The National Center for Genome Analysis Support and Galaxy

William K. Barnett, Ph.D. (Director)

Richard LeDuc, Ph.D. (Manager)

National Center for Genome Analysis Support

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Summary

- NCGAS and its mission
- NCGAS cyberinfrastructure
- The 100 Gigabit demonstration
- Scaling genomics analysis
- Trinity optimization

Changing genomics analytical needs

- Next Gen sequencers are generating more data and getting cheaper
- Sequencing is:
    - ➢ Becoming commoditized at large centers and
    - ➢ Multiplying at individual labs
- Analytical capacity has not kept up
    - ➢ Bioinformatics support
    - ➢ Computational support (thousand points solution)
    - ➢ Storage support

NCGAS widens the analytical bottleneck

- Funded by National Science Foundation
- Large memory clusters for assembly
- Bioinformatics consulting for biologists
- Optimized software for better efficiency
- Open for business at: http://ncgas.org

NSF

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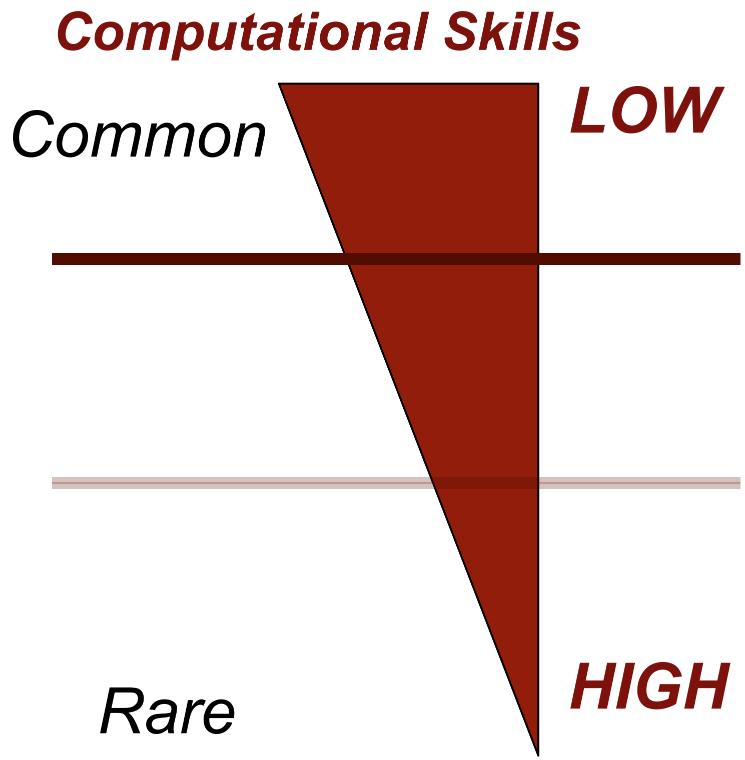
Making it easier for Biologists

- Galaxy interface provides a "user friendly" window to NCGAS resources
- Supports many bioinformatics tools
- Available for both research and instruction.

