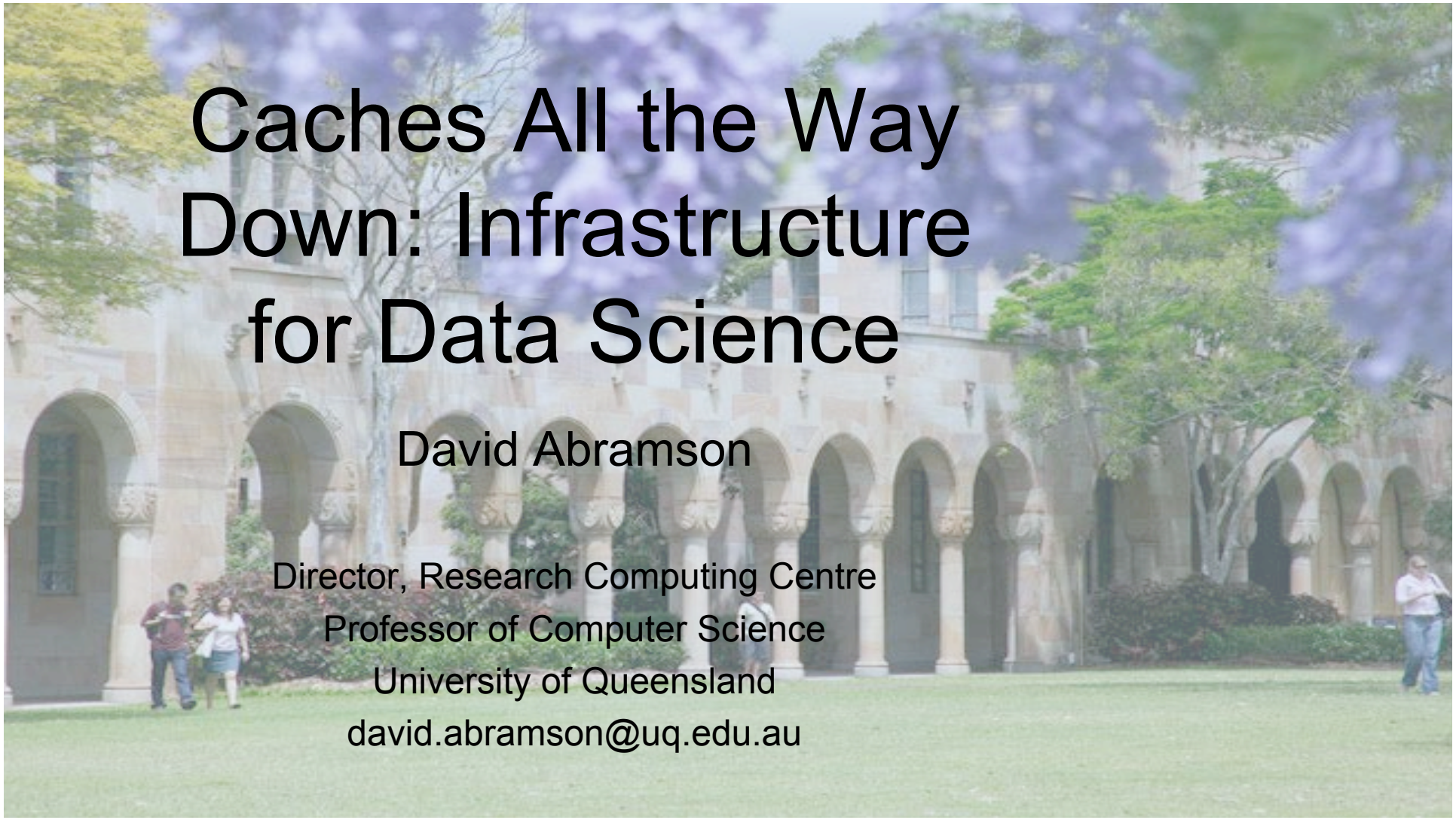


Caches All the Way Down: Infrastructure for Data Science

David Abramson

Director, Research Computing Centre
Professor of Computer Science
University of Queensland
david.abramson@uq.edu.au

“Purely Academic”

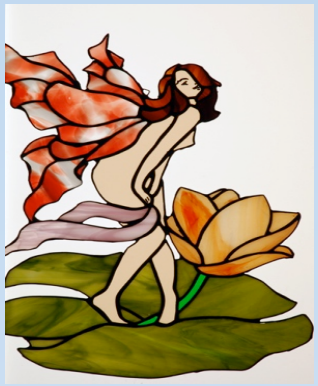
PURELY ACADEMIC

Cast

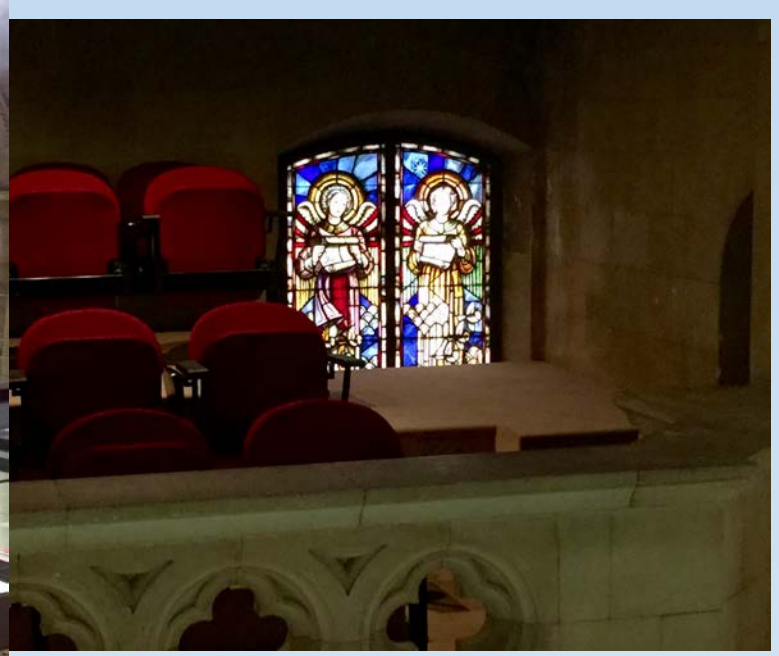
Prof John Holywell	Southern University academic in his early 50’s
Prof Martin Godson	Middleton University academic in his mid 50’s
Prof Mary Long	Southern University academic in her early 40’s
Charles Mittleman	Initially a 30 year old PhD student at Wooton College and Southern University, but then moves to Middleton University as a young academic.
Joanne	Southern University software developer in her mid 30’s. Works in Prof Holywell’s lab and is pregnant.
Prof Max Williams	St George College academic in his late 50’s. Serves as the chair of the Shaw Trust, a not for profit society that supports research projects with grants.
Anna	Middleton University administrator in her 30’s. She also serves as an administrator on the Shaw Trust, taking notes and helping with the grant assessment exercises.
Mark	Early career academic

Robin, Cheryle, Newsreader (voices only. Can be played by other actors)

This play starts in mid to late 1990’s.

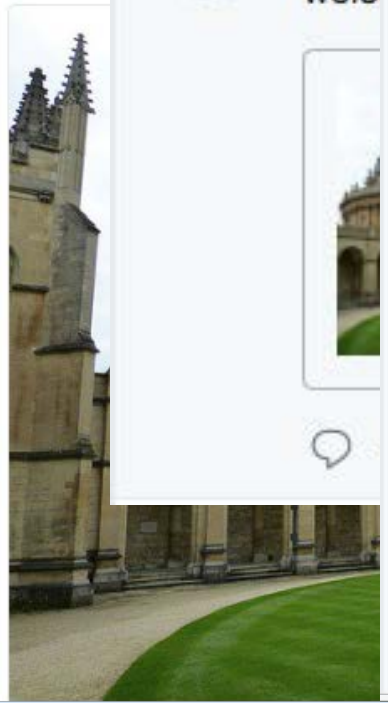


Inspired by the BSC



RCC UQ
@RCCUQ

RCC Director @da
at @
comp
rcc.u



Oxfo
Unfo
welc

Oxford e-Research @OxfordeResearch · 17 Mar 2017

Replying to @davidaabramson

Apologies for the mistake - this is the hoarding the builders were *meant* to have put up....

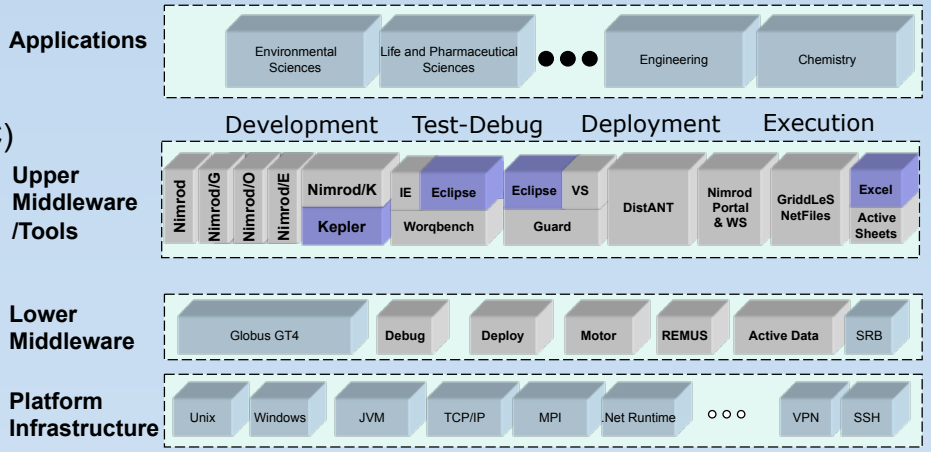
ted to

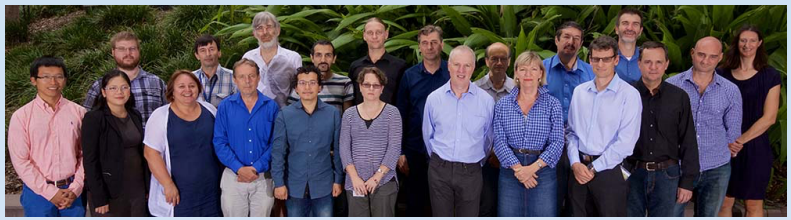
rastructure

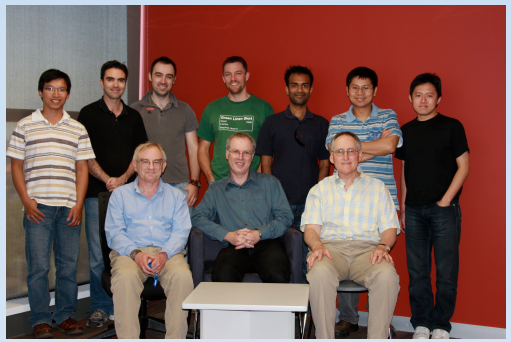
HPDC Award Thanks

- Blair Bethwaite
- Jin Chao
- Clement Chu
- Colin Enticott
- Slavisa Garic
- Greg Watson
- Rajkumar Buyya
- Andrew Lewis
- Nam Tran
- Wojtek Goscinski
- Aaron Searle
- Tim Ho
- Donny Kurniawan
- Tirath Ramdas
- Shahaan Ayyub
- Steve Quinette
- Ngoc Dinh (Minh)
- Hoang Nguyen

- Amazon
- Axceleon
- Australian Partnership for Advanced Computing (APAC)
- Australian Research Council
- Cray Inc
- CRC for Enterprise Distributed Systems (DSTC)
- GrangeNet (DCITA)
- Hewlett Packard
- IBM
- Microsoft
- Sun Microsystems
- US Department of Energy







PURELY ACADEMIC

Cast

Prof John Holywell	Southern University academic in his early 50's
Prof Martin Godson	Middleton University academic in his mid 50's
Prof Mary Long	Southern University academic in her early 40's
Charles Mittleman	Initially a 30 year old PhD student at Wooton College and Southern University, but then moves to Middleton University as a young academic.
Joanne	Southern University software developer in her mid 30's. Works in Prof Holywell's lab and is pregnant.
Prof Max Williams	St George College academic in his late 50's. Serves as the chair of the Shaw Trust, a not for profit society that supports research projects with grants.
Anna	Middleton University administrator in her 30's. She also serves as an administrator on the Shaw Trust, taking notes and helping with the grant assessment exercises.
Mark	Early career academic

Robin, Cheryle, Newsreader (voices only. Can be played by other actors)

This play starts in mid to late 1990's.

Data Intensive Computing

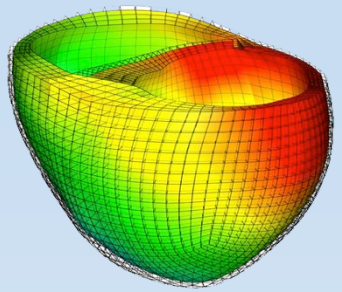
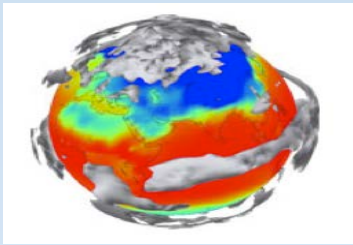
Data-Intensive Computing

- Very large data-sets or very large input-output requirements
- Two data-intensive application classes are important and growing



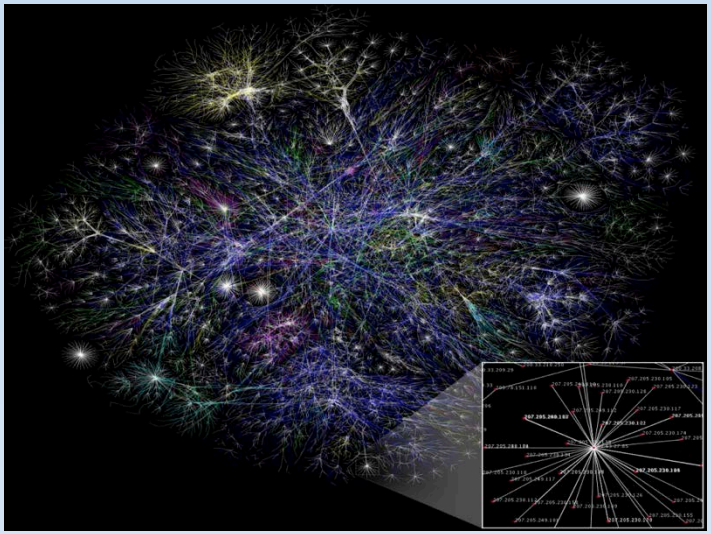


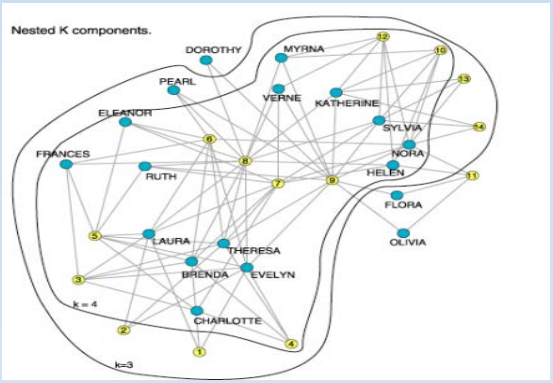
Data Mining &
Data Analytics

Data-Intensive Computing

- Examples Applications:
  - Genome sequence assembly
  - Climate simulation analysis
  - Social network analysis





