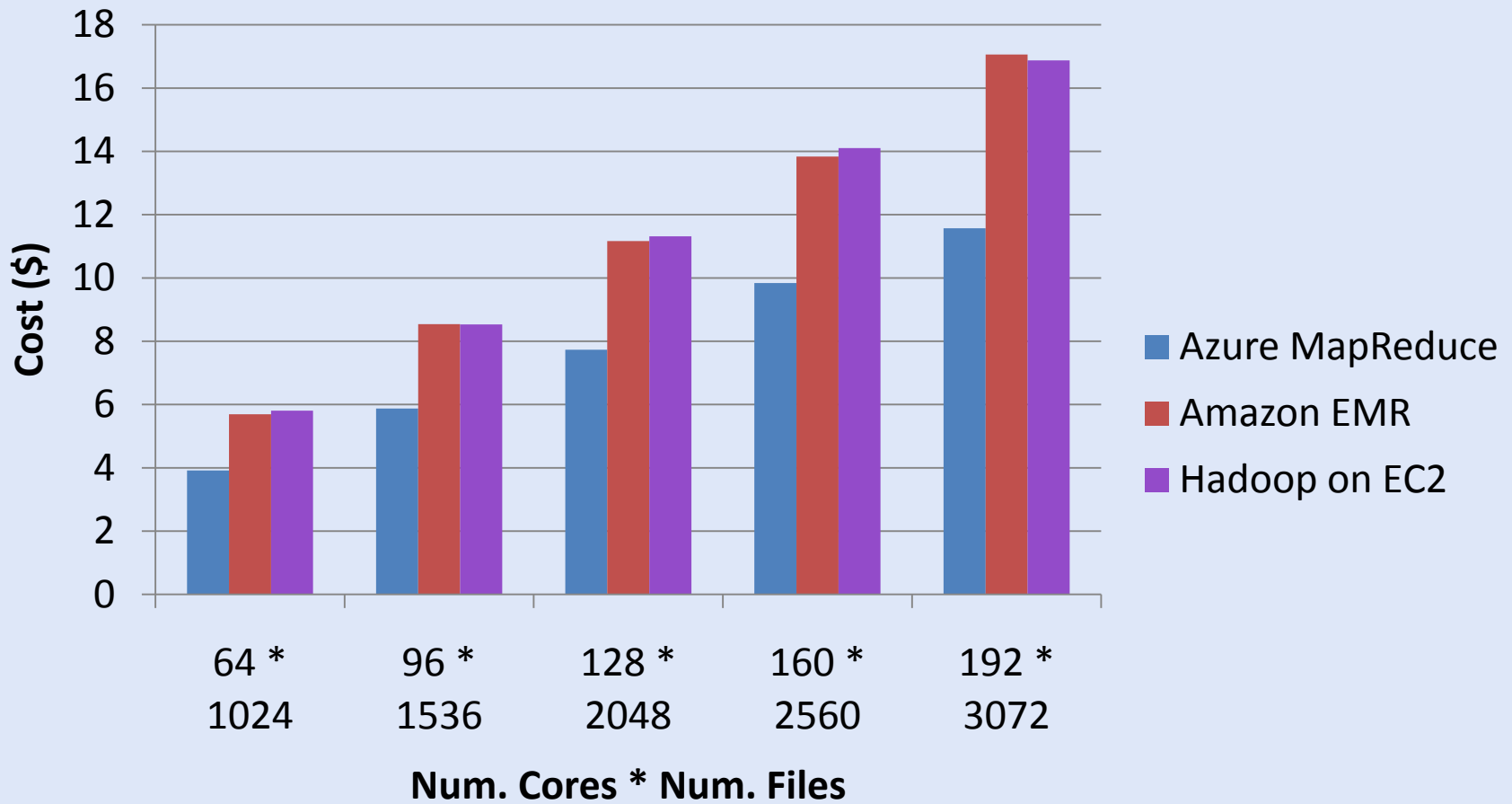# Early Results with Azure/Amazon MapReduce
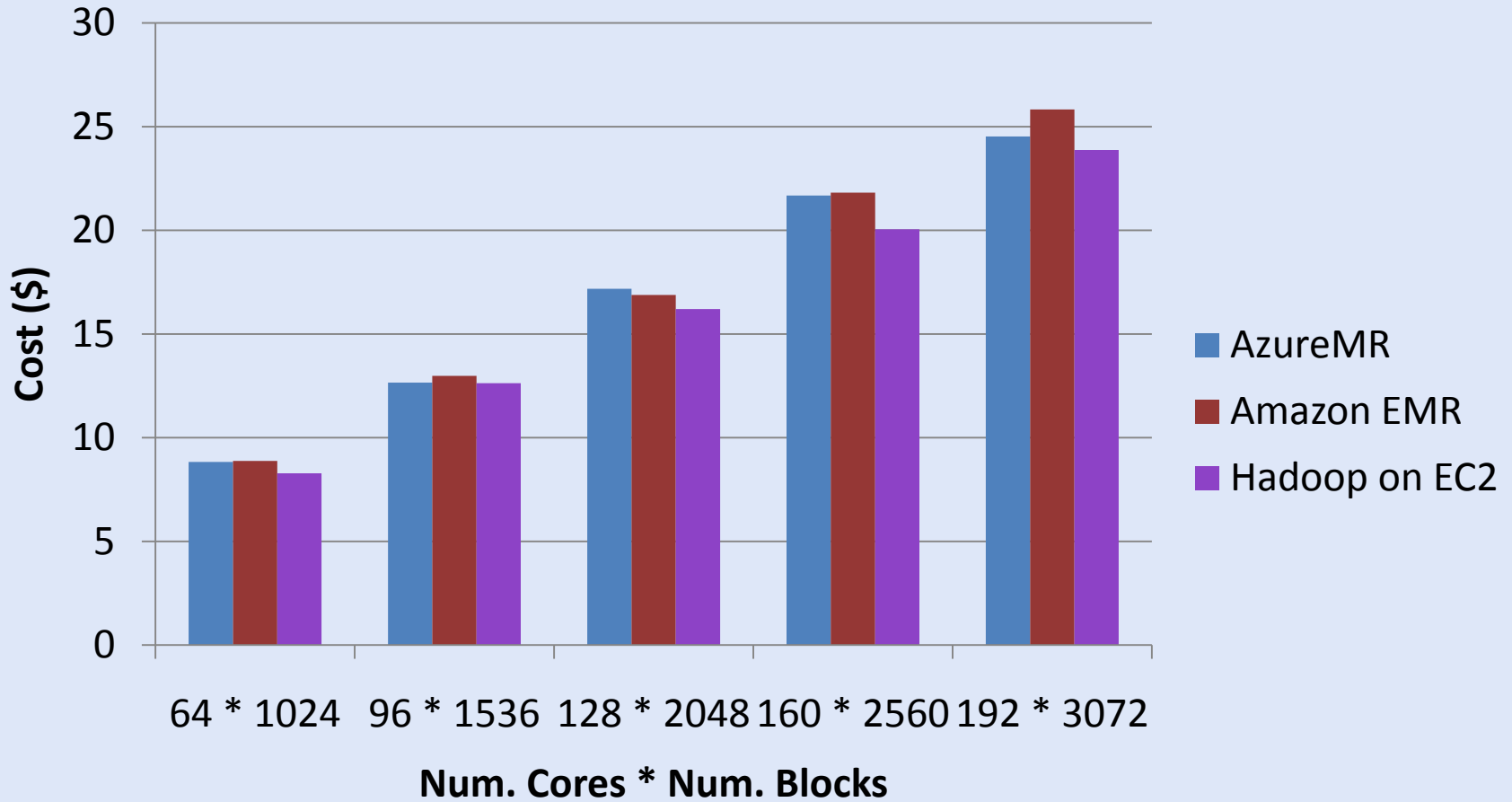
Cap3 Sequence Assembly

