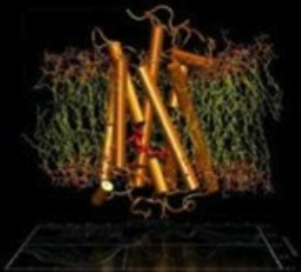


Research Computing Center
High-Performance Computing and
Research Technology Services

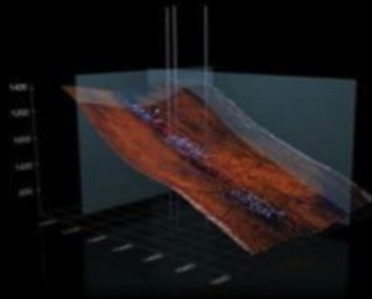
Robin Weiss

robinweiss@uchicago.edu

Computing – The 3rd Pillar of Science



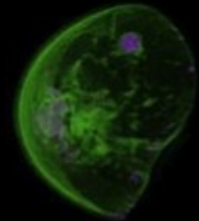
Drug Design
Molecular Dynamics



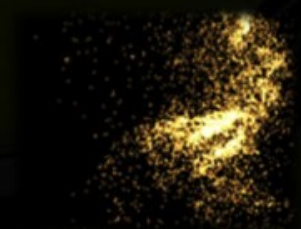
Seismic Imaging
Reverse Time Migration



Automotive Design
Computational Fluid Dynamics



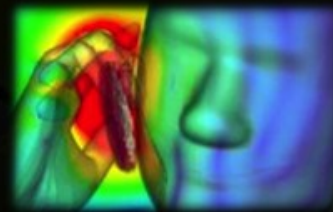
Medical Imaging
Computed Tomography



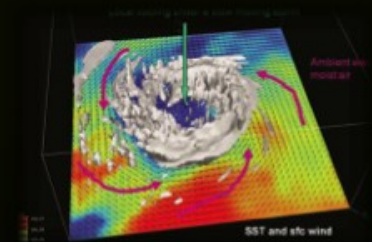
Astrophysics
n-body



Options Pricing
Monte Carlo



Product Development
Finite Difference Time Domain



Weather Forecasting
Atmospheric Physics

RCC's Mission

*The RCC mission is to **advance research and scholarship** by providing access to centrally managed high-end computing, storage and visualization resources. These resources include not just **hardware and software**, but also expert **technical user support**, education and training.*

Research Computing Center Services

“Provide access to hardware (computing, storage, and visualization resources), software and advanced technical support”

Hardware

High End Computing
Tightly Coupled & High Throughput

Research storage
Data Management

Special hardware:
GPU, Shared memory, fast Network

Software

Commercial software
Licensing

Public/Community
codes

Homegrown
codes

Technical Support

Scientific Computing
Visualization

Education and Training
Grants

Application Software
Development

Software

18 Commercial and 186 Publicly available software are installed and maintained at RCC (341 different modules)

- **System Tools and Math Libraries**

- Compilers: Intel, Portland, GCC
- Debugger
- Python, Perl, Ruby interpreters
- SWIFT
- MPI, MKL, FFTW, GSL, CUDA, etc.

- **Commercial software**

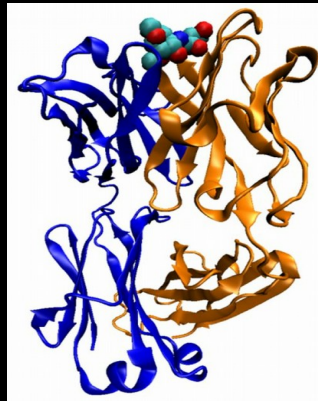
- MATLAB, STATA, AMIRA, Alinea DDT, etc.

- **Domain Specific Applications**

- chemistry
- Biology
- physics
- etc.