Infrastructure for Data Intensive Computing

- Computation
  - Large amounts of main memory
  - Parallel processors
  - Smooth out memory pyramid
- Storage
  - Significant long term storage
  - Smooth out the memory pyramid
  - Many views of same data
    - Parallel File System
    - Local access (POSIX)
    - Remote collaboration and sharing (Object store)
    - Sync-and-share
    - Web
    - Cloud

amazon web services™

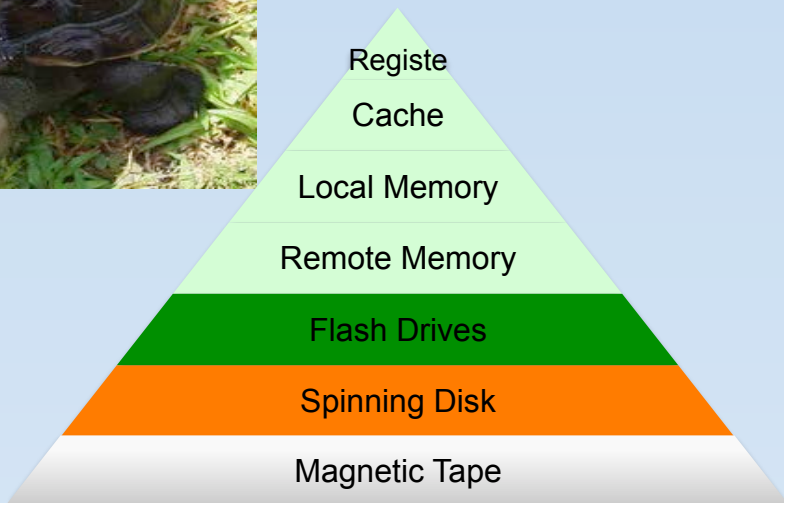
~~Turtles~~ Caches all the way down

“a jocular expression of the infinite regress problem in cosmology posed by the "unmoved mover" paradox.

The metaphor in the anecdote represents a popular notion of the theory that Earth is actually flat and is supported on the back of a World Turtle, which itself is propped up by a chain of larger and larger turtles.

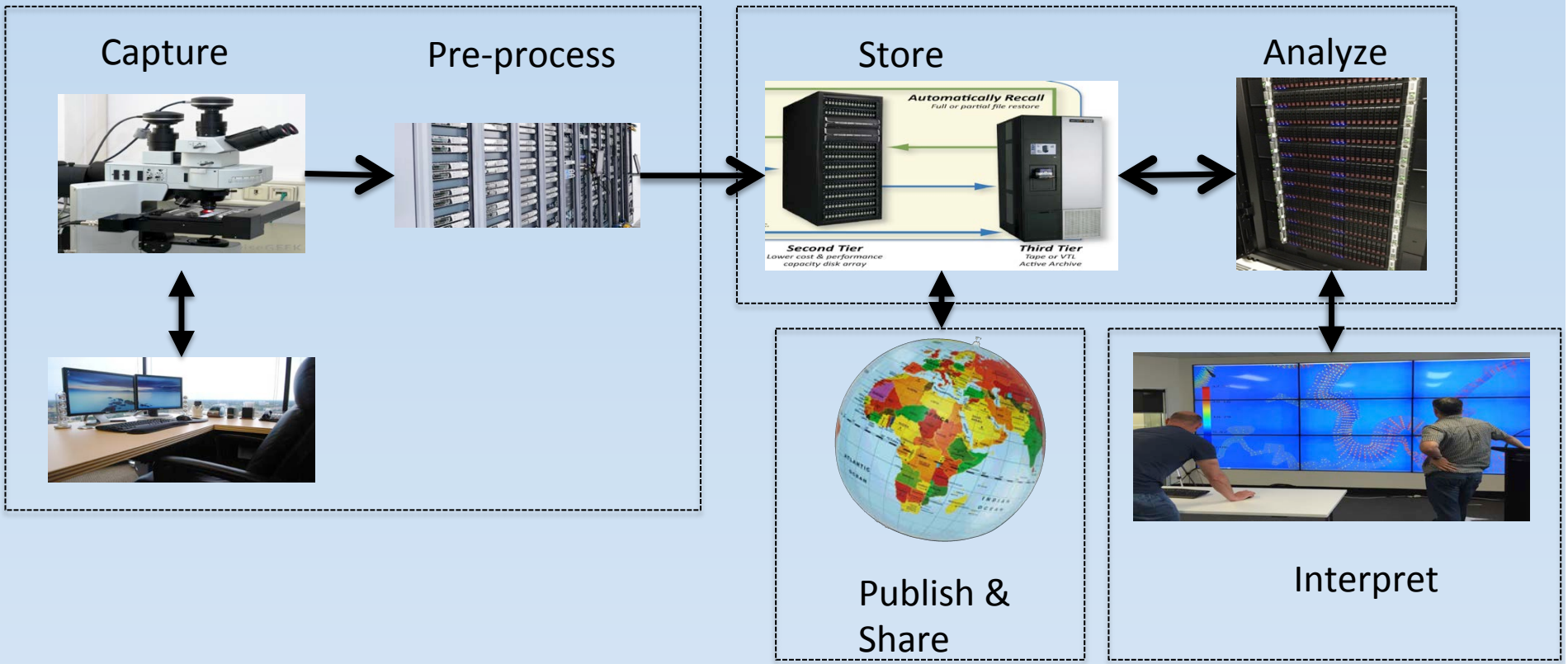
Questioning what the final turtle might be standing on, the anecdote humorously concludes that it is turtles all the way down””