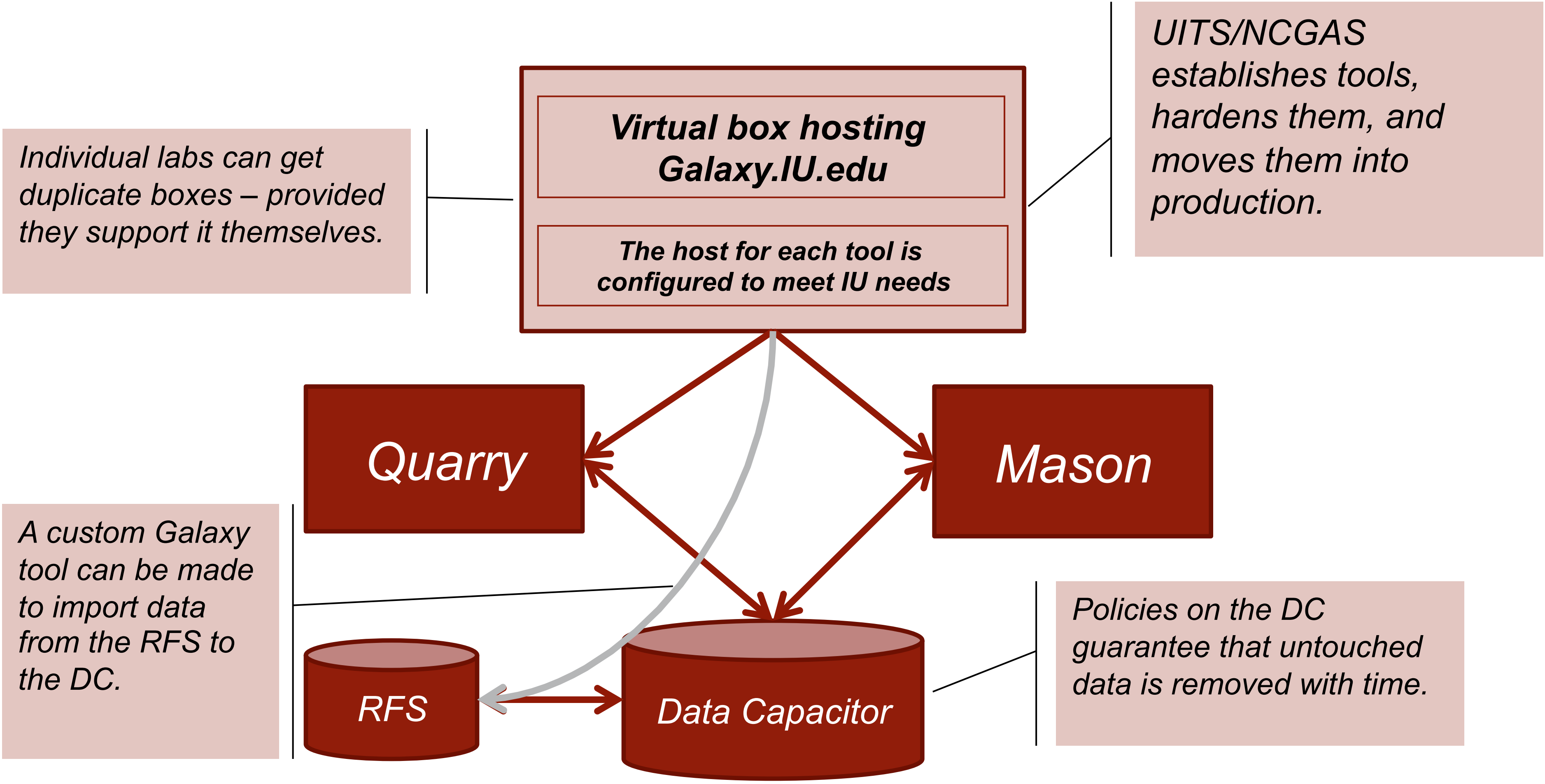
Galaxy



NCGAS Cyberinfrastructure at IU

- Mason large memory cluster (512 GB/node)
- Quarry cluster (16 GB/node)
- Data Capacitor (1 PB at 20 Gbps throughput)
- Research File System (RFS) for data storage
- Research Database Cluster for managing data sets.
- All interconnected with a high speed internal network (40 Gbps)

GALAXY.IU.EDU Model



Individual labs can get duplicate boxes – provided they support it themselves.

Virtual box hosting Galaxy.IU.edu

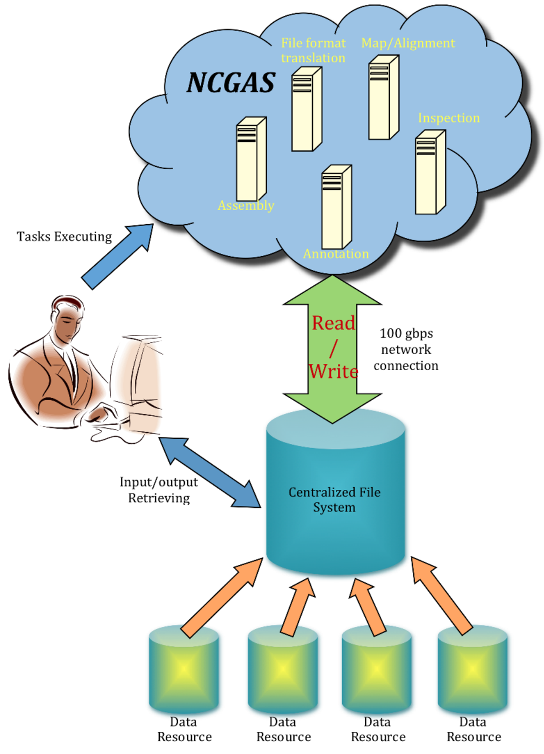
The host for each tool is configured to meet IU needs

UITS/NCGAS establishes tools, hardens them, and moves them into production.