Cap3 Cost

SWG Cost

Smith Waterman: Daily Effect

Some Issues with AzureTwister and AzureMapReduce

- Transporting data to Azure: Blobs (HTTP), Drives (GridFTP etc.), Fedex disks
- Intermediate data Transfer: Blobs (current choice) versus Drives (should be faster but don't seem to be)
- Azure Table v Azure SQL: Handle all metadata
- Messaging Queues: Use real publish-subscribe system in place of Azure Queues
- Azure Affinity Groups: Could allow better data-compute and compute-compute affinity

Research and Clouds I

- Clouds are suitable for "Loosely coupled" data parallel applications
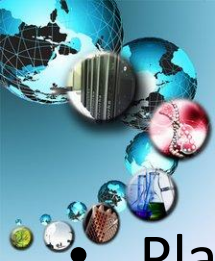- Quantify "loosely coupled" and define appropriate programming model
- "Map Only" (really pleasingly parallel) certainly run well on clouds (subject to data affinity) with many programming paradigms
- Parallel FFT and adaptive mesh PDA solver probably pretty bad on clouds but suitable for classic MPI engines
- MapReduce and Twister are candidates for "appropriate programming model"
- 1 or 2 iterations (MapReduce) and Iterative with large messages (Twister) are "loosely coupled" applications
- How important is compute-data affinity and concepts like HDFS

Research and Clouds II

- Platforms: exploit Tables as in SHARD (Scalable, High-Performance, Robust and Distributed) Triple Store based on Hadoop
  - What are needed features of tables
- Platforms: exploit MapReduce and its generalizations: are there other extensions that preserve its robust and dynamic structure
  - How important is the loose coupling of MapReduce
  - Are there other paradigms supporting important application classes
- What are other platform features are useful
- Are "academic" private clouds interesting as they (currently) only have a few of Platform features of commercial clouds?
- Long history of search for latency tolerant algorithms for memory hierarchies
  - Are there successes? Are they useful in clouds?
  - In Twister, only support large complex messages
  - What algorithms only need TwisterMPIReduce