https://en.m.wikipedia.org/wiki/Turtles_all_the_way_down

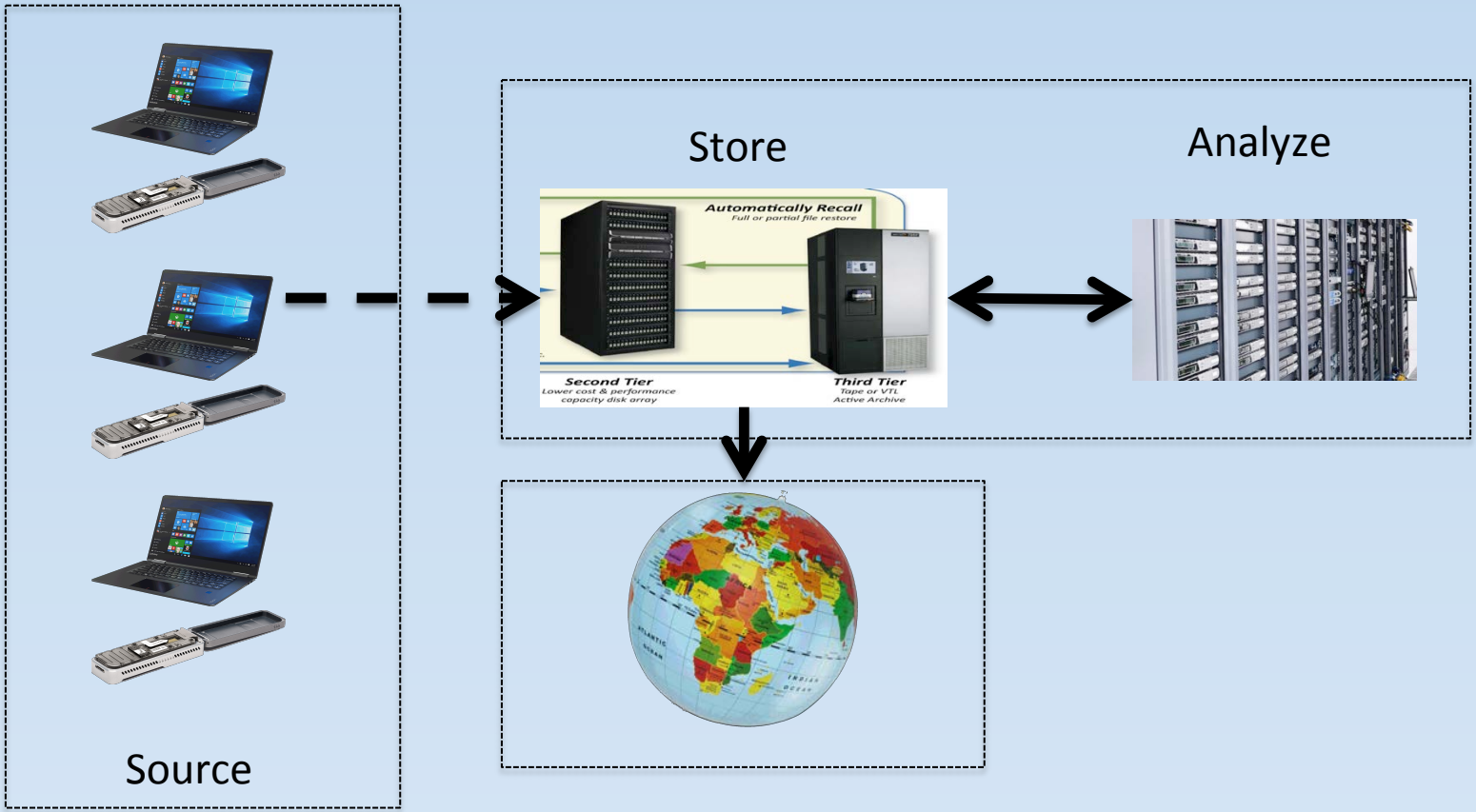


Use cases

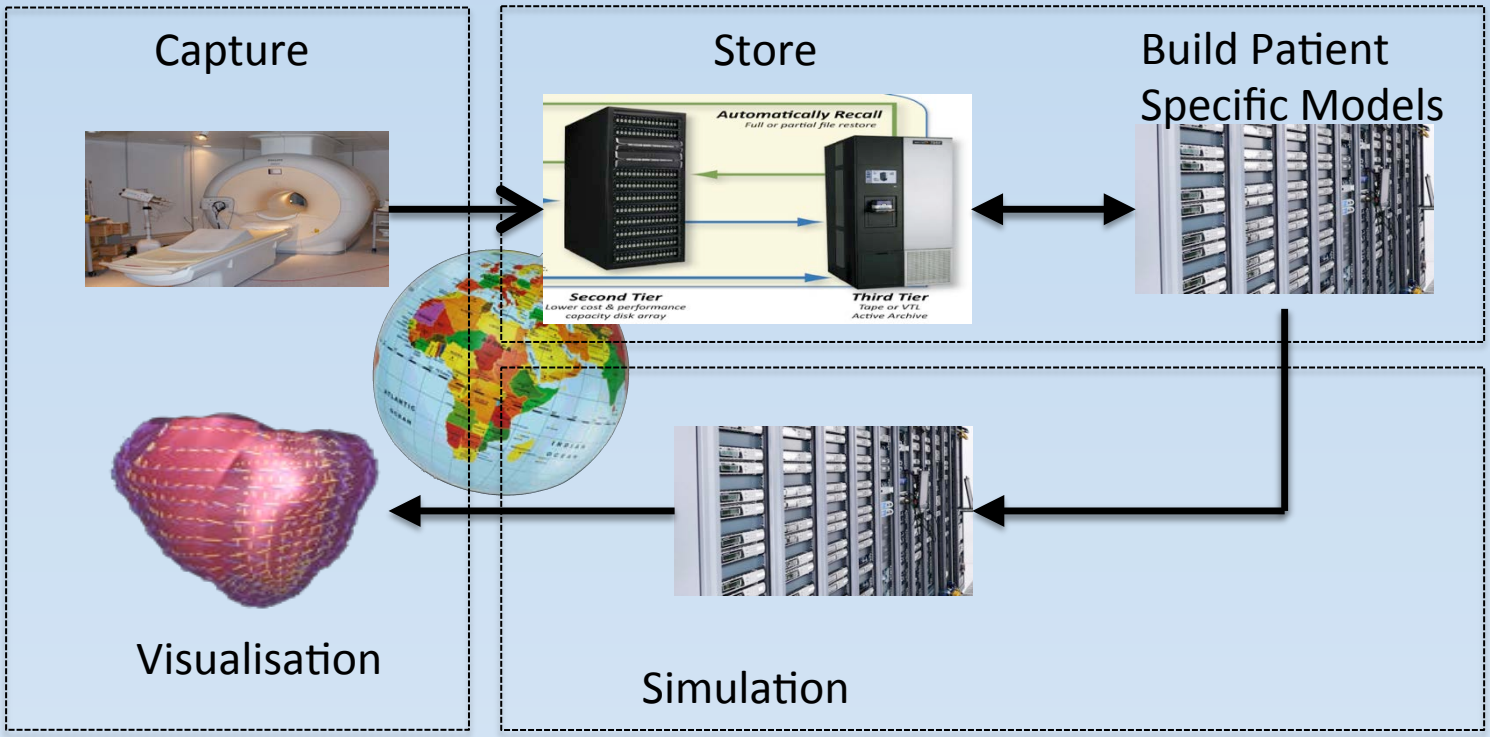
Use Case: Microscopy



Use Case: Personal Genomics

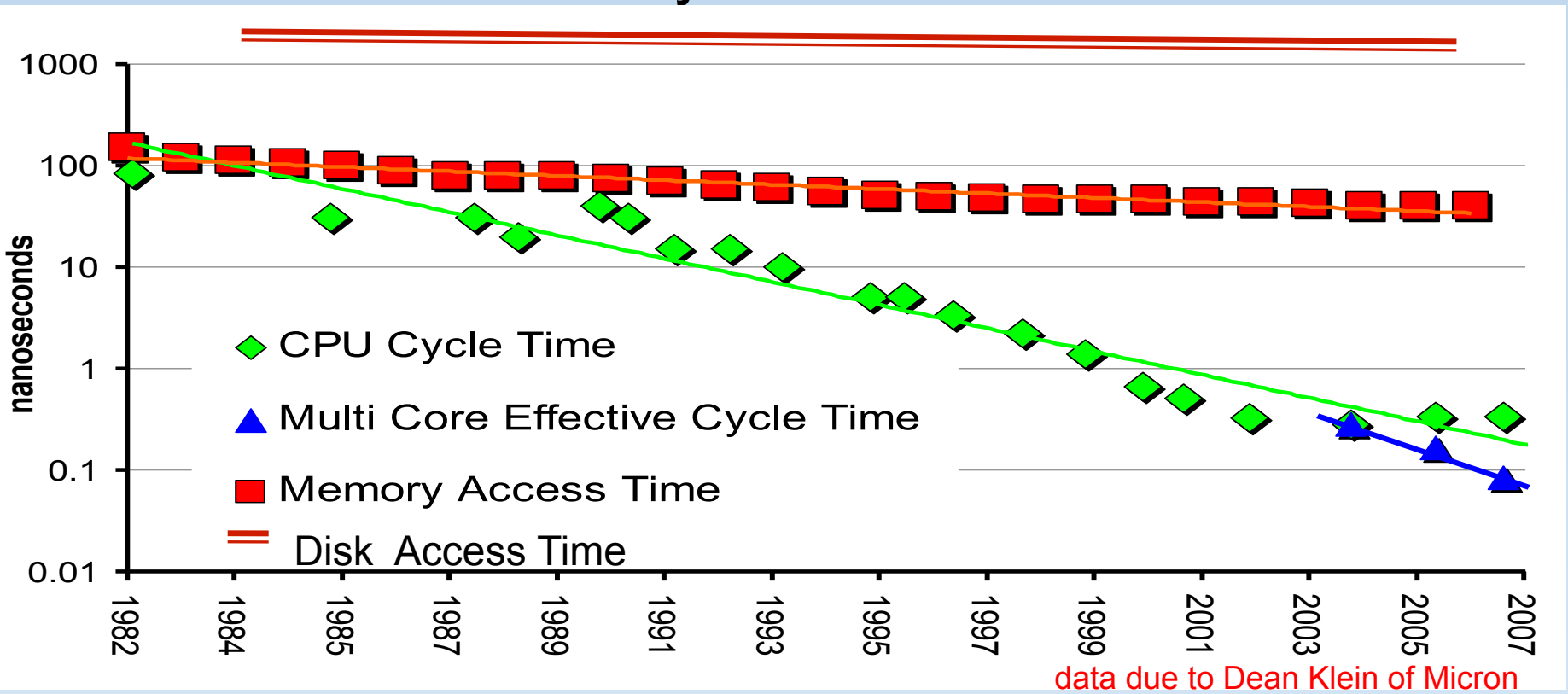


Use Case: Cardiac Science



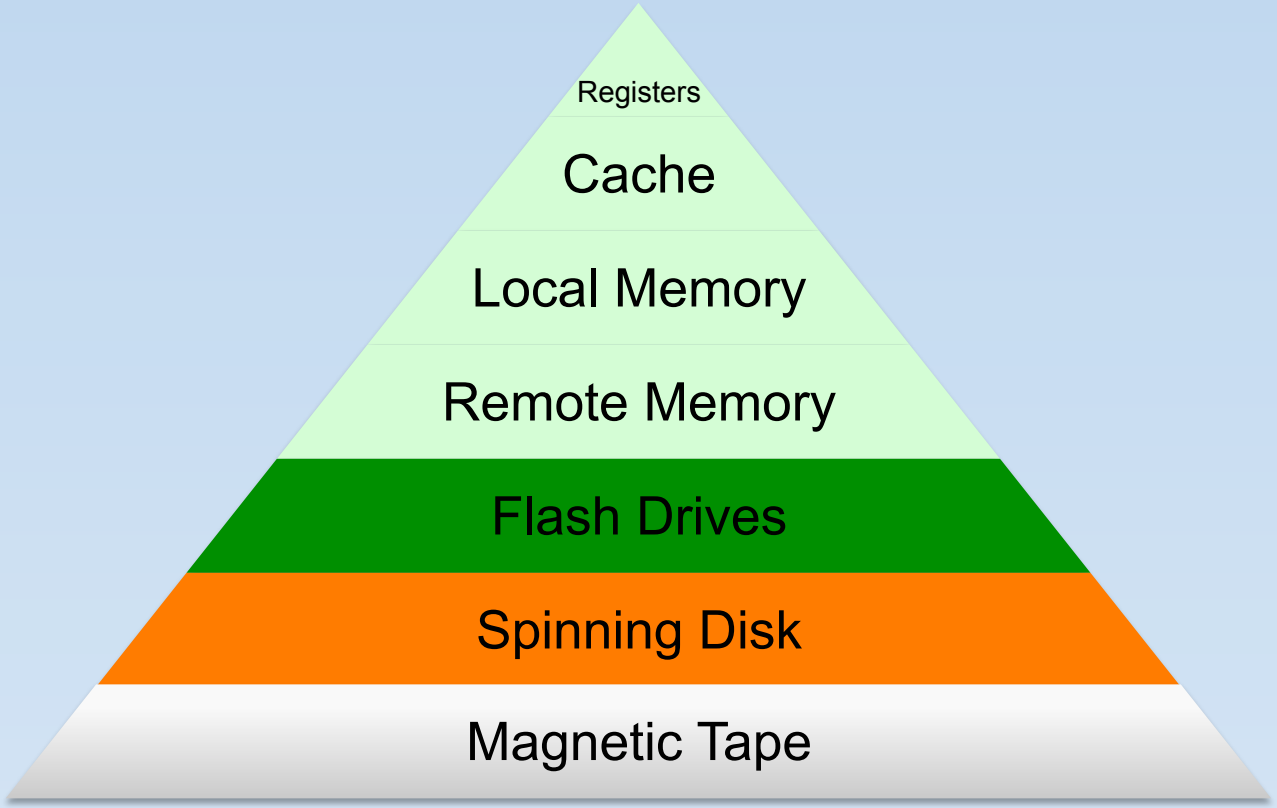
Infrastructure Challenges of Big Data

Red Shift: Data keeps moving further away from the CPU with every turn of Moore's Law



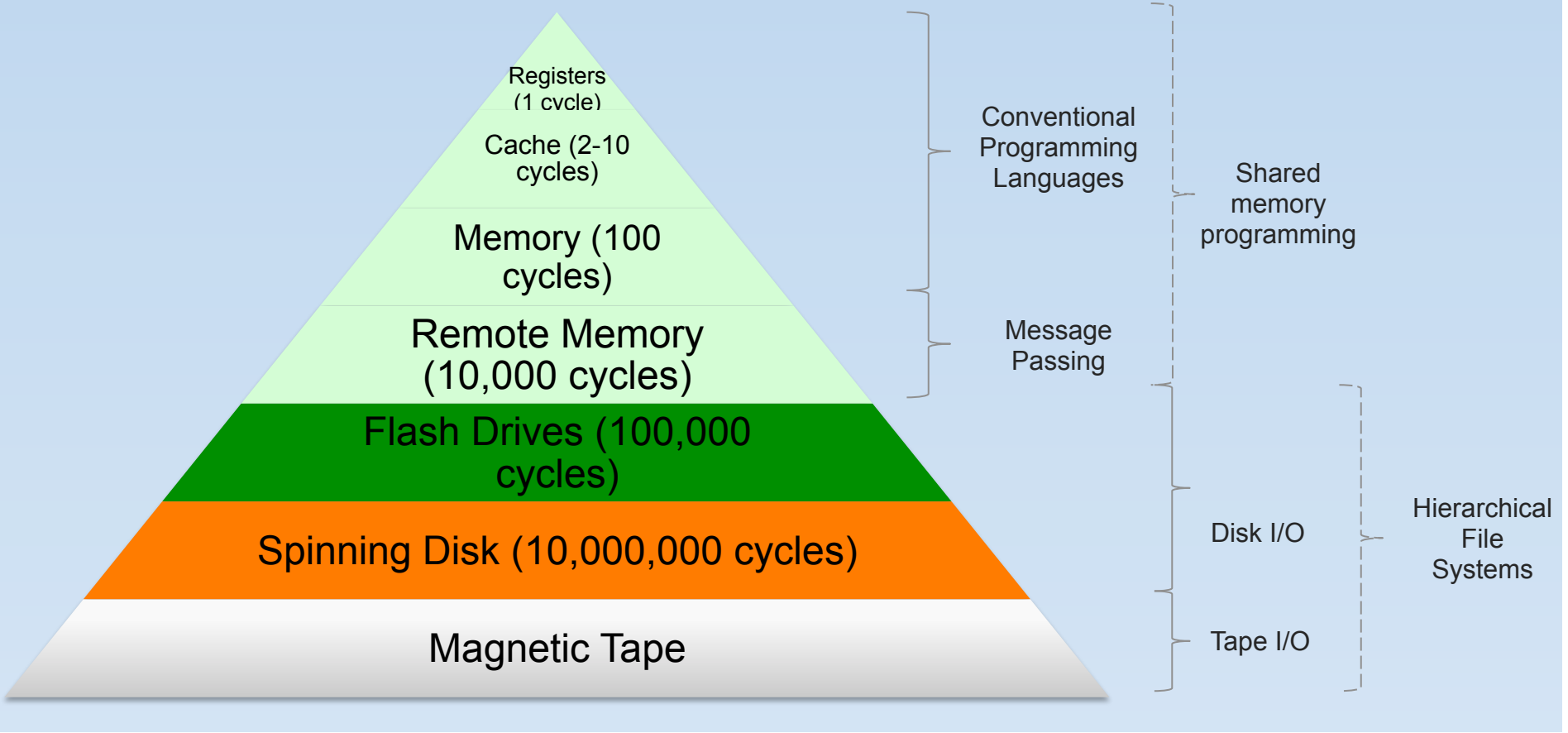
Slide courtesy Mike Norman, SDSC

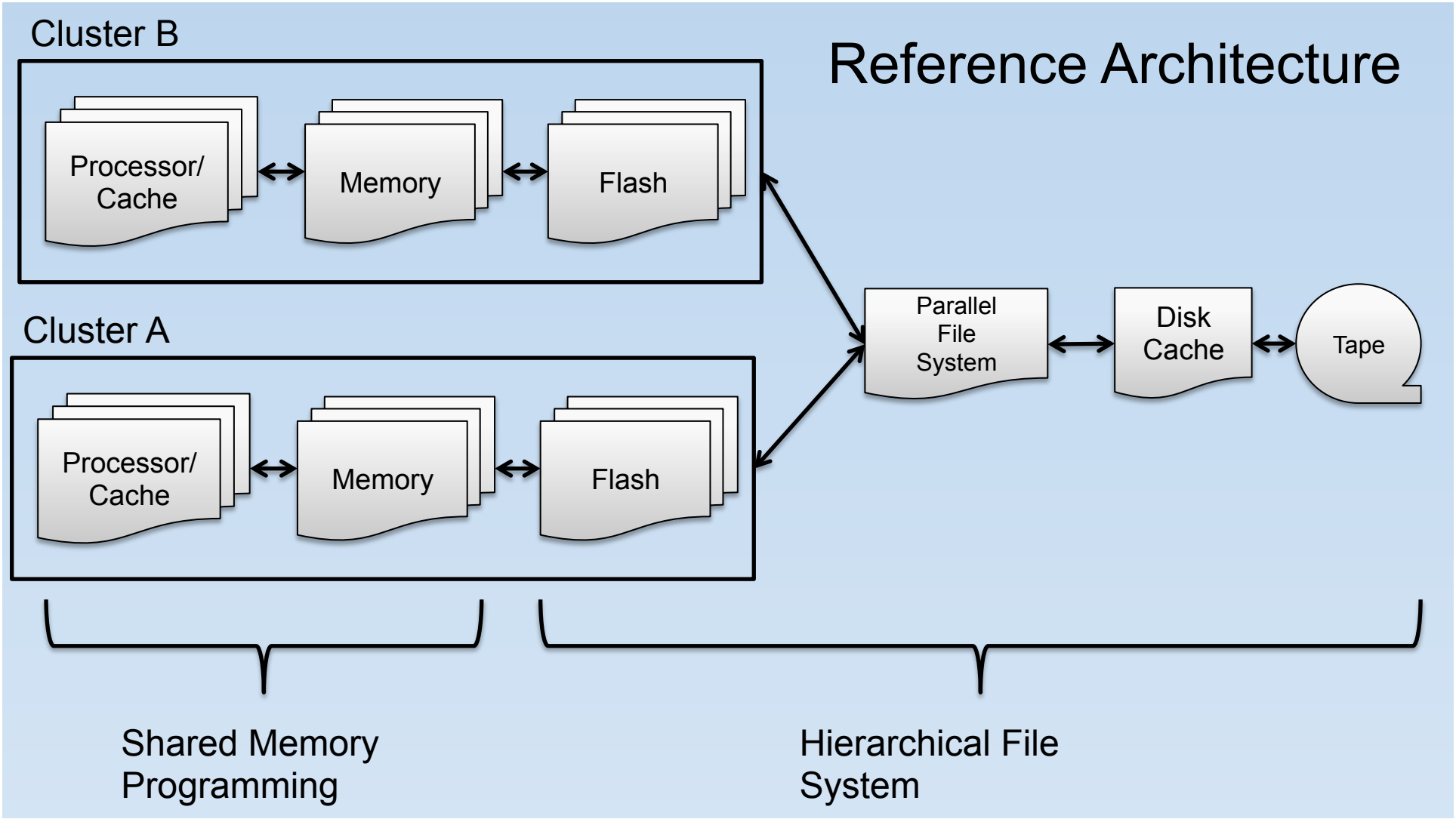
It’s always been caches all the way down