- **Use of module system**

- Example: *module load intel*



```
Q56940 R0YIN .....MREDAKSTVPLATEICLDQVCFYVAMTSKQMDLHSLGKAVPLGCTMMKATKGLNH--PAL 76
RLAO R0MAN .....MREDAKSTVPLATEICLDQVCFYVAMTSKQMDLHSLGKAVPLGCTMMKATKGLNH--PAL 76
RLAO R0MDE .....MREDAKSTVPLATEICLDQVCFYVAMTSKQMDLHSLGKAVPLGCTMMKATKGLNH--PAL 76
RLAO R0C .....MREDAKSTVPLATEICLDQVCFYVAMTSKQMDLHSLGKAVPLGCTMMKATKGLNH--PAL 76
RLAO R0CCK .....MREDAKSTVPLATEICLDQVCFYVAMTSKQMDLHSLGKAVPLGCTMMKATKGLNH--PAL 76
RLAO R0ANS .....MREDAKSTVPLATEICLDQVCFYVAMTSKQMDLHSLGKAVPLGCTMMKATKGLNH--PAL 76
Q7DNC3 R0ARE .....MREDAKSTVPLATEICLDQVCFYVAMTSKQMDLHSLGKAVPLGCTMMKATKGLNH--PAL 76
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RLAO D0CDE .....MREDAKSTVPLATEICLDQVCFYVAMTSKQMDLHSLGKAVPLGCTMMKATKGLNH--PAL 76
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RLAO S0LBO .....MREDAKSTVPLATEICLDQVCFYVAMTSKQMDLHSLGKAVPLGCTMMKATKGLNH--PAL 76
RLAO A0ERP .....MREDAKSTVPLATEICLDQVCFYVAMTSKQMDLHSLGKAVPLGCTMMKATKGLNH--PAL 76
RLAO PYRAE .....MREDAKSTVPLATEICLDQVCFYVAMTSKQMDLHSLGKAVPLGCTMMKATKGLNH--PAL 76
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RLAO ARCPY .....MREDAKSTVPLATEICLDQVCFYVAMTSKQMDLHSLGKAVPLGCTMMKATKGLNH--PAL 76
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RLAO PYRAB .....MREDAKSTVPLATEICLDQVCFYVAMTSKQMDLHSLGKAVPLGCTMMKATKGLNH--PAL 76
RLAO PYRBD .....MREDAKSTVPLATEICLDQVCFYVAMTSKQMDLHSLGKAVPLGCTMMKATKGLNH--PAL 76
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value 1.....10.....20.....30.....40.....50.....60.....70.....80.....90
```

Workshops and Advanced Training for Chicago Researchers

- RCC tutorials and Workshops
- Software vendors workshops
- Scheduled Workshops
 - Intro to Python
 - Intro to Linux
 - Intro to data visualization
 - Intro to OpenMP
 - Parallel programming with MPI
 - Programming with R
 - Introduction to Stata
 - Comsol Workshop
 - Python for HPC
 - GPU computing with Nvidia
 - Tips and Tricks for Midway



What is a Supercomputer?