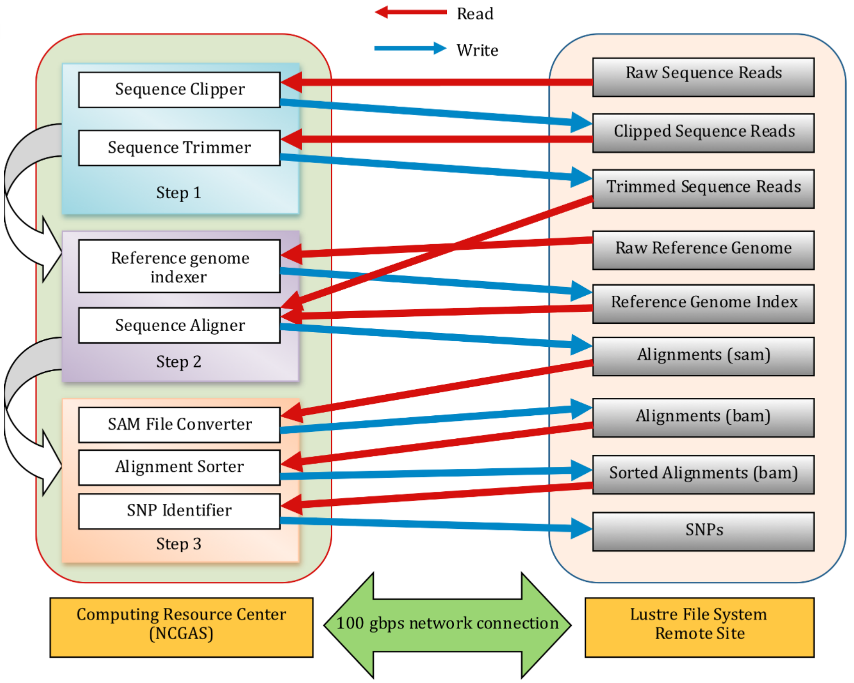
A custom Galaxy tool can be made to import data from the RFS to the DC.

Policies on the DC guarantee that untouched data is removed with time.