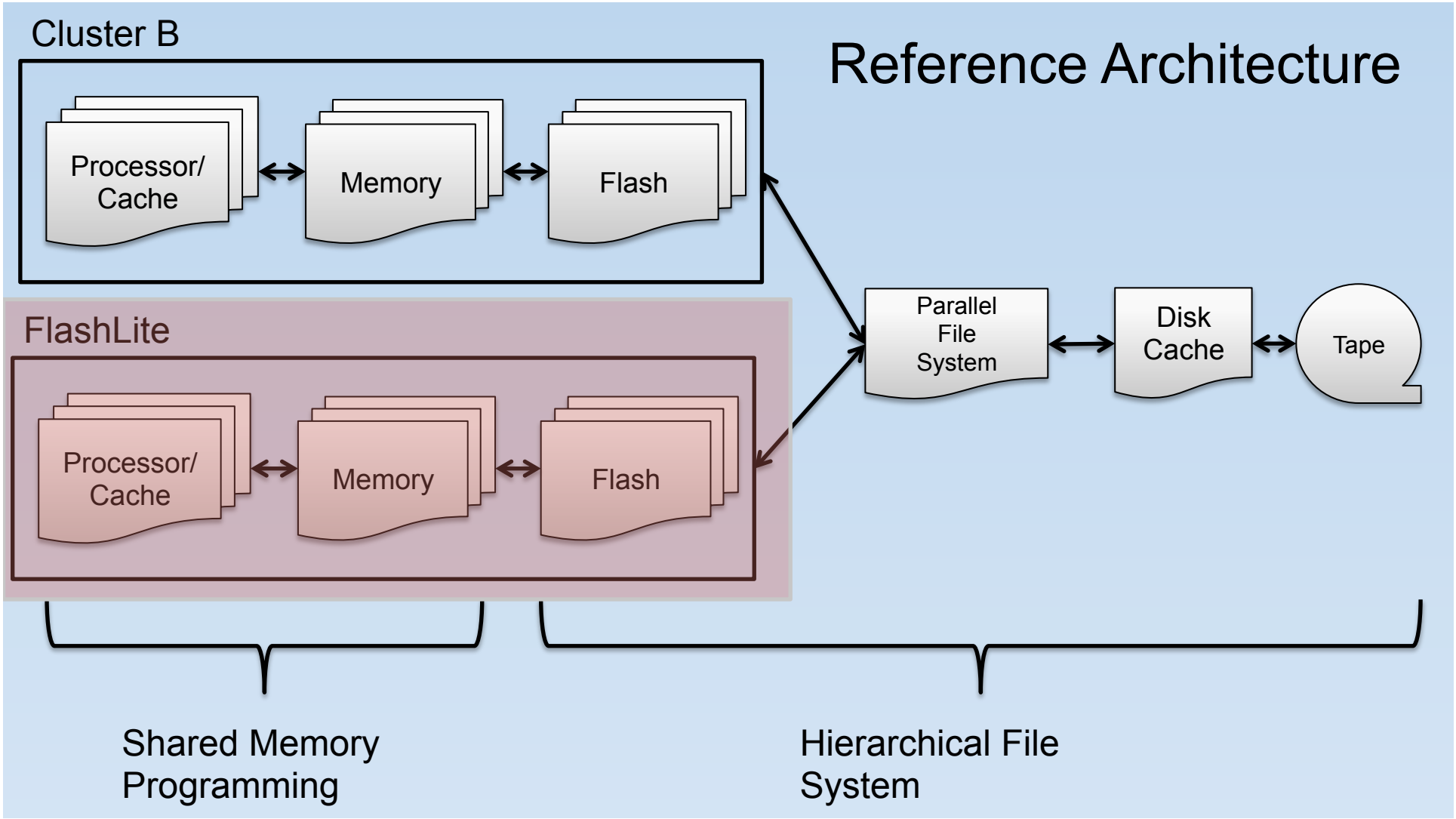


Explicit vs Implicit management

Memory Hierarchy




Cluster B
Reference Architecture
Processor/
Cache
Memory
Flash
Cluster A
Processor/
Cache
Memory
Flash
Parallel
File
System
Disk
Cache
Tape
Shared Memory
Programming
Hierarchical File
System


Cluster B
Reference Architecture
Processor/
Cache
Memory
Flash
FlashLite
Processor/
Cache
Memory
Flash
Parallel
File
System
Disk
Cache
Tape
Shared Memory
Programming
Hierarchical File
System

Data Intensive Computation Engine

- Parallel
  - High performance network
  - Good numeric performance
- Massive memory
  - Ability to hold whole data sets or data bases in memory
- High IO throughput

FlashLite

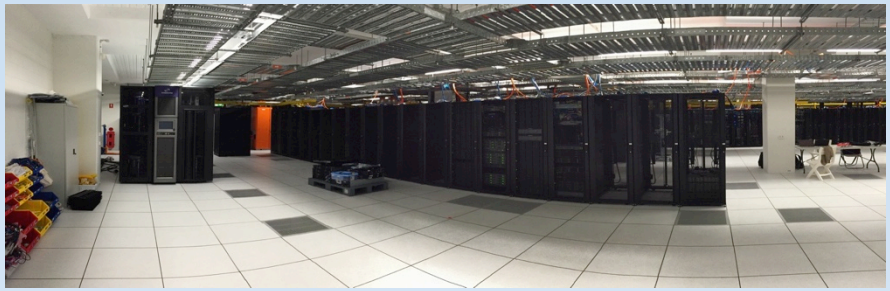
- High throughput solid state disk
- Large amounts of main memory
- Software shared memory
- Inspired by SDSC Gordon

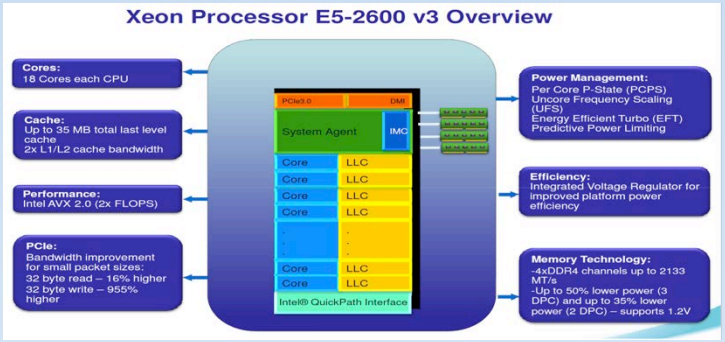
Why is flash SSD better than disk?

- Read latency for random IO is up to 100x faster than HDD (read head seek time)
- This speeds up database accesses enormously

What is FlashLite?

- FlashLite
  - ~ 70 compute nodes (~1600 cores)
    - Dual socket Intel E5-2680v3 2.5GHz (Haswell)
    - 512 GB DDR-2
    - 4.8 TB NVMe SSD
  - ScaleMP vSMP virtual shared memory
    - 4TB RAM aggregate(s)

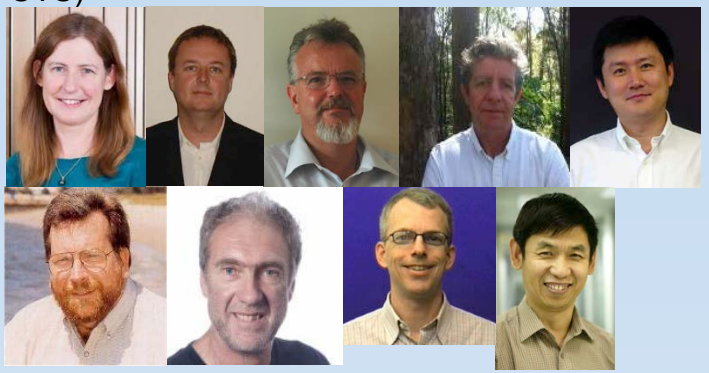




FlashLite: Data Intensive Themes

ARC LIEF grant

- Directly manipulate large amounts of data
  - Large Memory Database Systems (Zhou, UQ)
  - Machine Learning and Classification (Zhang, Zhu, Tao and Chen, UTS)
- Integrate observational data and computation
  - Astrophysics (Drinkwater, UQ)
  - Healthy hearts (Burrage, Turner, QUT; Abramson, UQ).
  - Coastal Management (Tomlinson, Griffith)
  - Climate Change (Mackey, Griffith)
  - LIDAR processing (Olley, Griffith)
- Large main memories to operate efficiently
  - Genomics (Edwards, UWA/UQ; Coppel, Monash; Griffiths, Griffith)
- Significant temporary storage requirements.
  - Computational Chemistry (Bernhardt, UQ; Du, QUT)



Results to date

Significant Temporary Storage

Marlies Hankel, AIBN

- Gaussian 90
- Coupled cluster with single and double (substitutions from Hartree-Fock)
  - 24 cores, 30GB of ram for jobs, 200GB MaxDisk, about 143GB used
    - Walltime with SSD= 120751 s
    - Walltime with GPFS = 239289 s
    - 1.98 speedup
- Moeller-Plesset second order correlation energy correction
  - 24 cores, 250GB of ram for job, 100GB MaxDisk, about 1GB used
    - Walltime with SSD= 21191 s
    - Walltime with GPFS = 34653 s
    - 1.63 speedup

MPI with lots of memory

Christoph Rohmann , AIBN

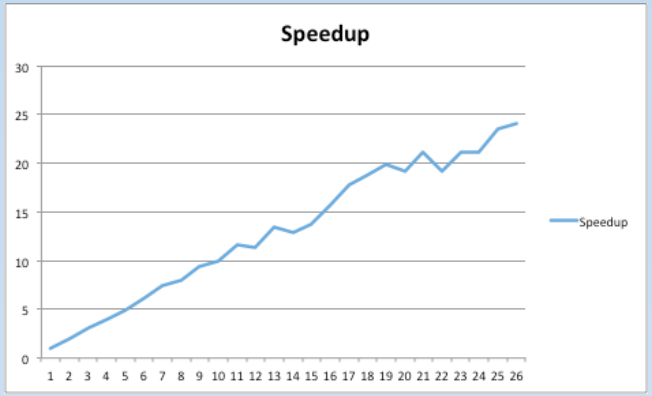
- VASP
- Job running within one node on FlashLite used ~232GB of memory.
- So need 48 cores with 5GB per core on Tinaroo to be able to run this job.

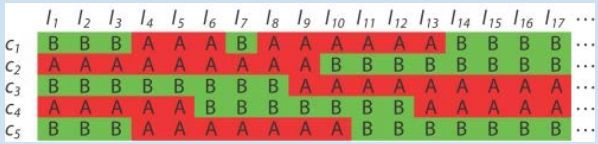
Cluster	cores	ram/core	flashdrive	walltime/s
Tinaroo	24			
FlashLite	24	6GB	no	Insufficient memory
FlashLite	24	10GB	no	10709
FlashLite	24	10GB	yes	8489
FlashLite	48	6GB	no	8705
Tinaroo	48	5GB	no	7799

Large Shared Memory Machine

Kevin Smith, RCC, UQ
Juan Daniel Montenegro, School of Agriculture & Food Science, UQ

- MSTMap
- The advent of the genomics era has increased exponentially the amount of data that needs to be analysed.
  - Marker datasets now contain millions of markers instead of thousands.
- Cluster and order markers on a genetic linkage map.
- Efficient in memory management and “large” data sets with thousands of genetic markers.
- It uses an “all vs all” distance calculation that can be parallelised.
- OpenMP & C, vSMP



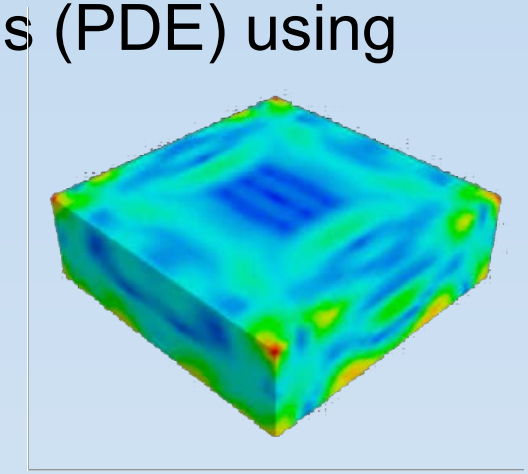


PLoS Genet. 2008 Oct; 4(10): e1000212.

Hybrid SMP and DMM

Lutz Gross, Cihan Altinay, School of Earth Sciences, UQ

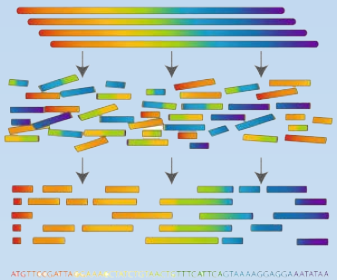
- eScript
- Solution of Partial Differential Equations (PDE) using Finite Elements (FEM)
- Timings @ 120 cores
  - MPI Only
    - Speedup: 54
  - MPI and OpenMP
    - Speedup: 52
  - OpenMP Only (vSMP)
    - Speedup of 41

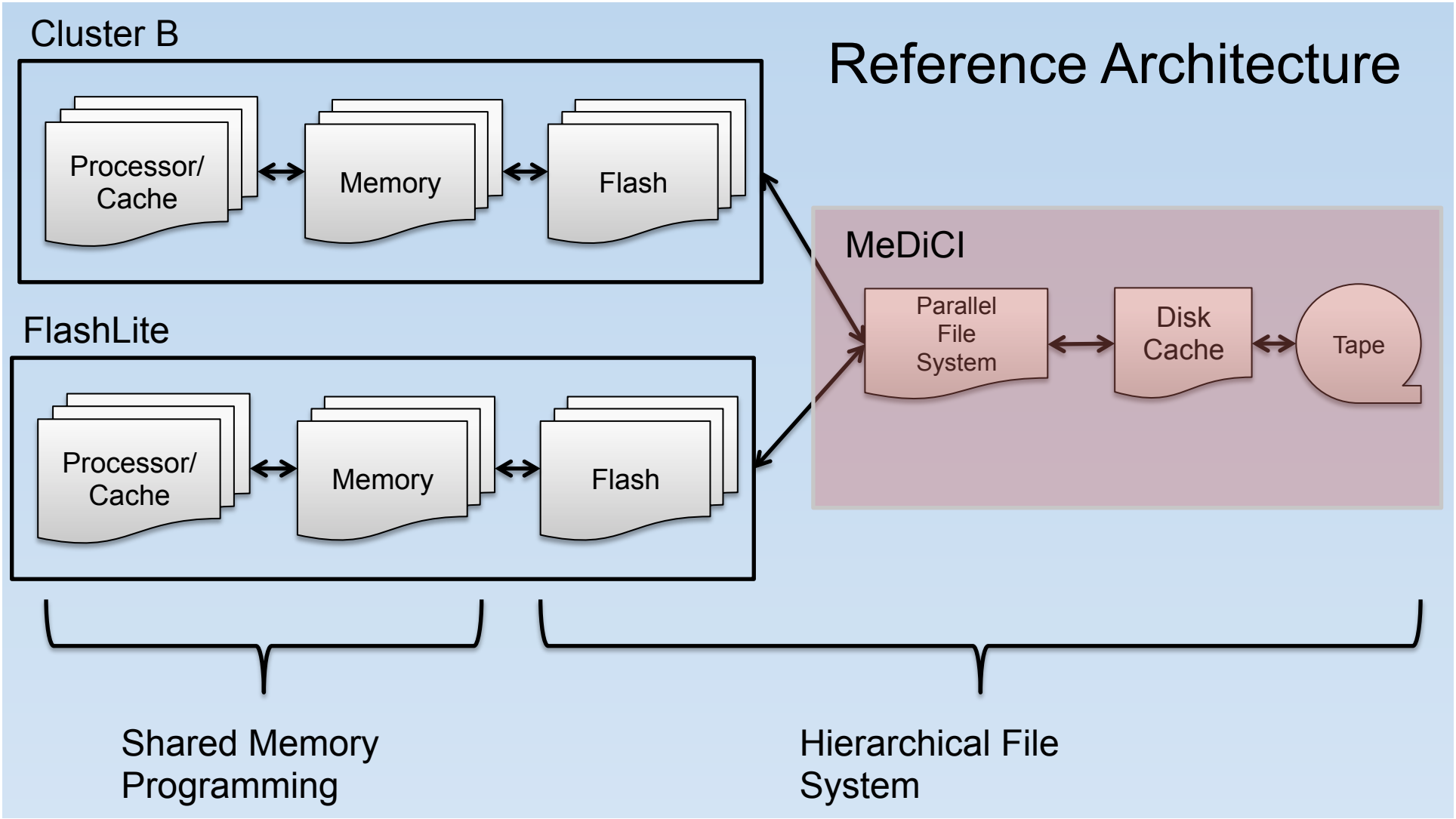


Large Memory

Ondrej Hlinka, Stuart Stephen, CSIRO

- BioKanga – Genome Assembly
- Integrated toolkit of high performance bioinformatics subprocesses targeting the challenges of next generation sequencing analytics.
- Highly efficient short-read aligner which incorporates an empirically derived understanding of sequence uniqueness within a target genome
  - Hamming distances between putative alignments to the targeted genome assembly for any given read as the discriminative acceptance criteria
  - can process billions of reads against targeted genomes containing 100 million contigs and totaling up to 100Gbp of sequence.
- A large synthetic dataset (Similar CPUs):
  - Dell blade with 48 (2.1GHz) cores 3TB of RAM 32.25 hours
  - SGI UV 3K 48 (2.6GHz) cores and 3TB RAM 36.80 hours
  - FlashLite (MEX mode) – 24 (2.5 GHz) cores and 3TB RAM (6 nodes) 38.62 hours