Research and Clouds III

- Can cloud deployment algorithms be devised to support compute-compute and compute-data affinity
- What platform primitives are needed by datamining?
  - Clearer for partial differential equation solution?
- Note clouds have greater impact on programming paradigms than Grids
- Workflow came from Grids and will remain important
  - Workflow is coupling coarse grain functionally distinct components together while MapReduce is data parallel scalable parallelism
- Finding subsets of MPI and algorithms that can use them probably more important than making MPI more complicated
- Note MapReduce can use multicore directly – don't need hybrid MPI OpenMP Programming models
- Develop Publish-Subscribe optimized for Twister communication
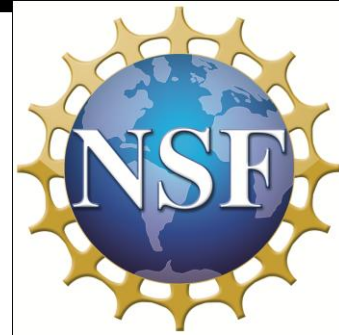
US Cyberinfrastructure Context

- There are a rich set of facilities
  - Production TeraGrid facilities with distributed and shared memory
  - Experimental "Track 2D" Awards
    - FutureGrid: Distributed Systems experiments cf. Grid5000
    - Keeneland: Powerful GPU Cluster
    - Gordon: Large (distributed) Shared memory system with SSD aimed at data analysis/visualization
  - Open Science Grid aimed at High Throughput computing and strong campus bridging

TeraGrid

- ~2 Petaflops; over 20 PetaBytes of storage (disk and tape), over 100 scientific data collections
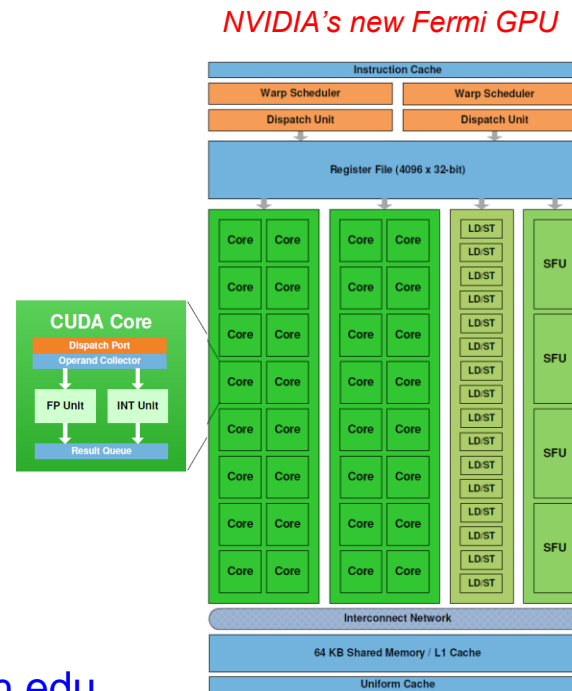
Keeneland – NSF-Funded Partnership to Enable Large-scale Computational Science on Heterogeneous Architectures

- NSF Track 2D System of Innovative Design
  - Georgia Tech
  - UTK NICS
  - ORNL
  - UTK
- Two GPU clusters
  - Initial delivery (~250 CPU, 250 GPU)
    - Being built now; Expected availability is November 2010
  - Full scale (> 500 GPU) – Spring 2012
  - NVIDIA, HP, Intel, Qlogic
- Operations, user support
- Education, Outreach, Training for scientists, students, industry
- Software tools, application development

http://keeneland.gatech.edu
http://ft.ornl.gov

- Exploit graphics processors to provide extreme performance and energy efficiency