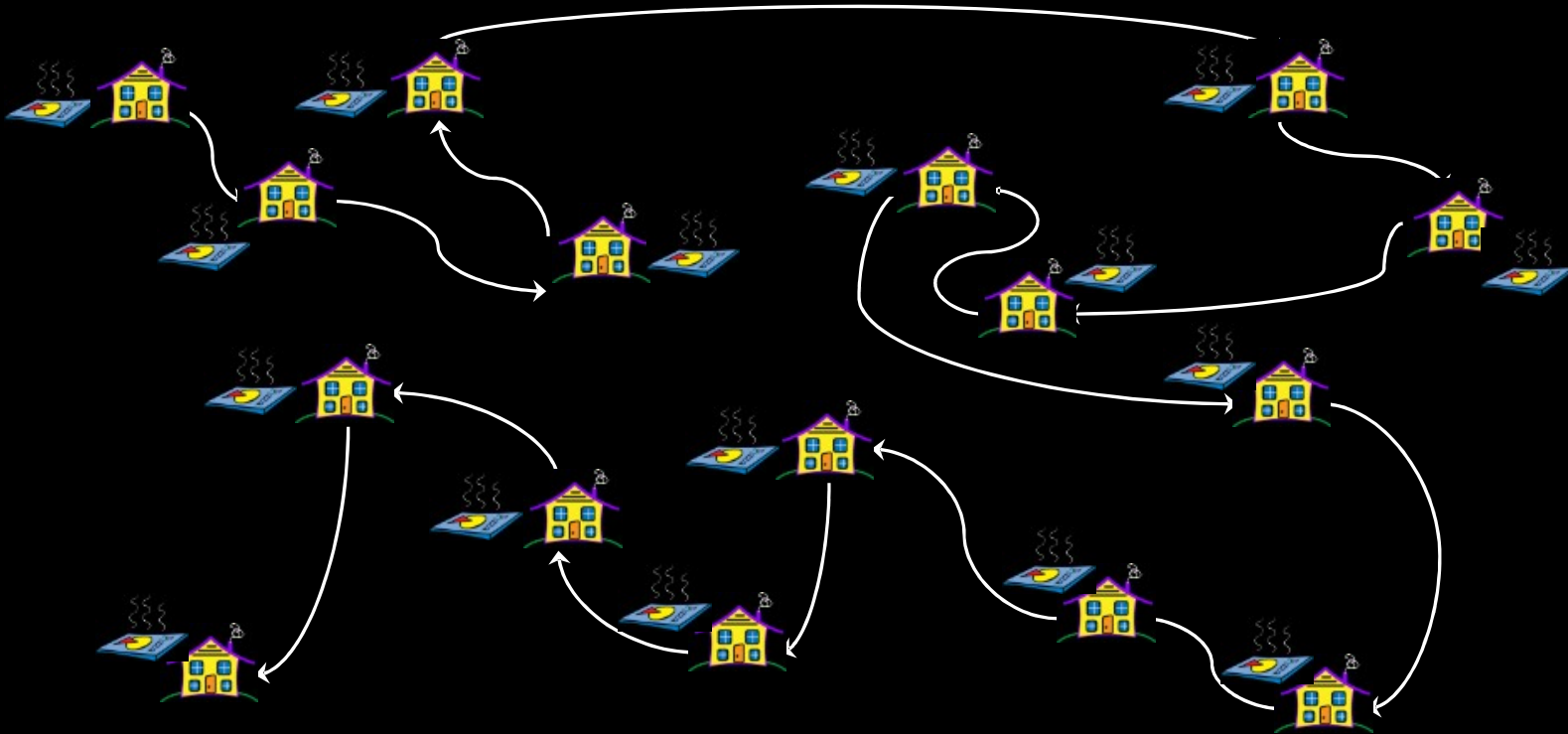
- A very fast computer...
... i.e.: A Super-Computer!
- It's all about math ($A + B = ?$)
- The “slowest” supercomputer does 153.4 Tflop/s
- The “fastest” does 33,862.7 Tflop/s
- (iPhone 5 does ~600 Mflop/s)

Serial Pizza Delivery



Process:

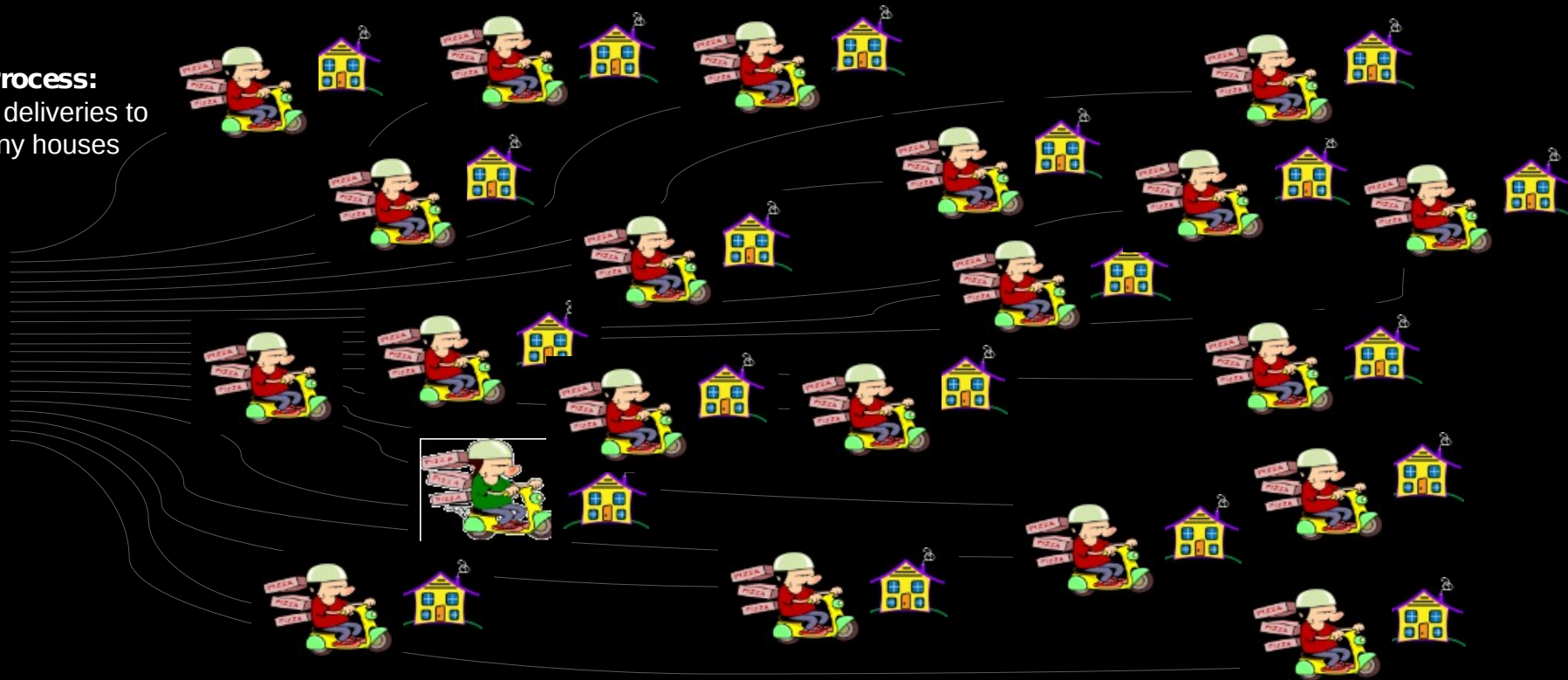
Delivery truck delivers one pizza and then moves to next house



Parallel Pizza Delivery

Process:

Many deliveries to many houses



So what's the secret?

- Take advantage of parallel processing
- Supercomputers are (usually) made up of many smaller computers
 - 10's of thousands or even millions
- Why go parallel? Because Intel has been lying to you ...

... Computers have not gotten
any faster in about 11 years

Pizza Delivery Problem

- The worlds faster supercomputer has 3,120,000 CPU cores
- If you have 3,120,000 drivers, you can deliver 3,120,000 pizzas at the same time

Midway Supercomputer is...

- In 2012 we were #447 in the world (80.6 Tflop/s)
- Scientific Linux 6.6
- Intel x86_64 based cluster
- ~895 Compute nodes (13,320 CPU cores)
 - Each with 16 CPUs and 32 GB memory
- 40 gbps infiniband network
 - 3-5 GB/s throughput
- ~1.5 PB storage
 - 900TB of tape backup

RCC capabilities continue to grow at Midway

RCC manages 895 nodes (13,320 cores) and 1.4 PB of storage

- **Compute**

 - Shared: 345 nodes**

 - **329** tightly coupled infiniband nodes (5376 cores)
 - **3** loosely coupled GigE nodes (48 cores)
 - **10** NVidia GPU nodes (176 cores)
 - **3** large shared memory nodes (up to 1TB) (64 cores)

 - Cluster Partnership Program: 270 nodes**

 - **160** tightly coupled infiniband nodes (2836 cores)
 - **109** loosely coupled nodes (1812 cores)
 - **1** large shared memory node (24 cores)

 - Cluster Partnership Program Special: 280 nodes**

 - **118** tightly coupled nodes (1040 cores)
 - **162** loosely coupled nodes (1944 cores)