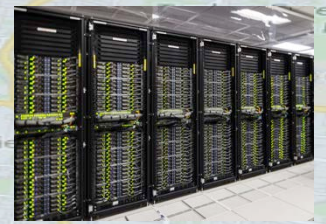



Cluster B
Reference Architecture
Processor/
Cache
Memory
Flash
MeDiCI
Parallel
File
System
Disk
Cache
Tape
FlashLite
Processor/
Cache
Memory
Flash
Shared Memory
Programming
Hierarchical File
System

But the caches continue …

MeDiCI

UQ Landscape: An inconvenient truth

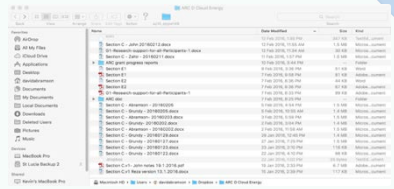


30 kms

Data Data everywhere anytime

ImageTrove | myTardis | OMERO

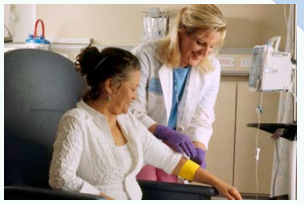
Managed Data



MeDiCI | ownCloud

Synchronous | Asynchronous

Unmanaged Data



OpenClinica

Clinical Data

S3, Swift

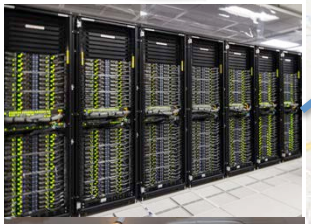
Cloud Access

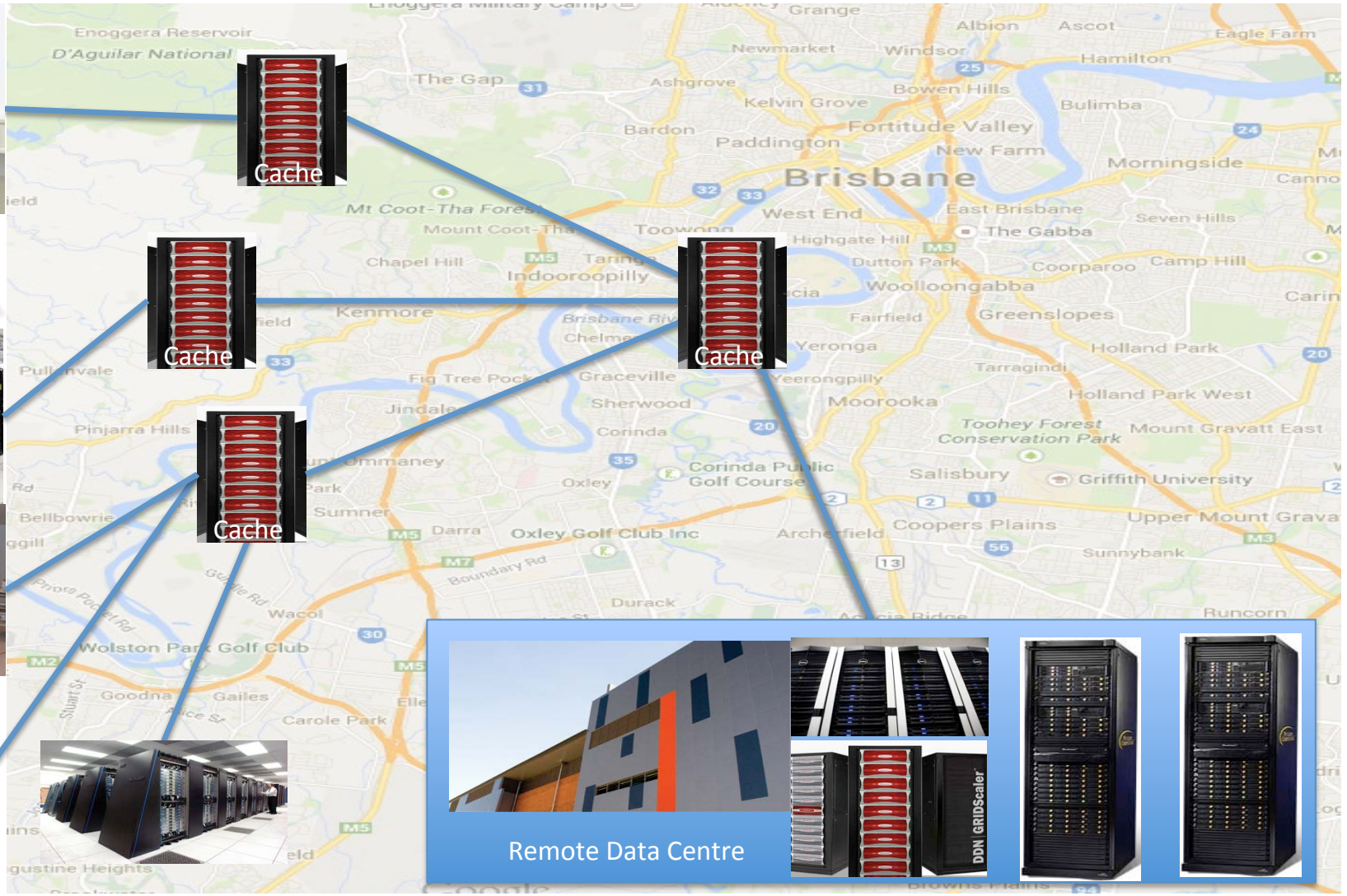
MeDiCI

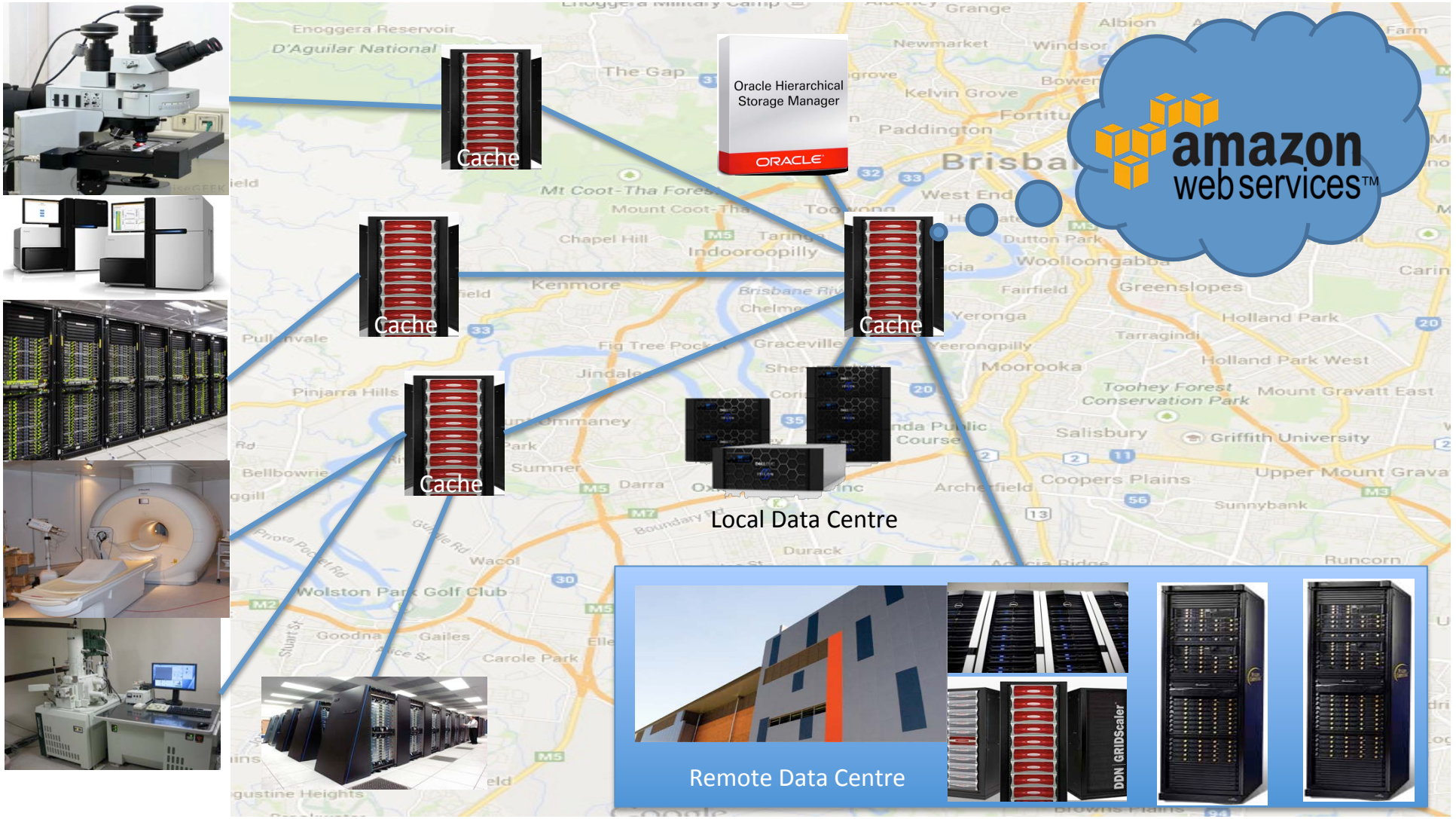
QRIScloud Compute and Storage Fabric

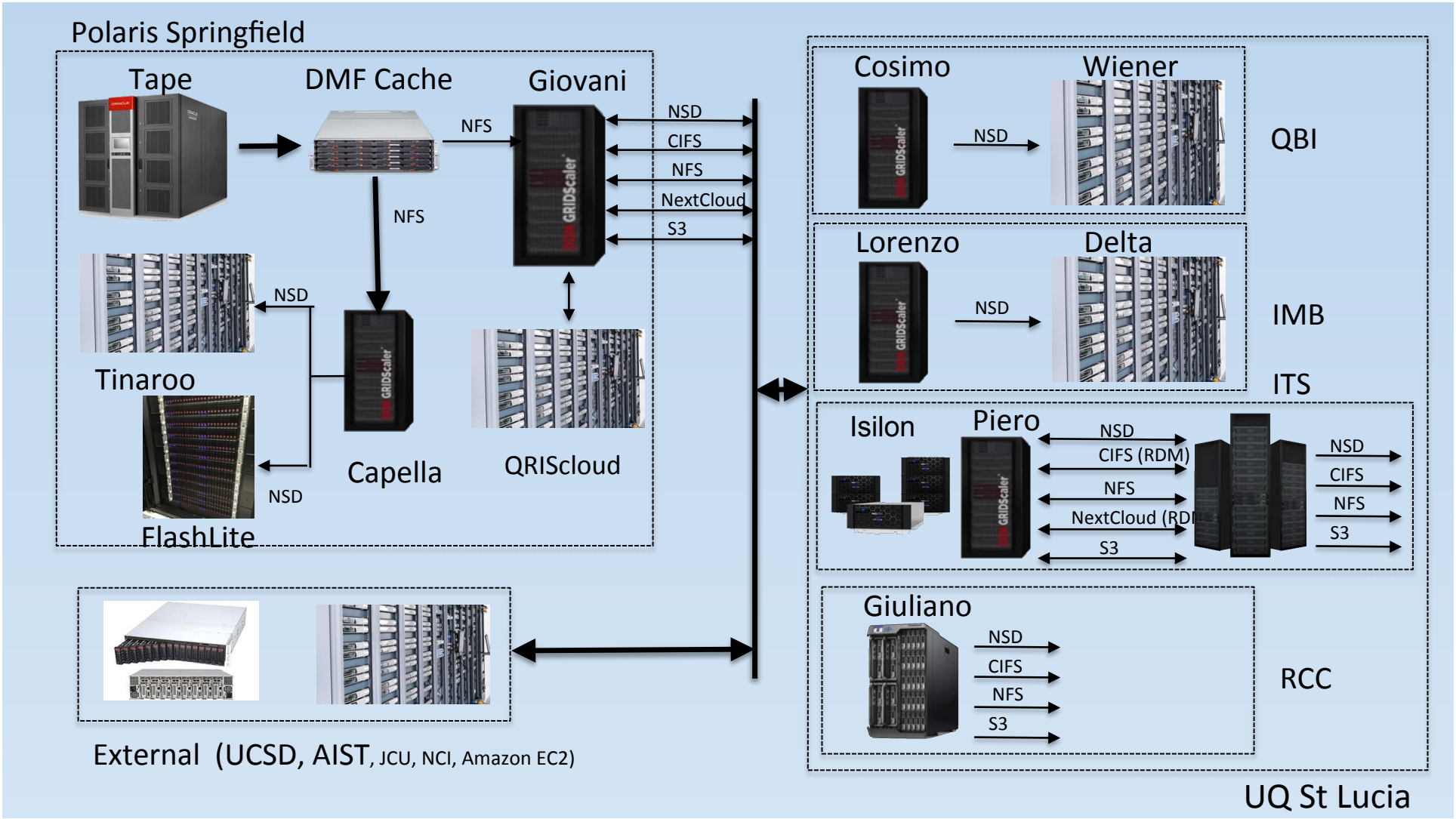
MeDiCI

- Centralising research data storage and computation
- Distributed data is further from both the instruments that generate it, some of the computers that process it, and the researchers that interpret it.
- Existing mechanisms manually move data
- MeDiCI solves this by
  - Augmenting the existing infrastructure,
  - Implementing on campus caching
  - Automatic data movement
- Current implementation based on IBM Spectrum Scale (GPFS) and SGI DMF

