Optimizing the National Cyberinfrastructure for Lower Bioinformatic Costs: Making the Most of Resources for Publicly Funded Research

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## Summary

- NCGAS and its mission and cyberinfrastructure.
- Overview NCGAS server-on-demand resources on a low cost fee-for-cycles basis.
- Overview XSEDE: When you need truly large-scale resources.

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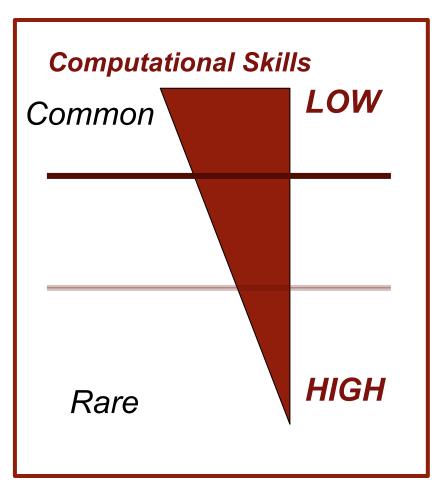
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- Funded by National Science Foundation
  - 1. Large memory clusters for assembly
  - 2. Bioinformatics consulting for biologists
  - 3. Optimized software for better efficiency



- Collaboration across IU, TACC, SDSC, and PSC.
- Open for business at: <u>http://ncgas.org</u>

## Making it easier for Biologists





- Web interface to NCGAS resources
- Supports many bioinformatics tools
- Available for both research and instruction.

## **NCGAS Cyberinfrastructure at IU**

- Rockhopper: 11 servers with 48 cores and 128 GB RAM.
- Mason large memory cluster: 16 nodes with 32 cores each and 512 GB RAM per node.
- Data Capacitor: 1 PB at 20 Gbps throughput.
- Research Database Cluster for managing data sets.
- All interconnected with high speed internal network (40 Gbps)
- 100 Gbps Internet2 Backbone



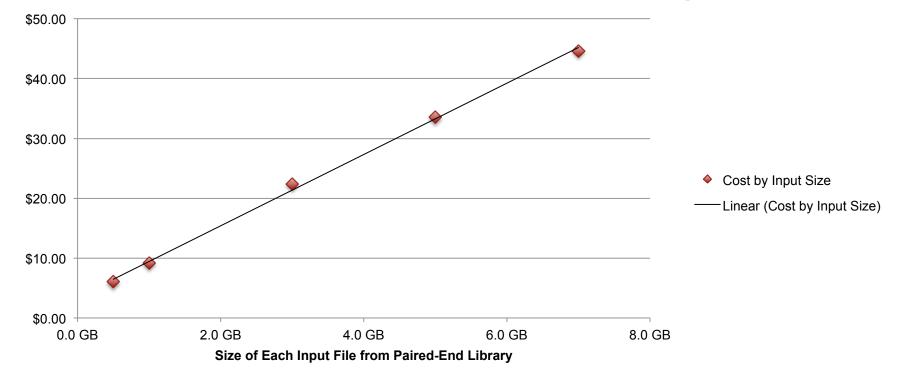
## Rockhopper

- Penguin Computing's Penguin-On-Demand (POD) supercomputing cloud appliance hosted by Indiana University.
- A collaborative effort between Penguin Computing, IU, the University of Virginia, the University of California Berkeley, and the University of Michigan.
- Provides supercomputing cloud services in a secure US facility.
- Researchers at US institutions of higher education and Federally Funded Research and Development Centers (FFRDCs) can purchase computing time from Penguin Computing, and receive access via high-speed national research networks operated by IU.