NVIDIA's new Fermi GPU
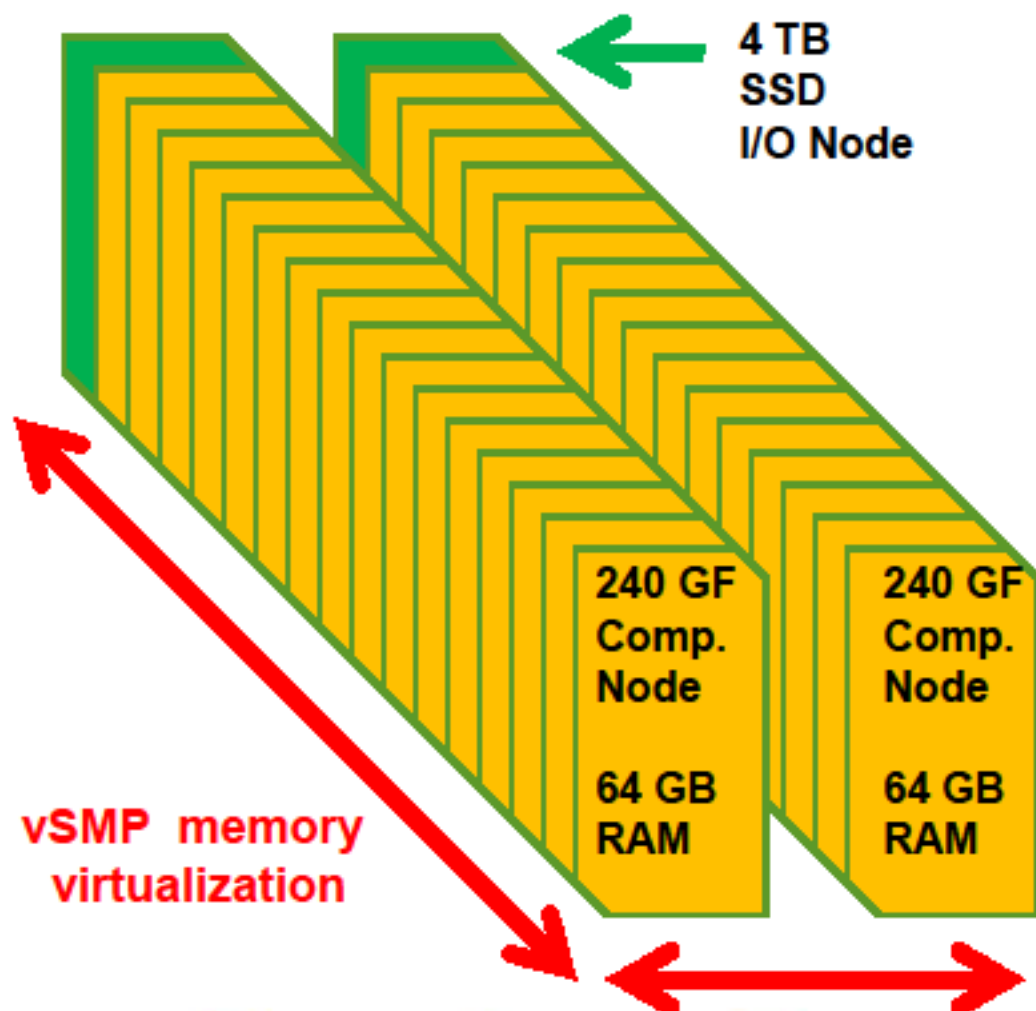

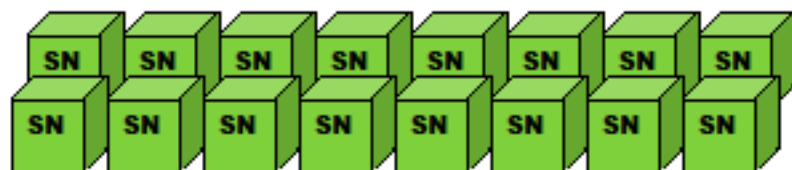| |
|---|
| Prof. Jeffrey S. Vetter |
| Prof. Richard Fujimoto |
| Prof. Karsten Schwan |
| Prof. Jack Dongarra |
| Dr. Thomas Schulthess |
| Prof. Sudha Yalamanchili |
| Jeremy Meredith |
| Dr. Philip Roth |
| Richard Glassbrook |
| Patricia Kovatch |
| Stephen McNally |
| Dr. Bruce Loftis |
| Jim Ferguson |
| James Rogers |
| Kathlyn Boudwin |
| Arlene Washington |
| *Many others…* |

Gordon Architecture: "Supernode"

- **32 Appro Extreme-X compute nodes**
  - Dual processor Intel Sandy Bridge
    - 240 GFLOPS
    - 64 GB

- **2 Appro Extreme-X IO nodes**
  - Intel SSD drives
    - 4 TB ea.
    - 560,000 IOPS

- **ScaleMP vSMP virtual shared memory**
  - 2 TB RAM aggregate
  - 8 TB SSD aggregate

4 TB SSD I/O Node

240 GF Comp. Node

64 GB RAM

240 GF Comp. Node

64 GB RAM

vSMP memory virtualization

SDSC **SAN DIEGO SUPERCOMPUTER CENTER**

UCSD

APPRO HPC Cluster Solutions

(intel)

ScaleMP

Gordon Architecture: Full Machine

- **32 supernodes = 1024 compute nodes**

- **Dual rail QDR Infiniband network**
  - 3D torus (4x4x4)