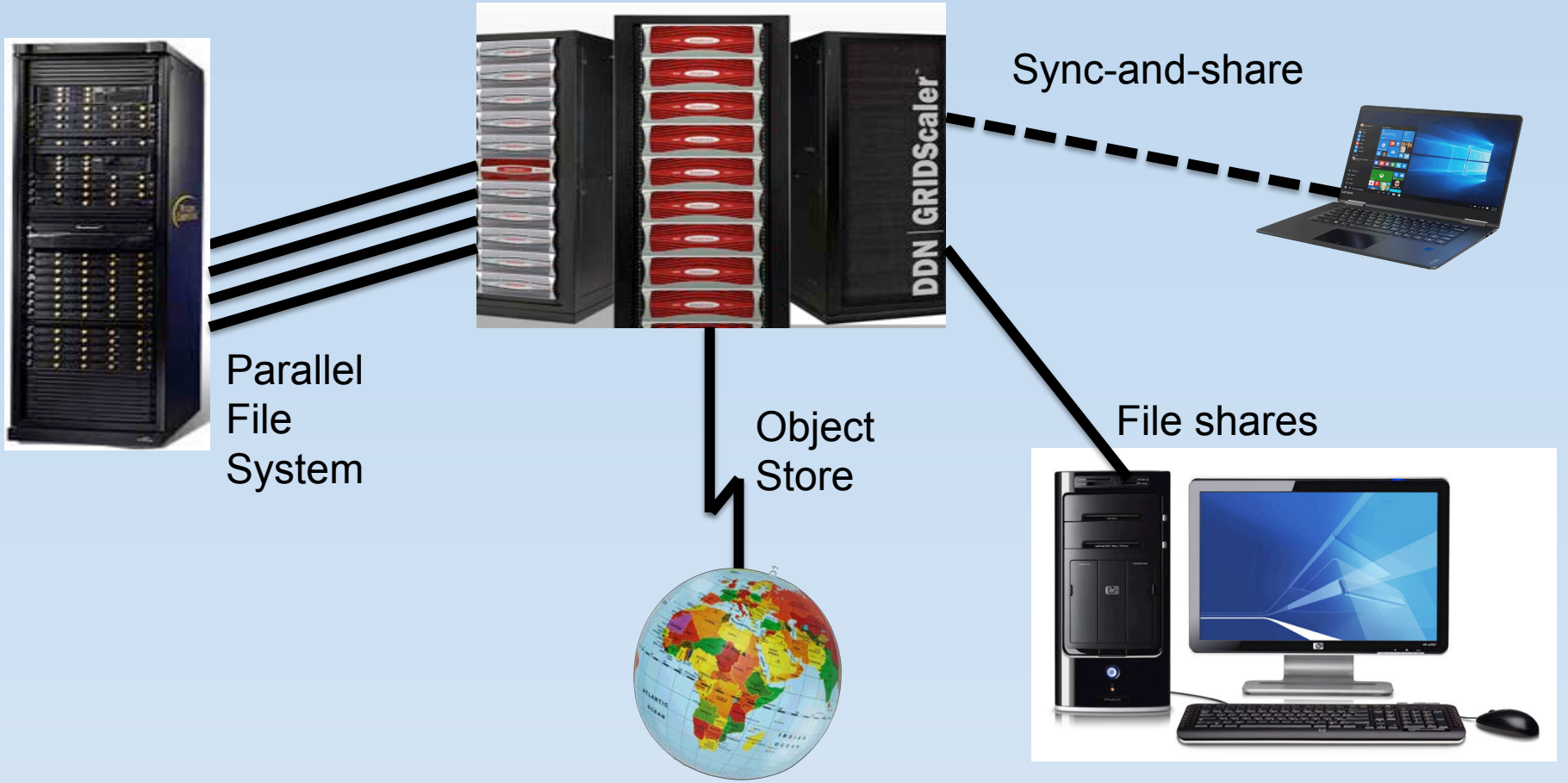



Cache
Cache
Cache
Cache
Remote Data Centre
DDN GRIDScaler

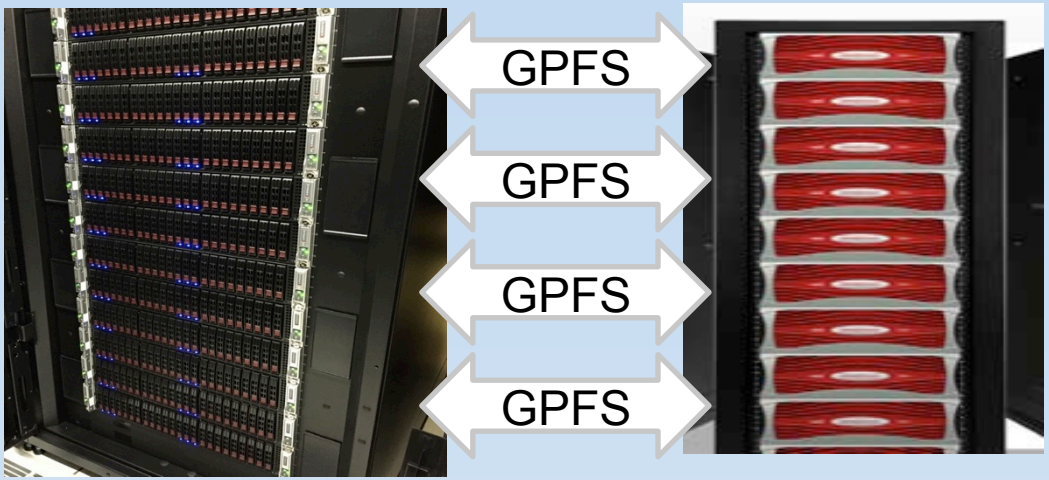

Cache
Cache
Cache
Cache
Oracle Hierarchical Storage Manager
ORACLE
amazon web services™
Local Data Centre
Remote Data Centre
DDN GRIDScaler


Polaris Springfield
Tape
DMF Cache
Giovani
NFS
NSD
CIFS
NFS
NextCloud
S3
NFS
NSD
Tinaroo
FlashLite
NSD
Capella
QRIScloud
Cosimo
Wiener
NSD
QBI
Lorenzo
Delta
NSD
IMB
ITS
Isilon
Piero
NSD
CIFS (RDM)
NFS
NextCloud (RDI
S3
NSD
CIFS
NFS
S3
Giuliano
NSD
CIFS
NFS
S3
RCC
External (UCSD, AIST, JCU, NCI, Amazon EC2)
UQ St Lucia

