# Shared Research Computing Policy Advisory Committee

Fall 2018 Meeting Friday, December 7<sup>th</sup>



# Welcome and Introductions

**Chris Marianetti** Chair of SRCPAC



Today's Agenda

Welcome and Introductions Chris Marianetti

HPC Update Kyle Mandli and George Garrett

*Foundations for Research Computing* Update Marc Spiegelman and Barbara Rockenbach

Research Data Survey Barbara Rockenbach **Potential for New Subcommittees** Chris Marianetti

**CUIT Updates** Research Computing Services Group

Closing Remarks Chris Marianetti

COLUMBIA RESEARCH Shared Research Computing Policy Advisory Committee HPC Update

Kyle Mandli Chair of Operating Committee **George Garrett** Manager of Research Computing Services



# High Performance Computing Update

#### Topics

- Governance
- Support
- Yeti
- Habanero
- Terremoto
- Data Center Cooling Expansion Update

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# HPC Governance

 Shared HPC is governed by the faculty-led HPC Operating Committee, chaired by Kyle Mandli.

• The committee **reviews business and usage rules** in open, semiannual meetings.



# HPC Support Services

#### Email

• <u>hpc-support@columbia.edu</u>

#### **Office Hours**

- In-person support from 3pm 5pm on 1<sup>st</sup> Monday of month
- RSVP required (Science & Engineering Library, NWC Building)

#### **Group Information Sessions**

- HPC support staff present with your group
- Topics can be general/introductory or tailored
- Contact <u>hpc-support@columbia.edu</u> to schedule an appointment



# Yeti Cluster Update

- Yeti Round 1 retired November 2017
- Yeti Round 2 to retire March 2019



## Habanero

#### **Specifications**

- 302 compute nodes (7,248 cores)
- 740 TB storage (DDN GS7K GPFS)
- 397 TFLOPS of processing power

#### Lifespan

- 222 nodes expire 2020
- 80 nodes expire 2021







# Habanero – Participation and Usage

- 44 groups
- 1,400 users
- 9 renters
- 120 free tier users
- Education tier
  - 13 courses since launch
- 2.7 million jobs completed



### Habanero – Cluster Usage in Core Hours





#### LIVE!! Wednesday, December 5!

- 24 research groups
- 5 year lifetime



# TERREMOTO Specifications

- 110 Compute Nodes (2640 cores)
  - 92 Standard nodes (192 GB)
  - 10 High Memory nodes (768 GB)
  - 8 GPU nodes with 2 x NVIDIA V100 GPUs
- 430 TB storage (Data Direct Networks GPFS GS7K)
- 255 TFLOPS of processing power
- Dell Hardware, Dual Skylake Gold 6126 CPUs, 2.6 Ghz, AVX-512
- 100 Gb/s EDR Infiniband, 480 GB SSD drives



### Data Center Cooling Expansion Update

- A&S, SEAS, EVPR, and CUIT contributed to expand Data Center cooling capacity
- Work to be completed by February 2019
- Assures HPC capacity for several generations



## Foundations for Research Computing Update

Marc Spiegelman Chair, *Foundations* Advisory Committee **Barbara Rockenbach** Associate University Librarian for Research and Learning



# Foundation's Goals

- 1. Address current **needs**, and **demand** for informal training in computational science to improve research capabilities
- 2. Provide a hierarchical training infrastructure to serve **novice**, **intermediate**, and **advanced** users
- 3. Develop and foster a Columbia-wide culture and community of research computing
- 4. Leverage existing University- and school-based investments in research computing infrastructure



# Hierarchical Program Structure

#### Novice

- Institutional Membership with *The Carpentries* (Software, Data, Library Carpentry)
- Pre-semester Boot Camps: ~200+ students per year
- Refresher Monthly Workshops & Help Room Office hours

#### Intermediate

- Help Room Office Hours
- Distinguished Lectures in Computational Innovation
- Research Symposium
- Monthly Workshops: Discipline-specific, use of advanced libraries

#### Advanced

Coordination with departmental curriculum

COLUMBIA UNIVERSITY Foundations for Research Computing

# Current Status

Columbia | Research

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### The Carpentries and CU Instructors

Silver membership with *The Carpentries* established July 2019

**Instructors trained** from CUIT, Libraries, Computer Science, and Business:

- 6 in July 2018
- 6 in October 2018

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# Fall 2018 Boot Camps

- August 27-28, 2018
- 462 registrations for 90 seats
- 90 seats filled in 4 Minutes
- 6 instructors from CUIT, Libraries, APAM
- 3 courses from the Software Carpentries
  - Programming in **Python** (x2)
  - **R** for Reproducible Scientific Analysis

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### Fall Bootcamp Attendance



#### Registration & Waitlist by School



Policy Advisory Committee

### Distinguished Lectures in Computational Innovation

All events held in Brown Institute for Media Innovation (Journalism School)

- September 13: **Bjarne Stroustrup** (creator of C++)
  - Registrations: 200 Attendance: 100+ (Standing Room Only)
- October 11: Lorena Barba (Reproducible Science and Open-Source Initiative)
  - Registrations: 90 Attendance: 40+
- November 8: **Eric Xing** (leader in commercialization of machine learning technologies)
  - Registrations: 191

Attendance: 80+



## Workshops Held

Three-Part *Introduction to HPC* Series (RCS held at Science and Engineering Library)

Additional workshops from Libraries:

- Panel and Survey Data Analysis Using Stata (2 sessions)
- Introduction to Data Visualization in R



### Office Hours

Four Graduate Students Staffing Two Locations Each Week:

- Mondays 3–5pm, Science and Engineering Library
- Fridays 1–3pm, Butler Library

Uptake has been slow:

• Will revisit allocation of student assistants for the spring



## Recruiting Program Coordinator

- Interviews conducted in several rounds throughout Fall semester
- Input from Advisory and Coordinating Committees
- Currently finalizing offer to top candidate



# Spring Look-Ahead: Boot Camps

- January 17-18, 2019: Butler Library
- Applications open December 11
- Expanding to 4 boot camps
  - Possibility of training additional instructors
- Experienced and novice instructors paired
  - CTL Microteaching Sessions in Arrangement
- Python groups will pilot new(er) curriculum in Plotting and Programming
- R group will use **R for Social Scientists** module

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## Spring Lectures Schedule

- February 14: Krishna Ratakonda (IBM Fellow & CTO, Blockchain Solutions)
- March 14: Runa Sandvik (computer security and encryption expert)
- April 11: Gina Helfrich (communications and diversity initiatives)
- May 9: Fernando Perez (creator of iPython computer environment)



# Future Plans and Opportunities

- Increase and Improve intermediate-level offerings: Need input and feedback from instructors/departments/students on most-needed content. Huge role for coordinator.
- Consider mechanisms for potential curriculum development (e.g. NRT/Carpentries, seed funding).
- Understand demand and scale to meet it while maintaining quality.
- Already some future discussions with additional units (CUIMC, SPS, etc).
- All input greatly appreciated.

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# Research Data Survey

**Barbara Rockenbach** Associate University Librarian for Research and Learning



# Potential New Subcommittees

**Chris Marianetti** Chair of SRCPAC



# Cloud Subcommittee

- A new subcommittee to determine how to make decisions such as:
  - When should a resident cluster **burst to a Cloud resource**?
  - How would **priorities** for use of resident vs. Cloud-based be established?
- SRCPAC membership, with support from staff should understand potential financing and charging models



## GPU Subcommittee

- GPU resources have increased astronomically in price.
- Some peer institutions and groups have set-up low cost, consumer grade GPU clusters.
- SRCPAC could establish a subcommittee to assess demand, risk, and support.



# CUIT Updates

**Michael Weisner** Research Systems Engineer, Columbia Population Research Center **George Garrett** Manager Research Computing Services **Jimmy Chiong** Lead Infrastructure Engineer, Configuration Management



## Secure Data Enclave (SDE)

#### Service

• The SDE Provides Columbia researchers with a secure, remotely accessible, virtual Windows 10 desktop environment to store and collaboratively analyze sensitive and identifiable information.

https://cuit.columbia.edu/sde

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### Secure Data Enclave – Usage Requirements

- Users must have a UNI and VPN access to use the SDE. (Outside collaborators may be approved for access through proper HR registration)
- Projects have a yearly cost of **\$526** per project per year
- Projects must have a sponsoring faculty member and provide a "Data Security Officer"



### Secure Data Enclave – Features

- Members get access to a 4-core 16GB RAM Windows 10 Desktop Image
- Allows for simultaneous work by project members on data
- Certified by the Columbia University Irving Medical Center Security group for HIPAA compliance
- Supports popular statistical software packages including Stata 15, R, STAN, QGIS, and more.



### Secure Data Enclave – Data

The SDE is currently approved for use of popular datasets, including:

- The Bureau of Labor Statistics National Longitudinal Surveys (NLS) datasets
- University of North Carolina Longitudinal Study of Adolescent Health (Add Health) datasets
- European Commission Eurostat restricted economic datasets
- Department of Health records
- Restricted National Economic Data



# Globus

- Provides secure, unified interface to research data.
- "*Fire and Forget*" high-performance data transfers between systems within and across organizations.
- Share data with collaborators.
- Columbia has procured an enterprise license.
- Contact rcs@columbia.edu to get started with Globus





# AWS Enterprise Agreement

- Multiple benefits over "click through" agreement:
  - 1. Improved security, privacy, and audit protections
  - 2. Branding and intellectual property protection
  - 3. Extended times to "exit" the service
  - 4. Compliance with procurement and IT security policies
  - 5. Ability to enroll in BAA (not automatic) PHI data
  - 6. Billing and pricing enhancements



# "Linked" vs. "Delegated" Accounts

- Existing AWS accounts can "link" to CUIT billing family
  - Allows for central ARC billing
  - Potential to realize volume discounts over time
  - Ensures compliance with University Finance and IT security policies



# "Linked" vs. "Delegated" Accounts

- For new requests, CUIT creates a "delegated" account:
  - SAML-based login with Columbia UNI
  - CUIT-managed CloudTrail log collection
  - Secure storage and management of the root credentials
- Researchers retain control of and responsibility for account



# AWS Direct Connect

- Activated January 2018
- Provides dedicated 10 Gbps link to US-East-1 Region
- Allows direct routing of RFC1918 addresses
- Envisioned as primary link for clients between campus and their AWS resources, with VPN as backup
- Public VIF enabled allowing dedicated network performance to AWS IP addresses



# Data Egress Waiver

 Research & Academic accounts can take advantage of Amazon's Data Egress Waiver program

 Credit for your data egress charges (network data traffic leaving AWS) of up to 15% of your total bill for a given month



## More Information

#### Account Information

https://cuit.columbia.edu/aws

Cloud Computing Consulting
<a href="https://cuit.columbia.edu/cloud-research-computing-consulting">https://cuit.columbia.edu/cloud-research-computing-consulting</a>

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# Closing Remarks

**Chris Marianetti** Chair of SRCPAC