- **4 PB rotating disk parallel file system**
  - >100 GB/s

FutureGrid key Concepts I

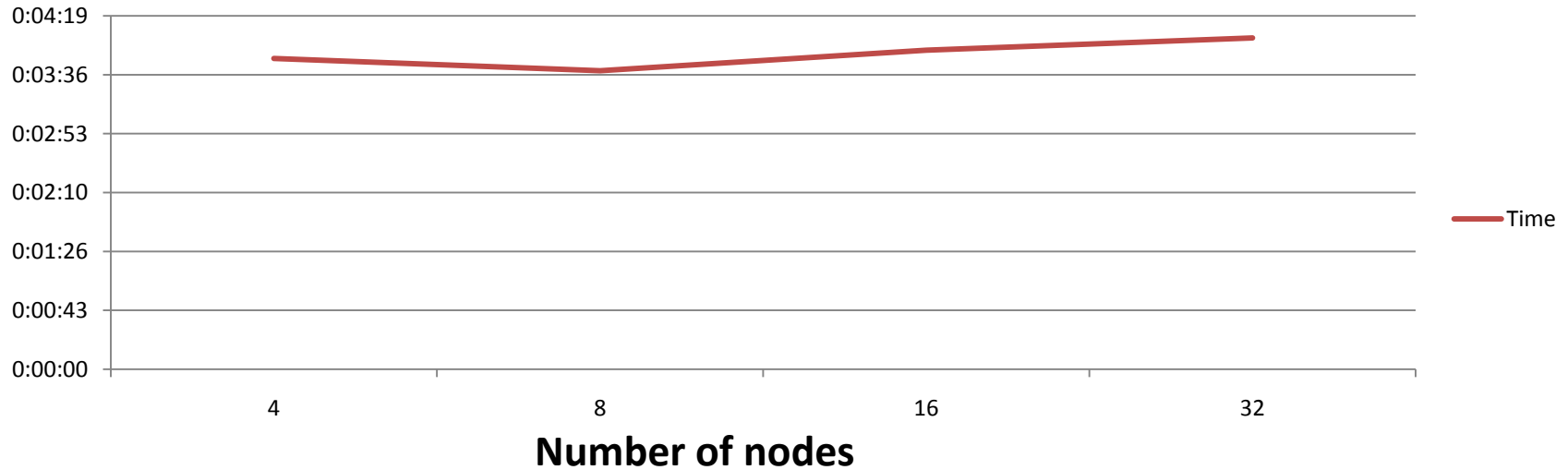- FutureGrid is an international testbed modeled on Grid5000

- Rather than loading images onto VM's, FutureGrid supports Cloud, Grid and Parallel computing environments by dynamically provisioning software as needed onto "bare-metal" using Moab/xCAT
  - Image library for MPI, OpenMP, Hadoop, Dryad, gLite, Unicore, Globus, Xen, ScaleMP (distributed Shared Memory), Nimbus, Eucalyptus, OpenNebula, KVM, Windows …..

- The FutureGrid testbed provides to its users:
  - A flexible development and testing platform for middleware and application users looking at interoperability, functionality and performance
  - Each use of FutureGrid is an experiment that is reproducible
  - A rich education and teaching platform for advanced cyberinfrastructure classes

- Growth comes from users depositing novel images in library

Dynamic Provisioning Results

Time minutes

Total Provisioning Time minutes

Time elapsed between requesting a job and the jobs reported start time on the provisioned node. The numbers here are an average of 2 sets of experiments.
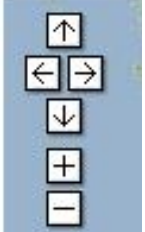
FutureGrid key Concepts II