MeDiCI also unifies data access



MeDiCI as a parallel file system



DDN SFA12KXE

FlashLite

Parallel file system

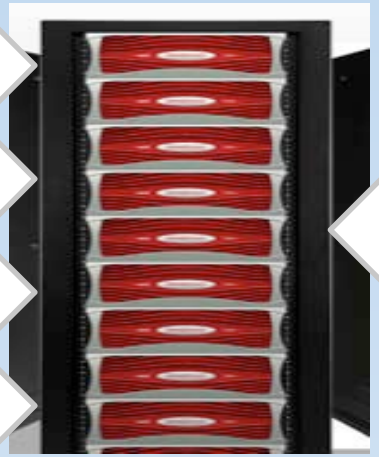
Accessing long term collections

GPFS

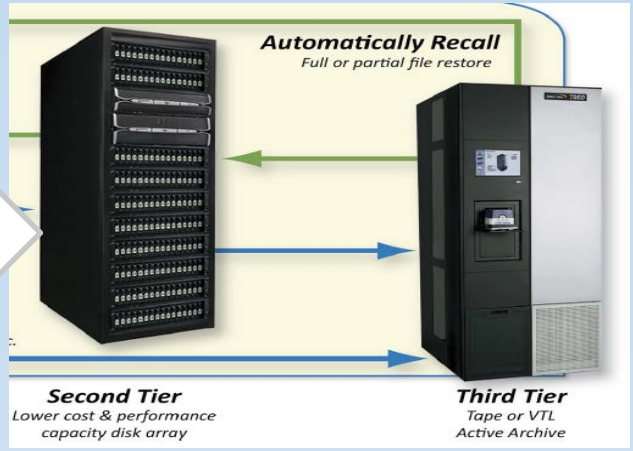
GPFS

GPFS

GPFS



NFS



DDN SFA12KXE

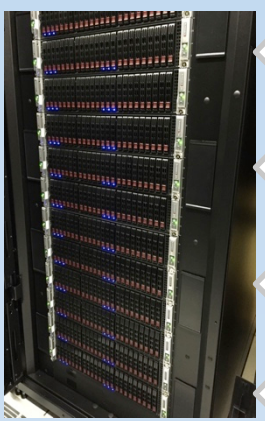
SGI DMF Disk/Tape

FlashLite

Parallel file system

Long term data collections

MeDiCI Wide Area Architecture

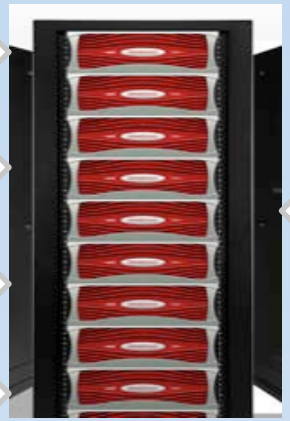


GPFS

GPFS

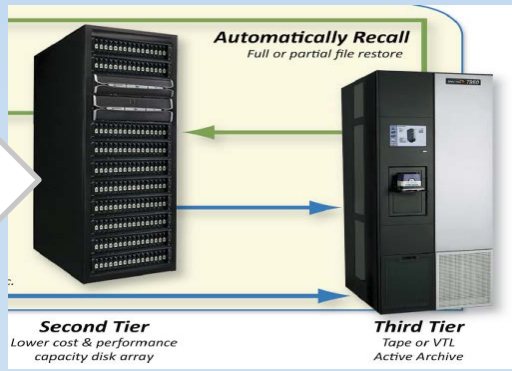
GPFS

GPFS



NFS

SGI DMF Disk/Tape



Machine Room Network

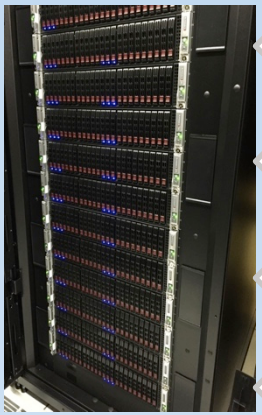
Compute

Parallel File System

Long term data collections

Cache

MeDiCI Wide Area Architecture

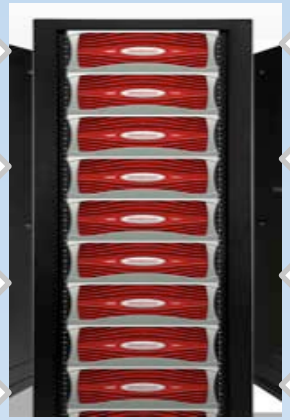


GPFS

GPFS

GPFS

GPFS

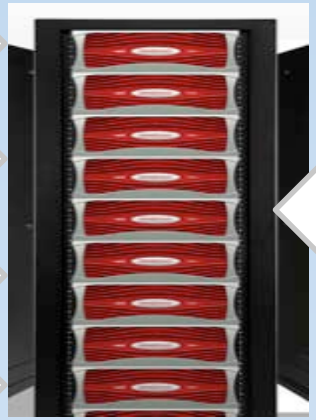


GPFS

GPFS

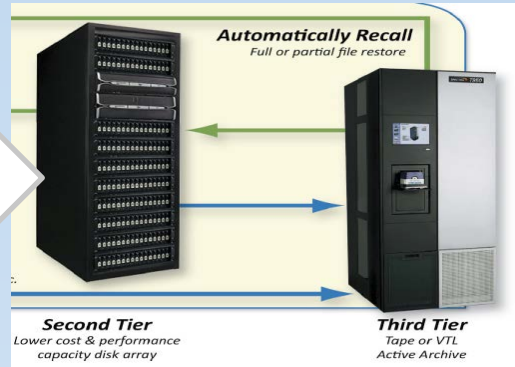
GPFS

GPFS



NFS

SGI DMF Disk/Tape



Machine Room Network

Wide Area Network

Long term data collections

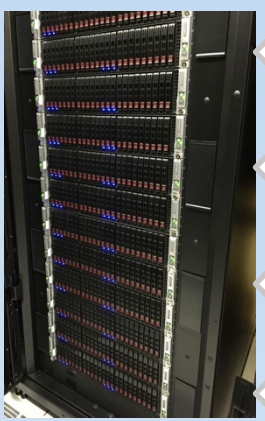
Compute

Parallel File System

Cache

Cache

MeDiCI Wide Area Architecture

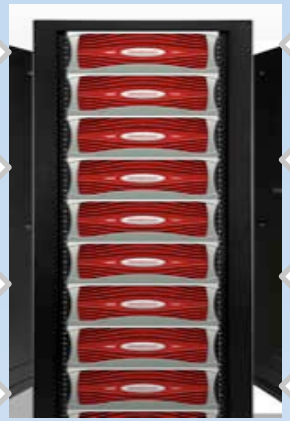


GPFS

GPFS

GPFS

GPFS

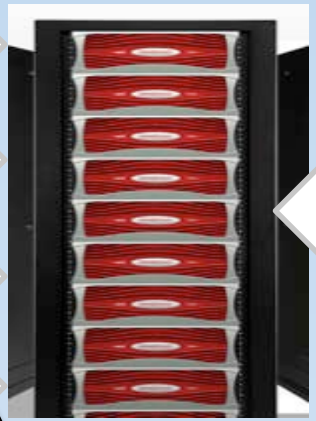


GPFS

GPFS

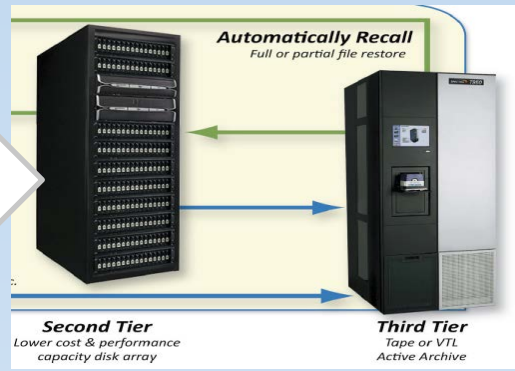
GPFS

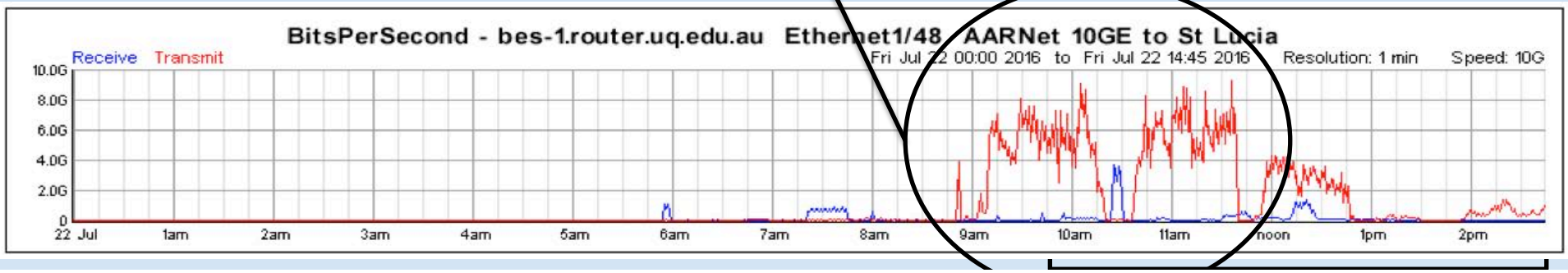
GPFS



NFS

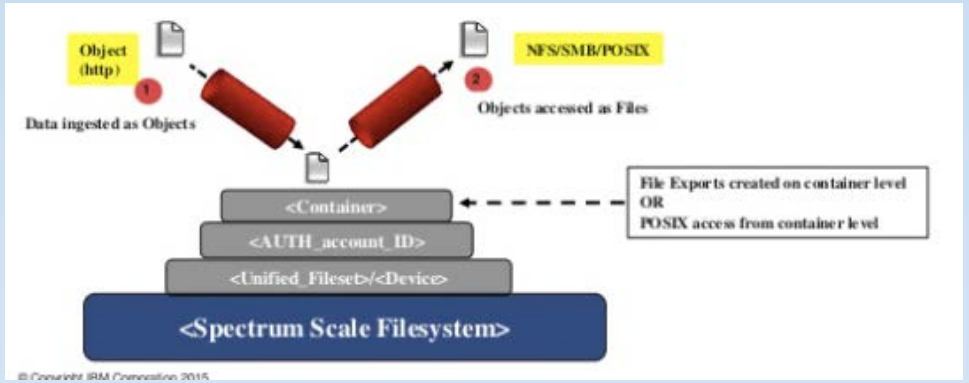
SGI DMF Disk/Tape





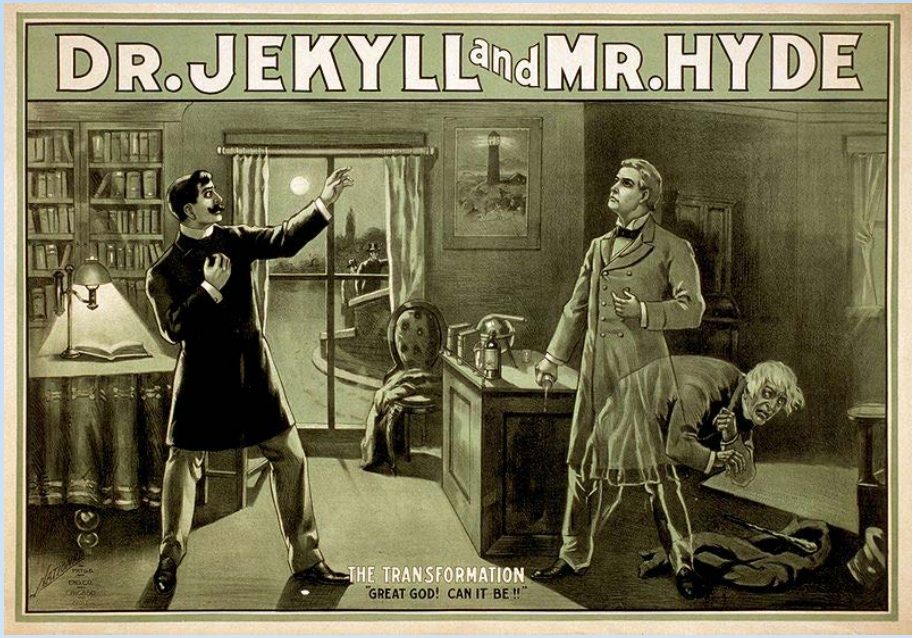
Object Storage

- S3 style objects becoming defacto standard for distributing data
- http put/get protocol
- Swift over GPFS
  - Unified Object/file interfaces



Identity!

- No single UID space across UQ/QCIF users
- Need to map UID space between UQ and Polaris
- GPFS 4.2
  - mmname2uid/mmuid2name

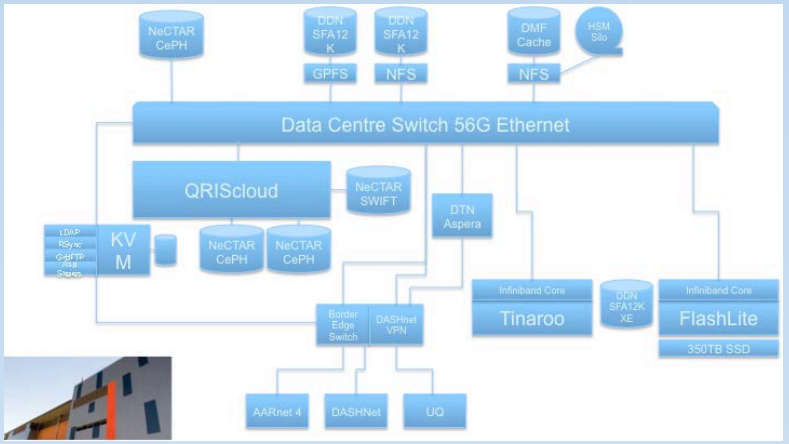


Building on basic architecture

- A Declarative Machine Room
- Leveraging Cloud Storage
- Very Very Wide Area File Systems
- Supporting repository stacks
- Orchestrating Workflows

A Declarative Machine Room?

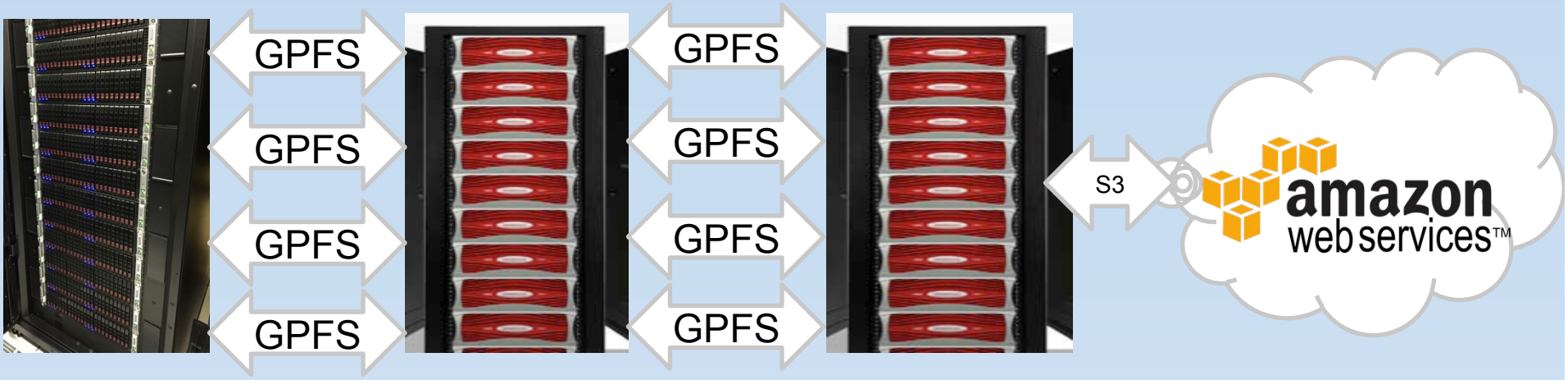
- Static allocation of disk and tape
- Policy driven allocation



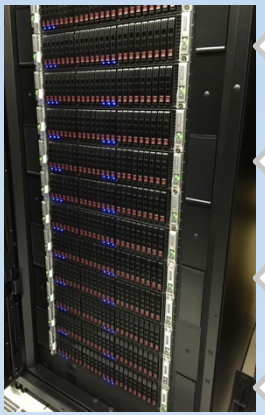

```
RULE 'prefetch-list'
LIST 'toevict'

WHERE  CURRENT_TIMESTAMP - ACCESS_TIME >
INTERVAL  '7' DAYS
  AND  REGEX(misc_attributes,'[P]') /* only list AFM managed files */
```