NCGAS Sandbox Demo at SC 11

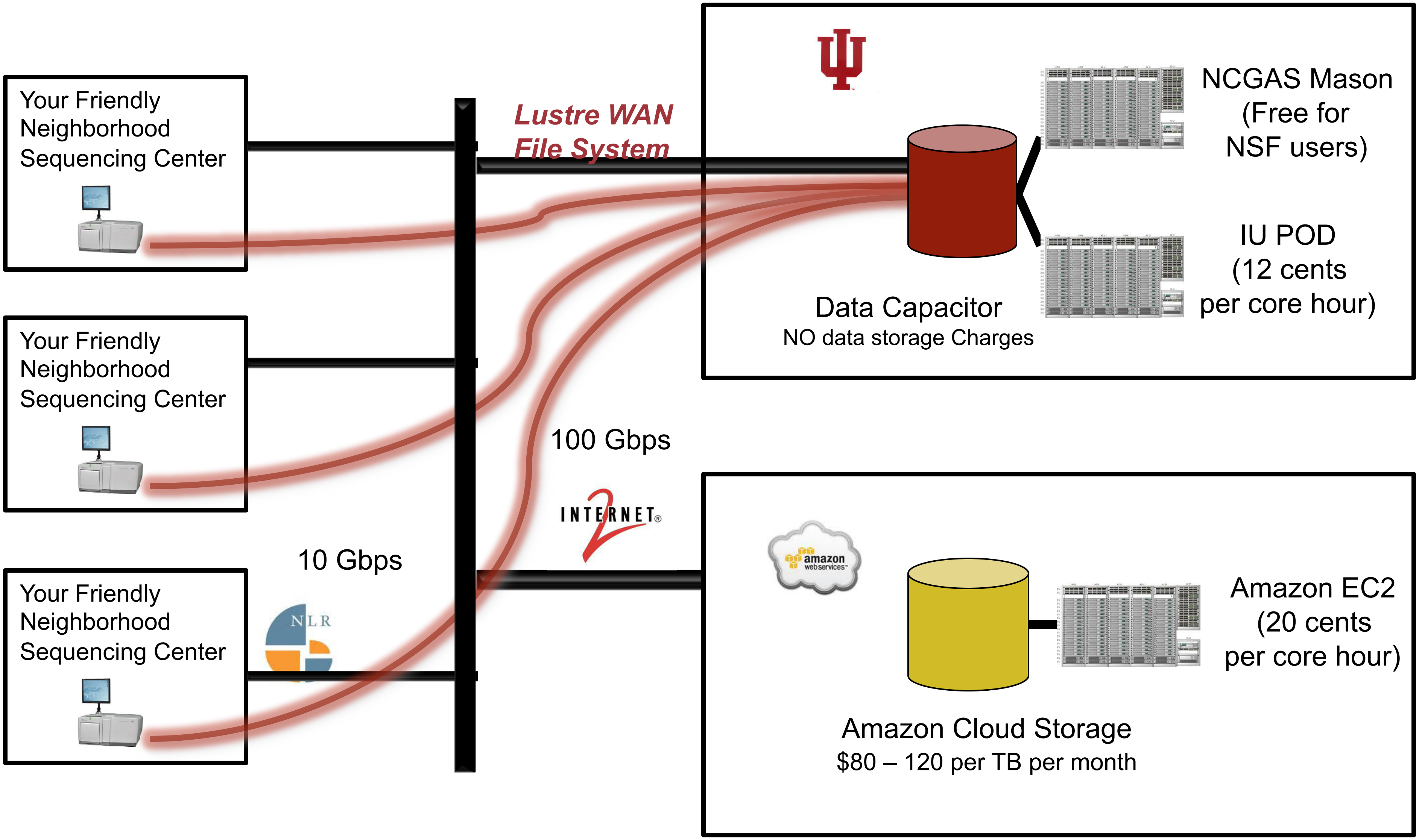


NCGAS with remote file system via 100 gbps link



- *STEP 1: **data pre-processing**, to evaluate and improve the quality of the input sequence*
- *STEP 2: **sequence alignment** to a known reference genome*
- *STEP 3: **SNP detection** to scan the alignment result for new polymorphisms*

Two Options for Computation and Storage


Your Friendly Neighborhood Sequencing Center
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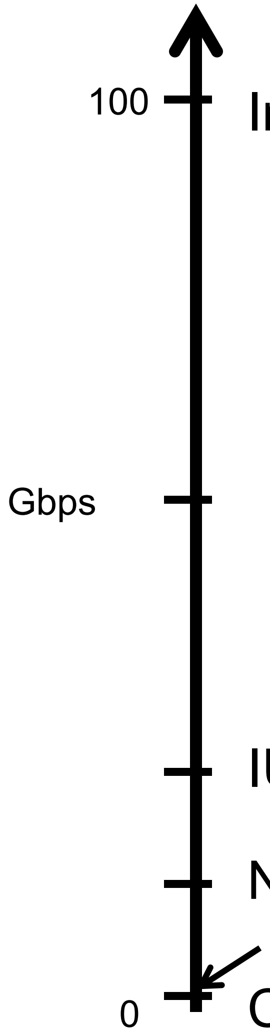
10 Gbps
NLR
Lustre WAN File System
100 Gbps
INTERNET2
NCGAS Mason (Free for NSF users)
IU POD (12 cents per core hour)
Data Capacitor
NO data storage Charges
amazon webservices
Amazon EC2 (20 cents per core hour)
Amazon Cloud Storage
$80 – 120 per TB per month

This Architecture Scales!