- Support Computer Science and Computational Science
  - Industry and Academia
  - Asia, Europe and Americas
- FutureGrid has ~5000 distributed cores with a dedicated network and a Spirent XGEM network fault and delay generator
- **Key early user oriented milestones:**
  - **June 2010** Initial users
  - **November 2010-September 2011** Increasing number of users allocated by FutureGrid
  - **October 2011** FutureGrid allocatable via TeraGrid process
  - 3 classes using FutureGrid this fall
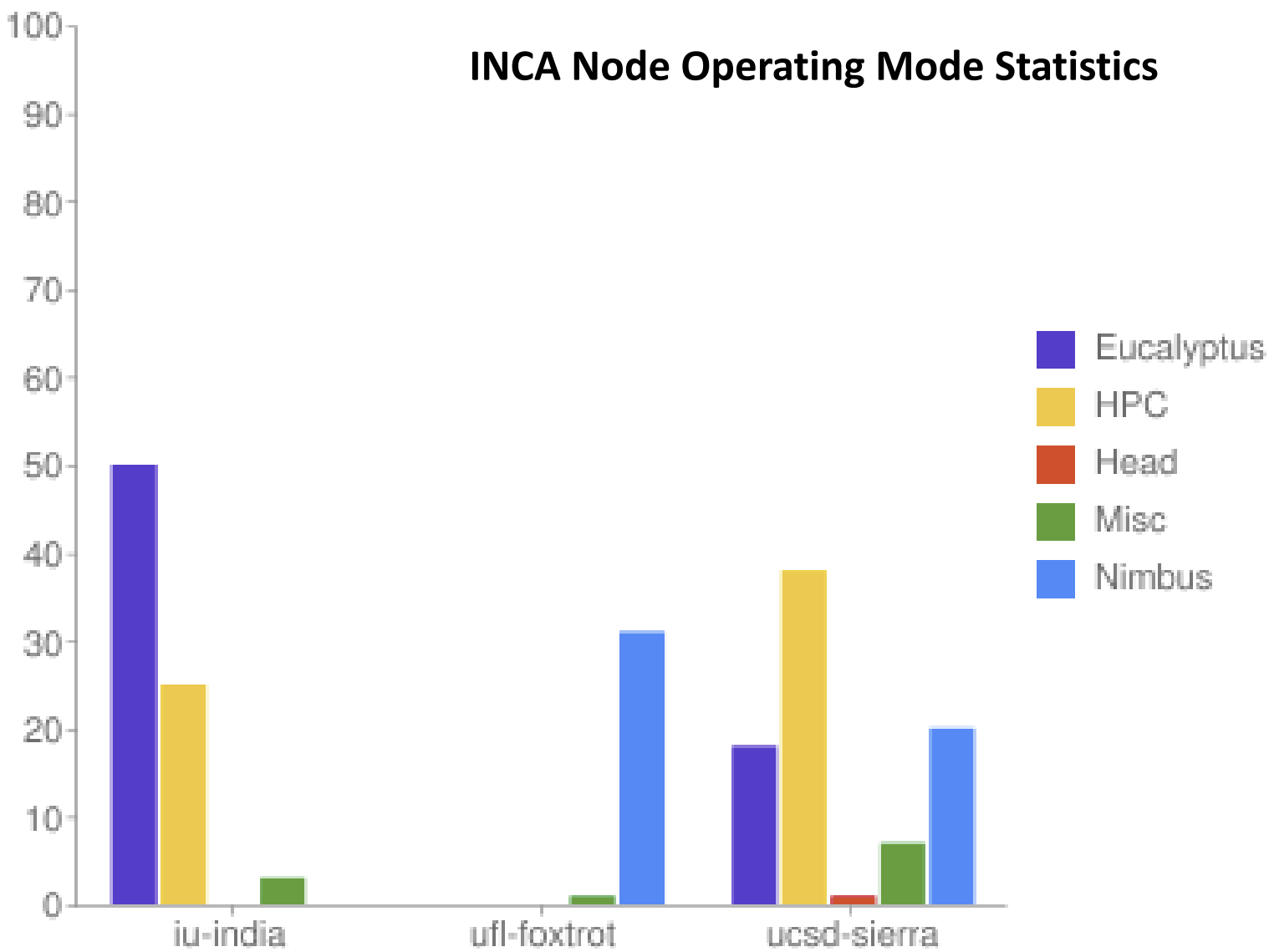- Apply **now** to use FutureGrid on web site www.futuregrid.org

FutureGrid Partners

- Indiana University (Architecture, core software, Support)
  - Collaboration between research and infrastructure groups
- Purdue University (HTC Hardware)
- San Diego Supercomputer Center at University of California San Diego (INCA, Monitoring)
- University of Chicago/Argonne National Labs (Nimbus)
- University of Florida (ViNE, Education and Outreach)
- University of Southern California Information Sciences (Pegasus to manage experiments)
- University of Tennessee Knoxville (Benchmarking)
- University of Texas at Austin/Texas Advanced Computing Center (Portal)
- University of Virginia (OGF, Advisory Board and allocation)
- Center for Information Services and GWT-TUD from Technische Universtität Dresden. (VAMPIR)
- Red institutions have FutureGrid hardware

FutureGrid: a Grid/Cloud/HPC

INCA Node Operating Mode Statistics

Legend:
- Eucalyptus
- HPC
- Head
- Misc
- Nimbus

iu-india · ufl-foxtrot · ucsd-sierra

Network & Internal Interconnects

- FutureGrid has dedicated network (except to TACC) and a network fault and delay generator
- Can isolate experiments on request; IU runs Network for NLR/Internet2
- (Many) additional partner machines will run FutureGrid software and be supported (but allocated in specialized ways)

Machine	Name	Internal Network
IU Cray	xray	Cray 2D Torus SeaStar
IU iDataPlex	india	DDR IB, QLogic switch with Mellanox ConnectX adapters Blade Network Technologies & Force10 Ethernet switches
SDSC iDataPlex	sierra	DDR IB, Cisco switch with Mellanox ConnectX adapters Juniper Ethernet switches
UC iDataPlex	hotel	DDR IB, QLogic switch with Mellanox ConnectX adapters Blade Network Technologies & Juniper switches
UF iDataPlex	foxtrot	Gigabit Ethernet only (Blade Network Technologies; Force10 switches)
TACC Dell	alamo	QDR IB, Mellanox switches and adapters Dell Ethernet switches

Network Impairment Device

- Spirent XGEM Network Impairments Simulator for jitter, errors, delay, etc
- Full Bidirectional 10G w/64 byte packets
- up to 15 seconds introduced delay (in 16ns increments)
- 0-100% introduced packet loss in .0001% increments
- Packet manipulation in first 2000 bytes
- up to 16k frame size
- TCL for scripting, HTML for manual configuration