MeDiCI Very Wide Area Architecture



Alternative Backends

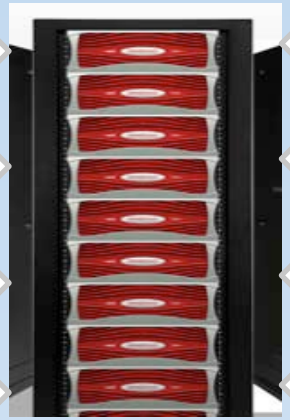


GPFS

GPFS

GPFS

GPFS

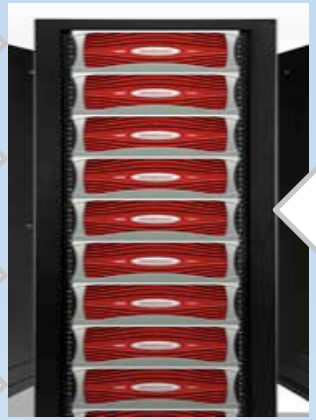


GPFS

GPFS

GPFS

GPFS



S3

Machine Room Network

Wide Area Network

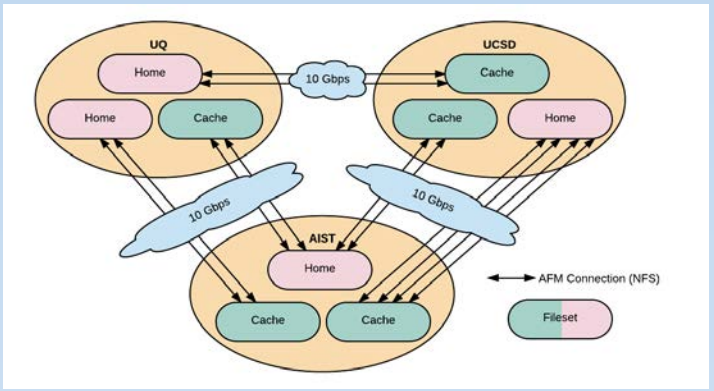
Compute

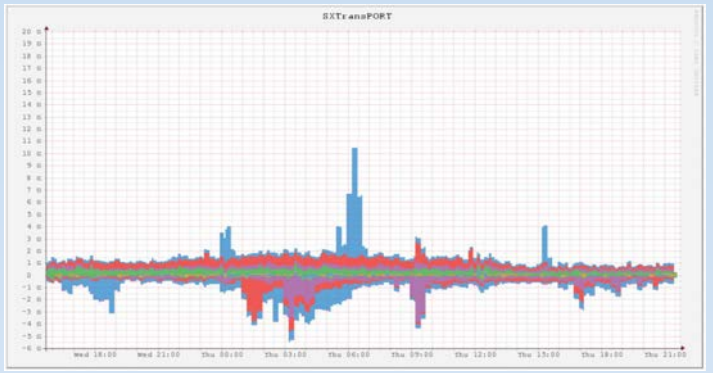
Parallel File System

Cache

HSM

MeDiCI goes East





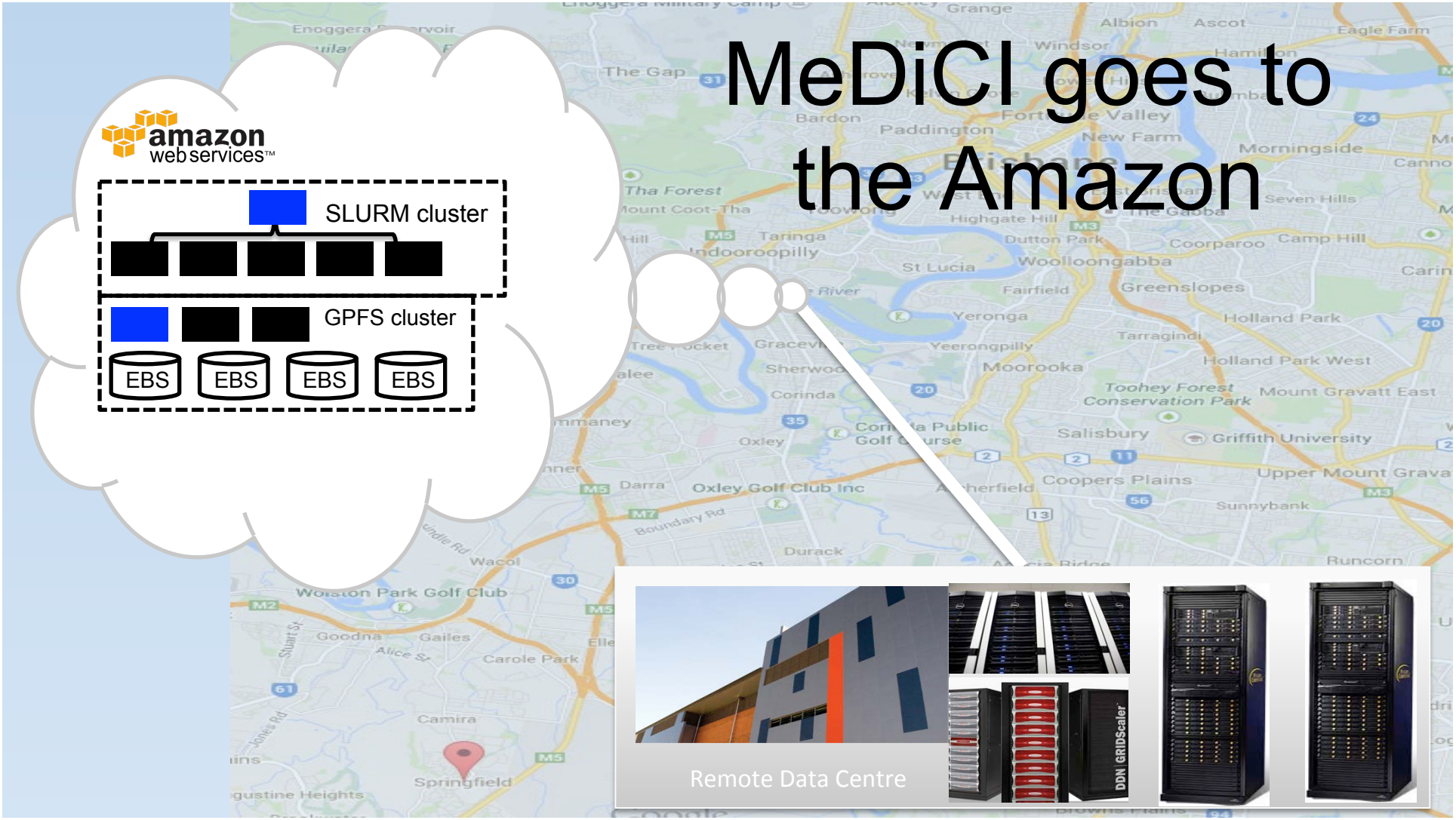
MeDiCI goes South and West

AARnet X

Magnus, Pawsey

Raijin, NCI

MeDiCI goes to the Amazon

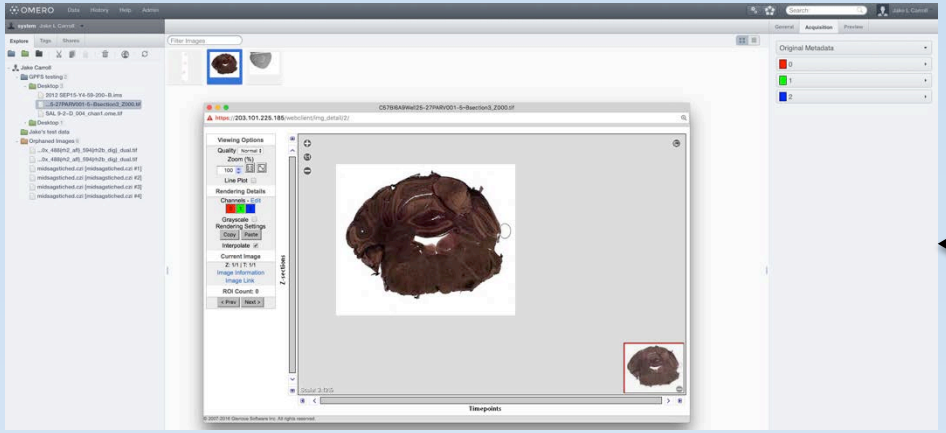


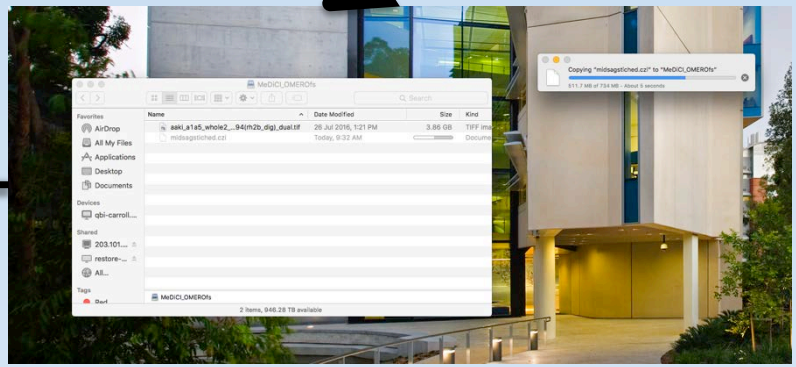
Caches under Managed Data Stacks

3.66 GB

http: 60 seconds

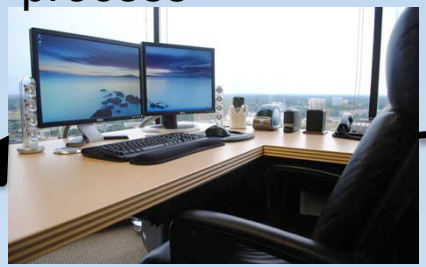
GPFS: 5 seconds

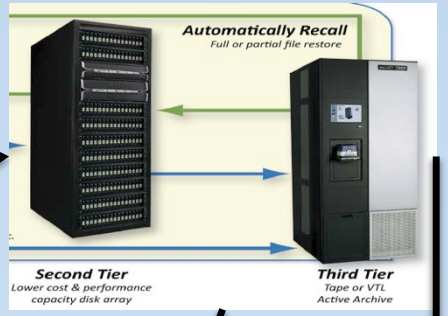




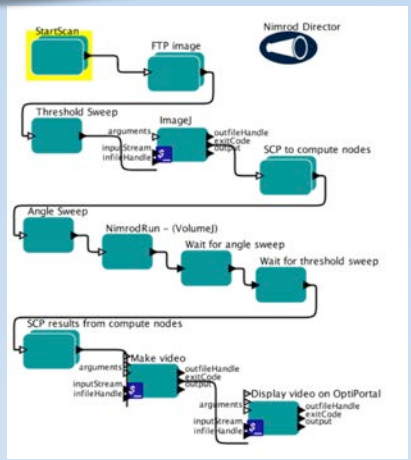
Caches under workflows

Capture & Pre-process

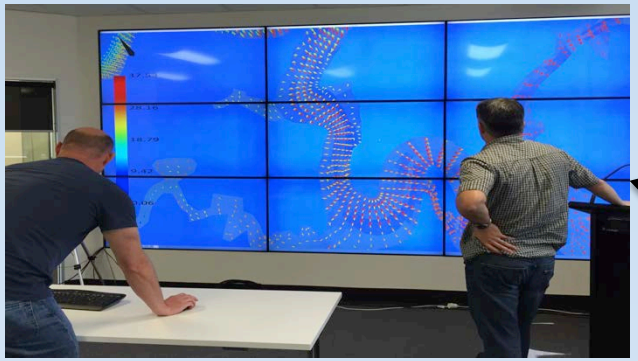




Store

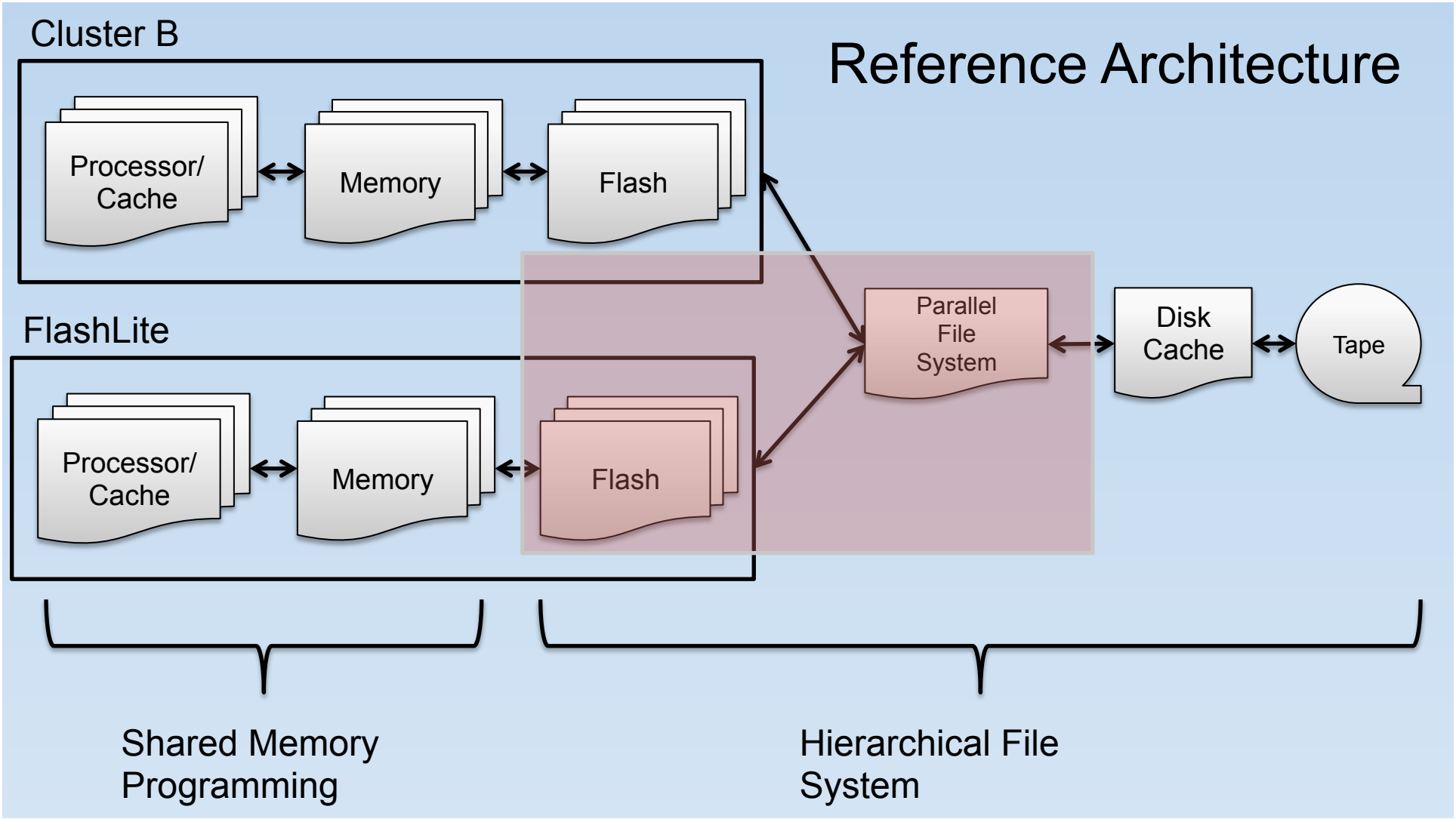


Process

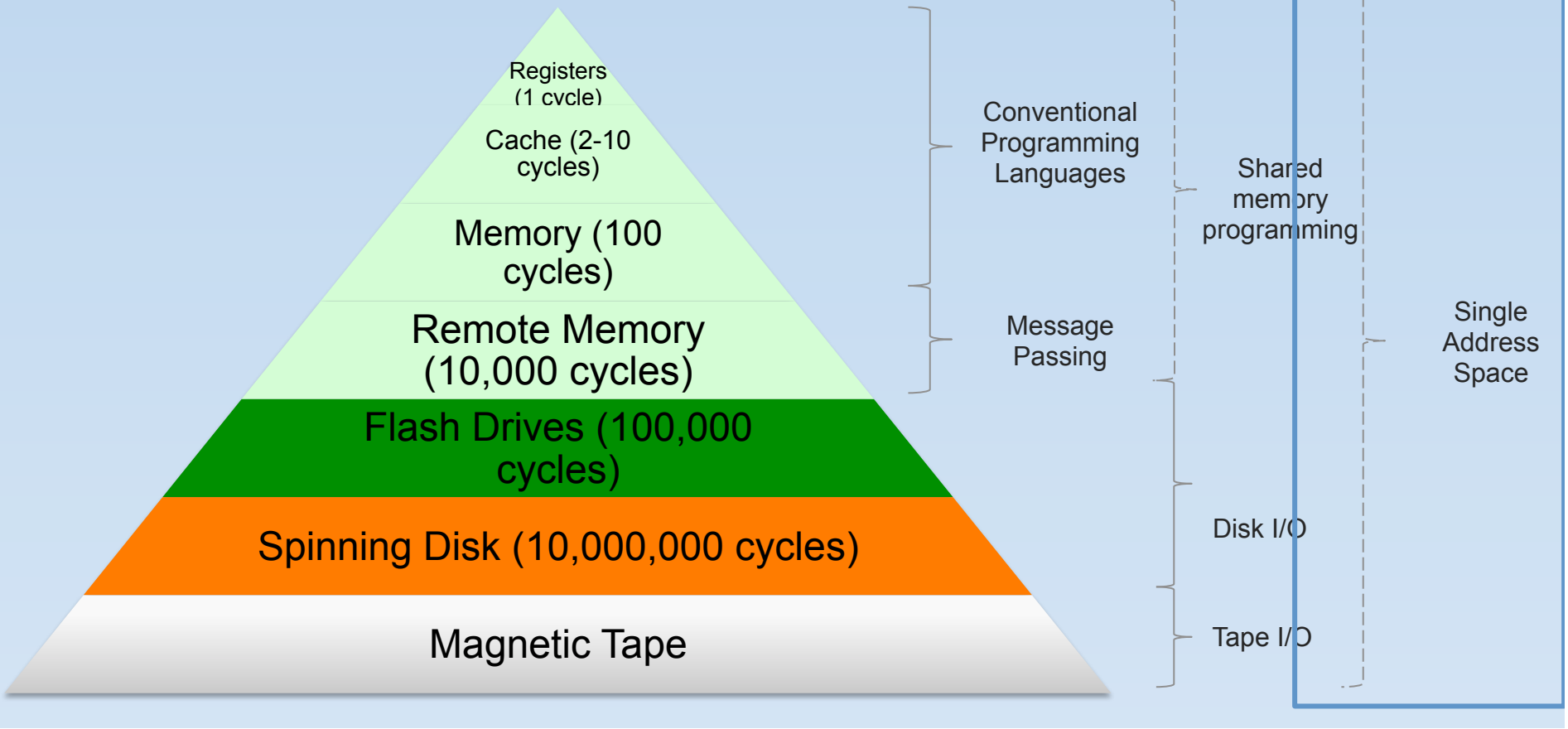


Interpret

What’s missing?


Cluster B
Reference Architecture
Processor/
Cache
Memory
Flash
FlashLite
Processor/
Cache
Memory
Flash
Parallel
File
System
Disk
Cache
Tape
Shared Memory
Programming
Hierarchical File
System

Memory Hierarchy



Proceedings of the Eighteenth Annual Hawaii International Conference on System Sciences, 1985.

IMPLEMENTING A LARGE VIRTUAL MEMORY IN A DISTRIBUTED COMPUTING SYSTEM

D. A. Abramson
Department of Computer Science
Monash University
Clayton 3168
Victoria
Australia

and

J. L. Keedy
Institut fuer Praktische Informatik,
Technische Hochschule Darmstadt,
Alexanderstr. 24,
D-6100 Darmstadt,
West Germany.

Conclusions

- FlashLite
  - Parallel computer
  - Very large amounts of local memory and Flash disk
  - Still learning what works
- MeDiCI
  - Caches all the way down
  - IBM Spectrum Scale & HPE DMF
- Need to remove the speed bumps

Conclusions

- Caches all the way down
- IBM Spectrum Scale & HPE DMF
- From Metro to Wide area
  - North (JCU)
  - East (US)
  - West (Pawsey)
  - South (NCI)
  - … to the Amazon

Acknowledgments and Questions

- Australian Research Council
  - Zhou, Bernhardt, Zhang, Zhu, Tao, Chen, Drinkwater, Tomlinson, Coppel, Gu, Burrage, Griffiths, Turner, Mackey, Du, Mengersen, Edwards
- Queensland Cyber Infrastructure Foundation (QCIF)
- CSIRO
  - Ondrej Hlinka, Stuart Stephen
- University of Queensland
  - Jake Carroll, Michael Mallon, Kevin Smith, Marlies Hankel ,Lutz Gross ,Cihan Altinay Christoph Rohmann
- SDSC
  - Mike Norman
- AARnet
  - Peter Elford