Internet2 (100Gbps)

DDR3 SDRAM (51.2 Gbps, 6.4GBps,)

IU Data Capacitor (20 Gbps throughput)

NLR to Sequencing Centers (10Gbps/link)

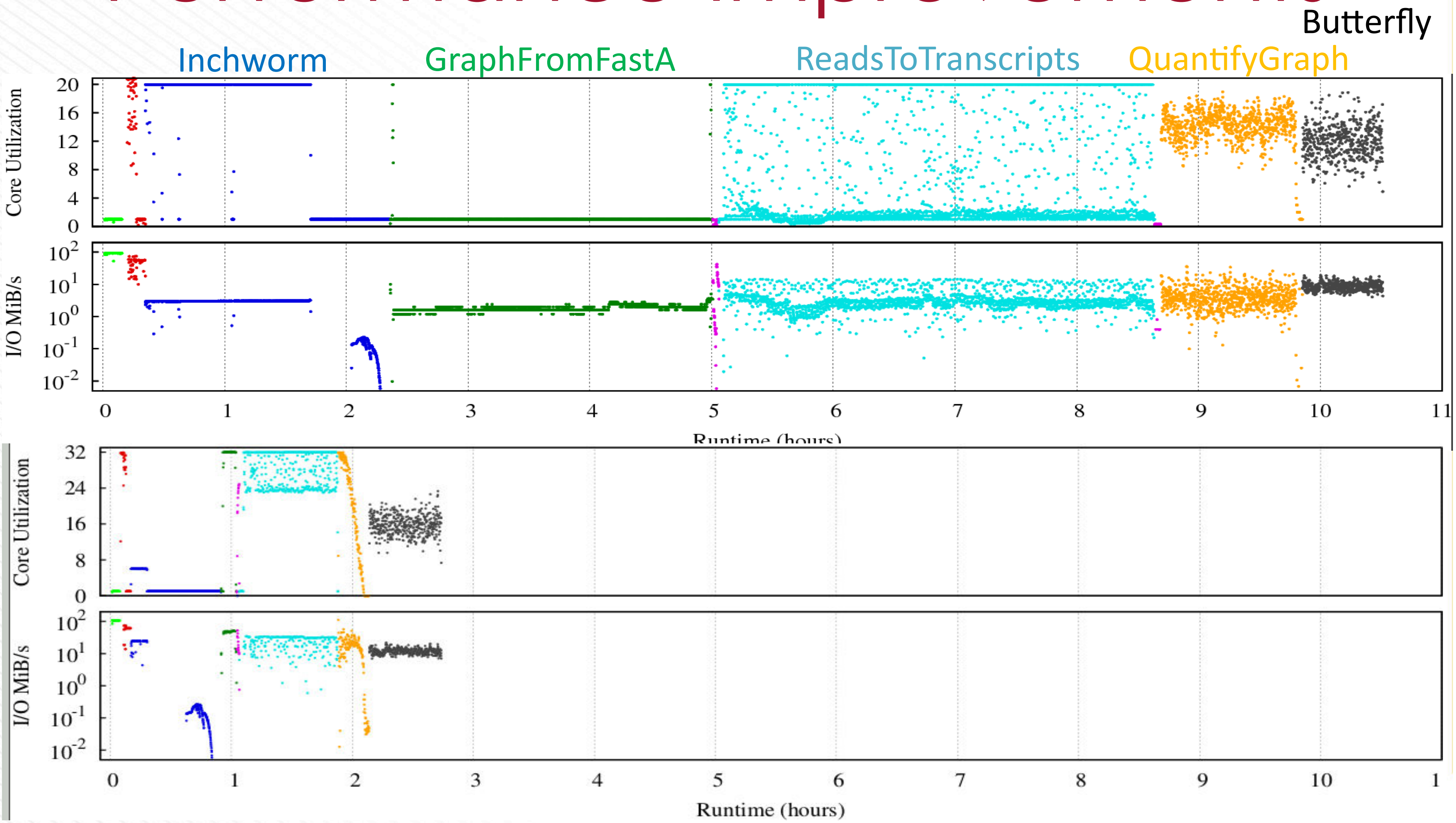
Ultra SCSI 160 Disk (1.2 Gbps, 160 MBps)

Commodity Internet (1Gbps but highly variable)

How would this work at scale?