## **Standardized Trinity Analyses**

Cost by Input Size for Trinity Jobs on POD@IU

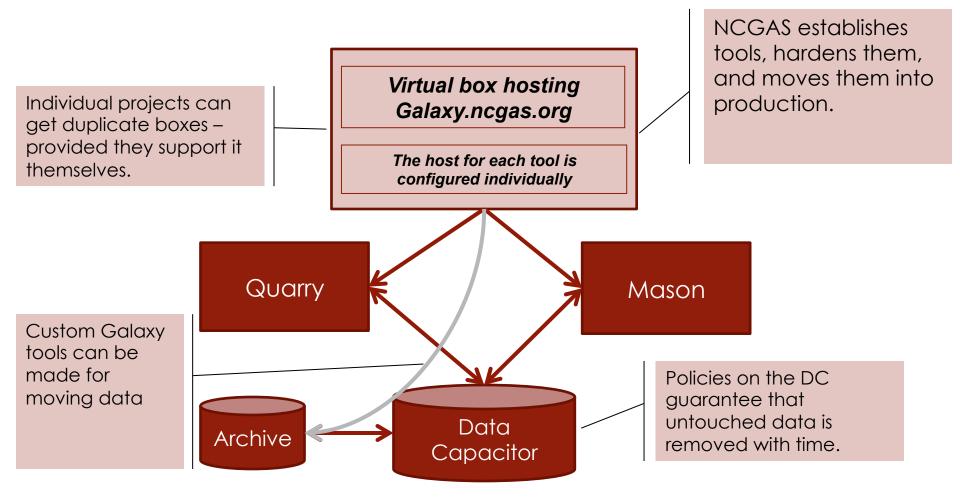


National Center for Genome Analysis Support: http://ncgas.org

- Galaxy	Analyze Data Workflow Shared Data * Visualization * Admin Help * User *	Using 14.9 M	1B
Tools 🌣		History	¢
Import Data Sequence QC De novo Assembly Trinity De novo assembly of	NCGAS National Center for Genome Analysis Support	<ul> <li>☑ — Ø I I I I I I I I I I I I I I I I I I</li></ul>	-
RNA-Seq data <ul> <li><u>Celera</u> De novo assembly of wgs DNA sequences</li> </ul>	at Indiana University	8 lines format: tabular, database: dm3 (a) (b) (b) (c) (c) (c) (c) (c) (c) (c) (c) (c) (c	
<ul> <li><u>SOAPdenovo</u> De novo assembly of Illumina GA short reads</li> </ul>	Welcome to the Galaxy Instance at Indiana University	1 2 FBtr0078013 chr2L:825963-833245	
<ul> <li><u>Newbler</u> De novo assembly of 454 GS data</li> </ul>		FBtr0078015 chr2L:825963-833245 FBtr0078014 chr2L:825963-833245	
<u>Assembly QC</u> Workflows	This instance of the Galaxy is installed and maintained by National Center for Genome Analysis Support <u>NCGAS</u>	FBtr0302612 chr2L:833583-851071	
All workflows	The Computing power is provided by the Indiana University <u>Mason Compute Cluster</u>	FBtr0302121 chr2L:833583-842691 FBtr0302120 chr2L:833583-851071	
	The storage is provided by the Indiana University <u>Data Capacitor</u>		
	The web server is hosted on the Indiana University <u>Quarry Gateway Hosting</u>	<u>56: Merge Columns on</u> ● Ø X data 55	
	The Galaxy project is supported in part by <u>NSF</u> , <u>NHGRI</u> , and <u>the Huck Institutes of the Life Sciences</u> .	<u>55: Cut on data 53</u> ● Ø X	
	The NCGAS projects is supported by <u>NSF</u> Questions? <u>help@ncqas.orq</u>	<u>53: Add column on data</u>	
	WINCGAS © 2012   National Center for Genome Analysis Support   Pervasive Technology Institute	<u>52: Add column on data</u> ④ ℓ ※ <u>48</u>	
		48: D. melanogaster       ● 𝔅 X         chr2L:826001-851000       𝔅         8 regions       format: bed, database: dm3         Im ① ♥ 𝔅       𝔅 🖉 👘	
		display at UCSC <u>main test</u> view in <u>GeneTrack</u> display at Ensembl <u>Current</u>	
		1.Chrom 2.Start 3.End 4.Name chr2L 825963 833245 FEtr0078013	
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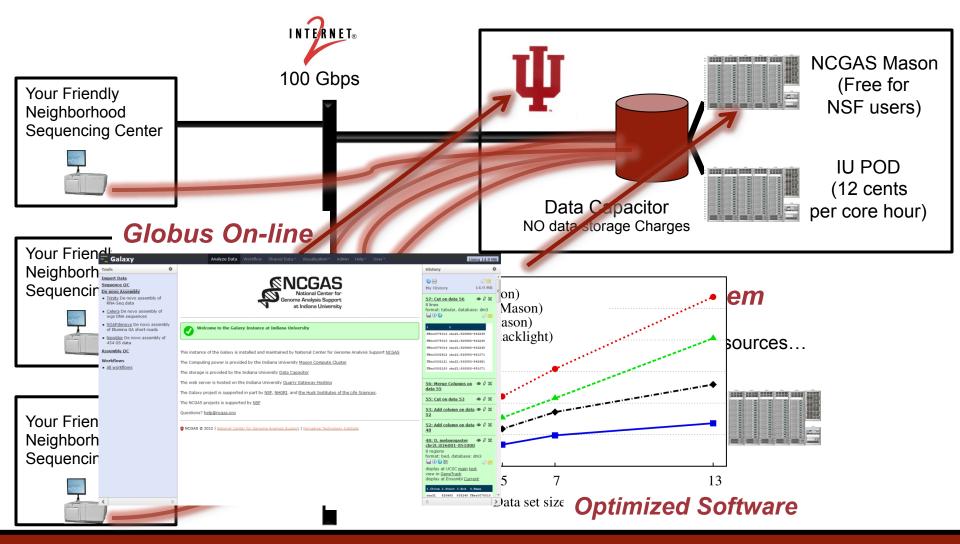