FutureGrid Usage Model

- The goal of FutureGrid is to support the research on the future of distributed, grid, and cloud computing
- FutureGrid will build a robustly managed simulation environment and test-bed to support the development and early use in science of new technologies at all levels of the software stack: from networking to middleware to scientific applications
- The environment will mimic TeraGrid and/or general parallel and distributed systems – FutureGrid is part of TeraGrid (but not part of formal TeraGrid process for first two years)
  – Supports Grids, Clouds, and classic HPC
  – It will mimic commercial clouds (initially IaaS not PaaS)
  – Expect FutureGrid PaaS to grow in importance
- FutureGrid can be considered as a (small ~5000 core) Science/Computer Science Cloud but it is more accurately a virtual machine or bare-metal based simulation environment
- This test-bed will succeed if it enables major advances in science and engineering through collaborative development of science applications and related software

Two Recent Projects

FG10-803

Title	TIS Technology Evaluation Laboratory
Submitted By	John Lockman
Institution	Texas Advanced Computing Center Research Office Complex 1.101, J.J. Pickle Research Campus 10100 Burnet Road (R8700) Austin, Texas 78758-4497
Discipline	
Subdiscipline	
Orientation	Research
Hardware Systems	Hotel (IBM iDataPlex at U Chicago); India (IBM iDataPlex at IU); Sierra (IBM iDataPlex at SDSC); XRay (Cray XM5 at IU)
Software	

Use of FutureGrid
Future Grid will be used in part by the TIS team for the Technology Evaluation Process.

Software Contributions
This project WILL NOT generate software that can be used by other FutureGrid users.

Scale
comparisons of different software...

FG10-802

Title	Peer-to-peer overlay networks and applications in virtual networks and virtual clusters
Submitted By	Renato Figueiredo
Institution	University of Florida 336 Larsen Hall Gainesville, FL 32611
Discipline	Computer Science and Engineering
Subdiscipline	Distributed Systems
Web Page	http://www.grid-appliance.org
Orientation	Research
Hardware Systems	Hotel (IBM iDataPlex at U Chicago); India (IBM iDataPlex at IU); Sierra (IBM iDataPlex at SDSC)
Software	Eucalyptus VM; Nimbus VM

Use of FutureGrid
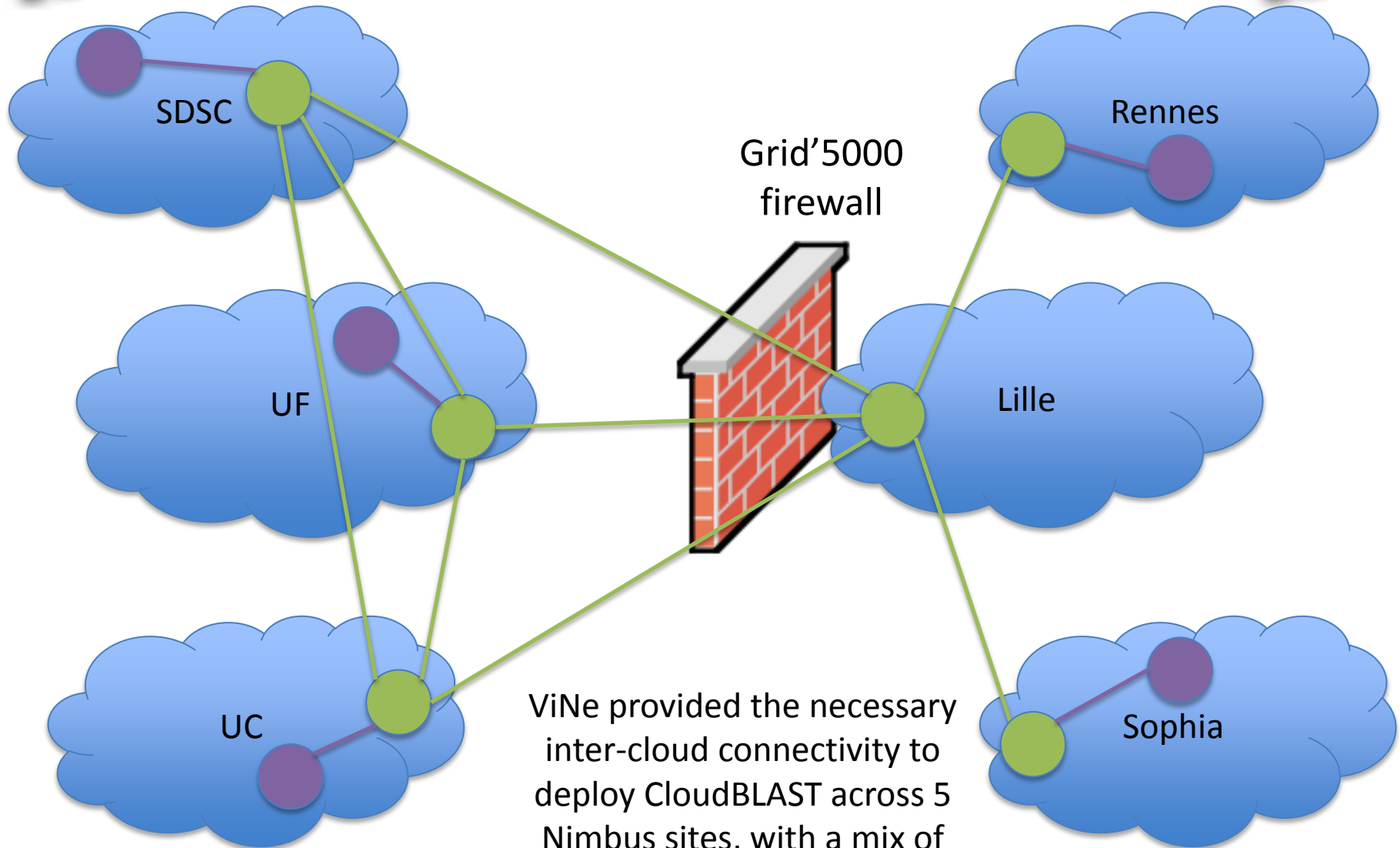FutureGrid will be used in experiments that evaluate various aspects...