1. Biologists use Galaxy to execute workflows
2. Sequence data mounted via Lustre WAN or automatically transferred using Internet2
3. Data Capacitor flows data into Mason or other computational clusters
4. Data Capacitor mounts or mirrors reference data from NCBI or other sources
5. Results delivered through web interfaces and to visualization or other science tools

Performance Improvements



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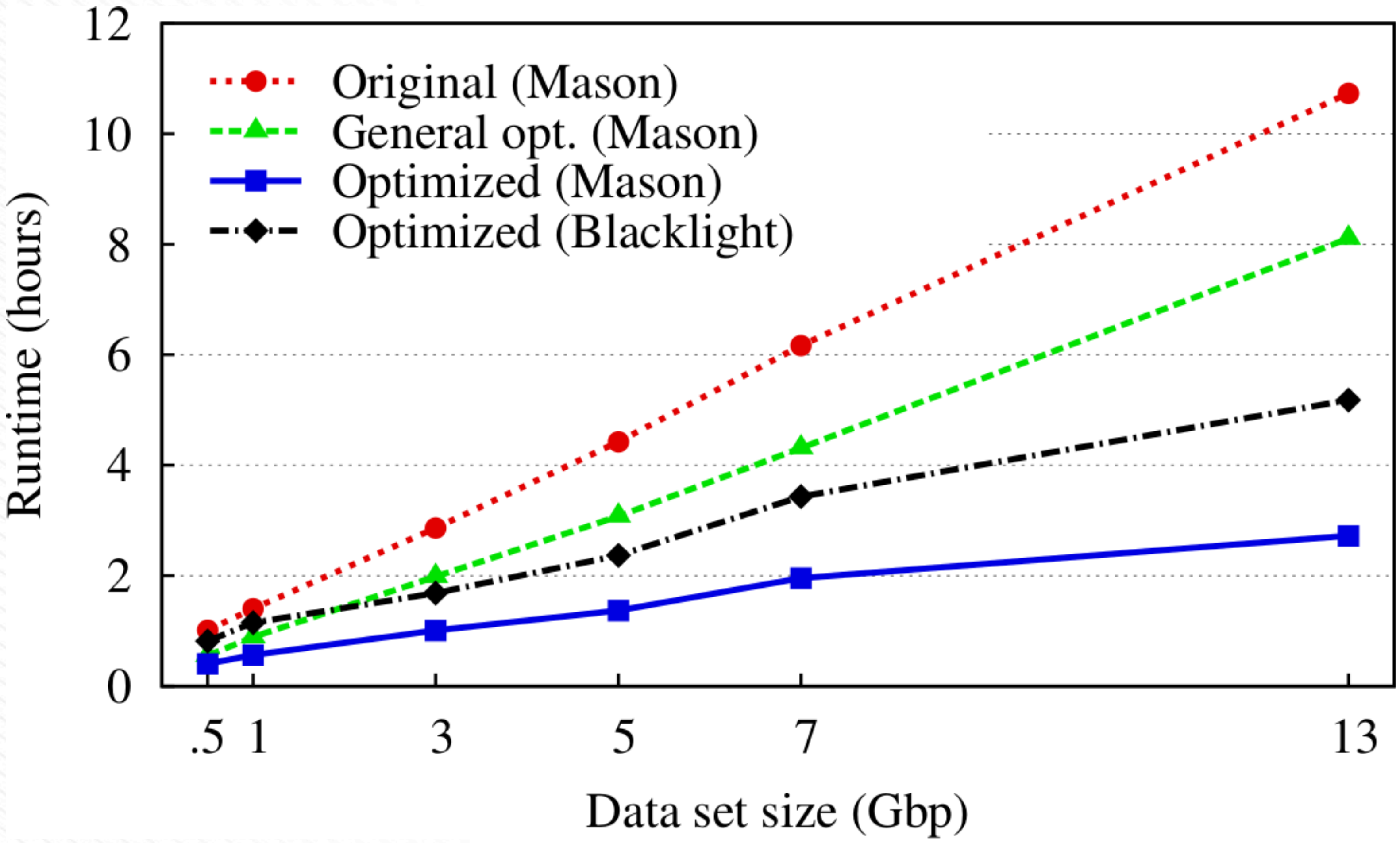
Final Results



Trinity Results

- Significantly reduced runtime, while maintaining correctness of results
- Results are published
- Source code is commit to official SourceForge repository
- Continued support for HPC optimization for Trinity
- Brian Haas at Broad is developing Trinity workflows for Galaxy

In Sum…

- NG Sequencing is creating a analytical problem that cannot be solved at sequencing centers
- NCGAS can provide a global scale infrastructure to better serve the needs of biologists who cannot become bioinformaticians to accomplish their research.
- Trinity is no longer a resource hog

Thank You

Questions?

Bill Barnett (barnettw@iu.edu)

Rich LeDuc (rleduc@iu.edu)

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