## GALAXY.NCGAS.ORG Model



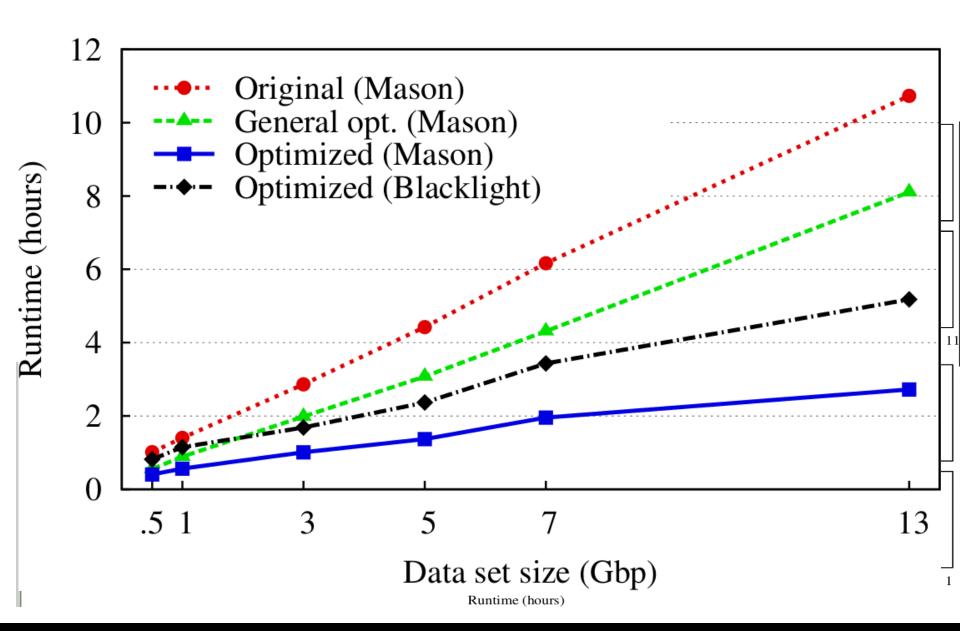
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## **Moving Forward**



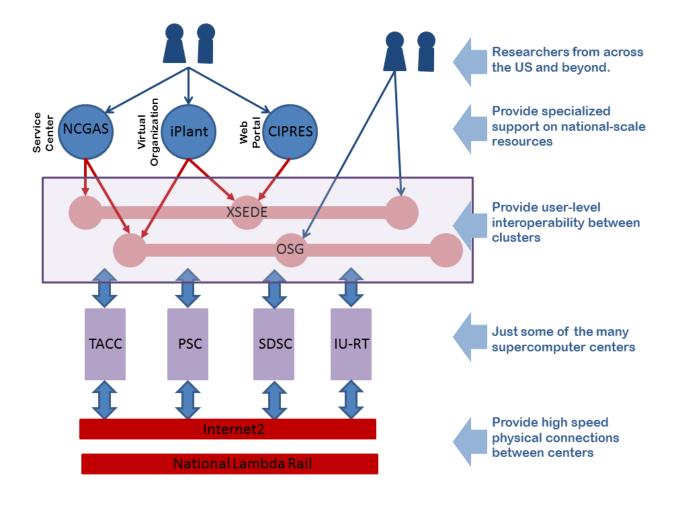
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## **The National Cyberinfrastructure**





# **XSEDE: Extreme Science and Engineering Discovery Environment**





- About 100 requests every quarter.
- About 50% of need is met.
- 75% from two systems.
- Allocations in the millions of SU.



# XSEDE

ALASKA

HAWAII

Extreme Science and Engineering Discovery Environment

#### Campus Champion Institutions

★



- EPSCoR States 46
- Minority Serving Institutions 12
- EPSCoR States and Minority Serving Institutions 8
  - Total Campus Champion Institutions 146

VIRGIN ISLANOS

## 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.
- XSEDE allows scaling to larger projects.



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