Grid Interoperability
from Andrew Grimshaw

- Colleagues,
- FutureGrid has as two of its many goals the creation of a Grid middleware testing and interoperability testbed as well as the maintenance of standards compliant endpoints against which experiments can be executed. We at the University of Virginia are tasked with bringing up three stacks as well as maintaining standard-endpoints against which these experiments can be run.
- We currently have UNICORE 6 and Genesis II endpoints functioning on X-Ray (a Cray). Over the next few weeks we expect to bring two additional resources, India and Sierra (essentially Linux clusters), on-line in a similar manner (Genesis II is already up on Sierra). As called for in the FutureGrid program execution plan, once those two stacks are operational we will begin to work on g-lite (with help we may be able to accelerate that). Other standards-compliant endpoints are welcome in the future , but not part of the current funding plan.

We RENKEI/NAREGI project are interested in the participation for interoperation demonstrations or projects for OGF and SC. We have a prototype middleware which can submit and receive jobs using the HPCBP specification. Can we have more detailed information of your endpoints(authentication, data staging method, and so on) and the participation conditions of the demonstrations/projects.

OGF'10 Demo

SDSC

Rennes

Grid'5000 firewall

UF

Lille

UC

Sophia

ViNe provided the necessary inter-cloud connectivity to deploy CloudBLAST across 5 Nimbus sites, with a mix of public and private subnets.

Big Data for Science

300+ Students learning about Twister & Hadoop MapReduce technologies, supported by FutureGrid.
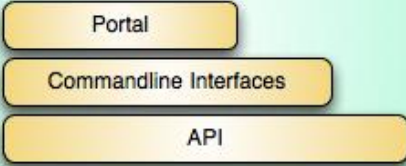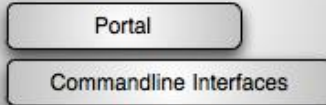
July 26-30, 2010 NCSA Summer School Workshop
http://salsahpc.indiana.edu/tutorial

Software Components

- **Portals** including "Support" "use FutureGrid" "Outreach"
- **Monitoring** – INCA, Power (GreenIT)
- **Experiment Manager**: specify/workflow
- **Image** Generation and Repository
- **Intercloud** Networking ViNE
- **Virtual Clusters** built with virtual networks
- **Performance** library
- **Rain** or **R**untime **A**daptable **I**nsertio**N** Service: Schedule and Deploy images
- **Security** (including use of isolated network), Authentication, Authorization,

FutureGrid Layered Software Stack

FutureGrid Interaction with Commercial Clouds

- We support experiments that link Commercial Clouds and FutureGrid with one or more workflow environments and portal technology installed to link components across these platforms

- We support environments on FutureGrid that are similar to Commercial Clouds and natural for performance and functionality comparisons

– These can both be used to prepare for using Commercial Clouds and as the most likely starting point for porting to them

– One example would be support of MapReduce-like environments on FutureGrid including Hadoop on Linux and Dryad on Windows HPCS which are already part of FutureGrid portfolio of supported software

- We develop expertise and support porting to Commercial Clouds from other Windows or Linux environments

- We support comparisons between and integration of multiple commercial Cloud environments – especially Amazon and Azure in the immediate future

- We develop tutorials and expertise to help users move to Commercial Clouds from other environments

FutureGrid Viral Growth Model

- Users apply for a project

- Users improve/develop some software in project

- This project leads to new images which are placed in FutureGrid repository

- Project report and other web pages document use of new images

- Images are used by other users

- And so on ad infinitum ………

194 papers submitted to main track; 48 accepted; 4 days of tutorials