- **Storage**

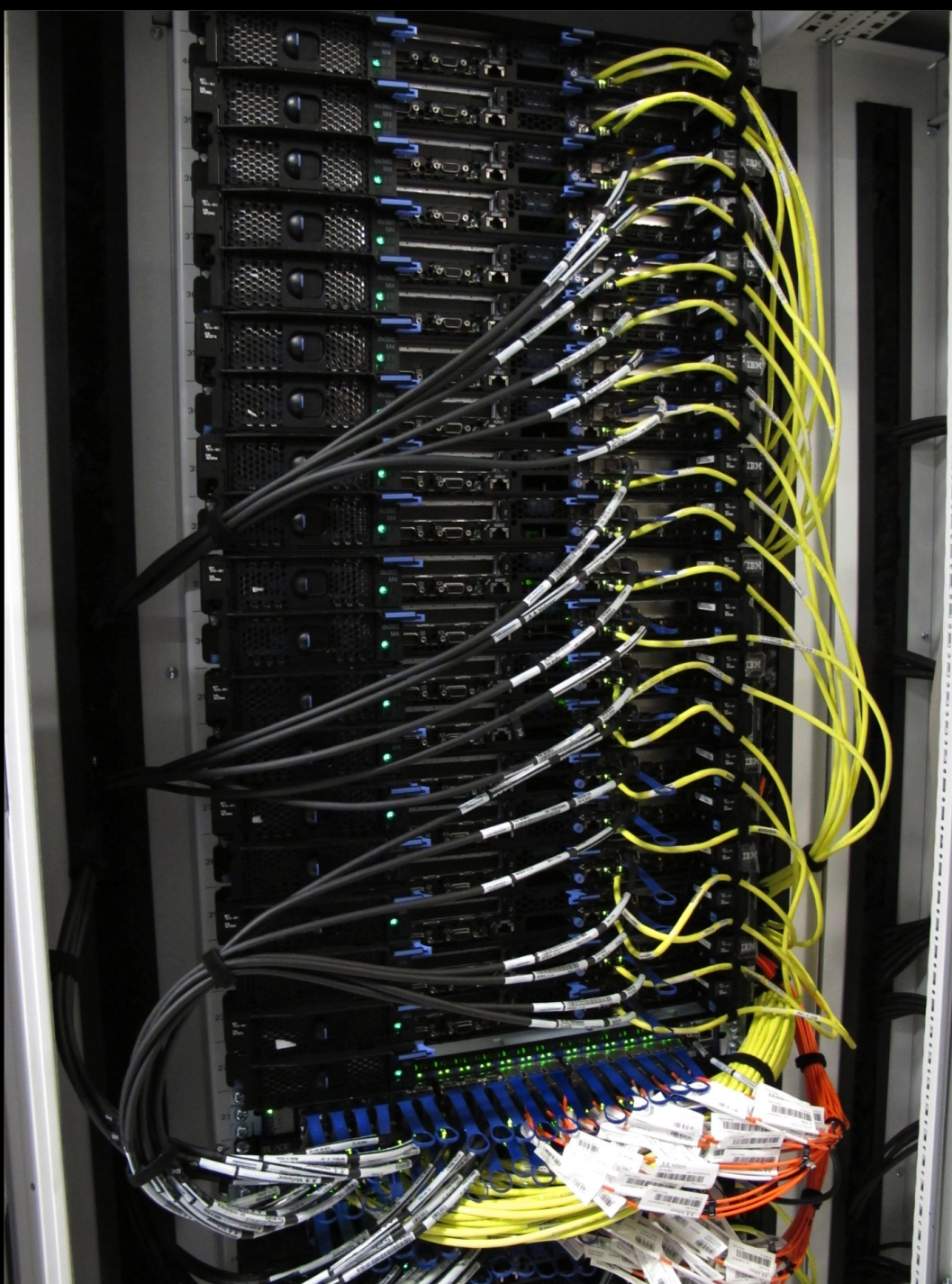
 - High-performance storage (**96 TB** usable)
 - Capacity storage: **1.4 PB** usable
 - Cluster Partnership Program Storage: **750 TB** usable
 - Backed up and snapshotted

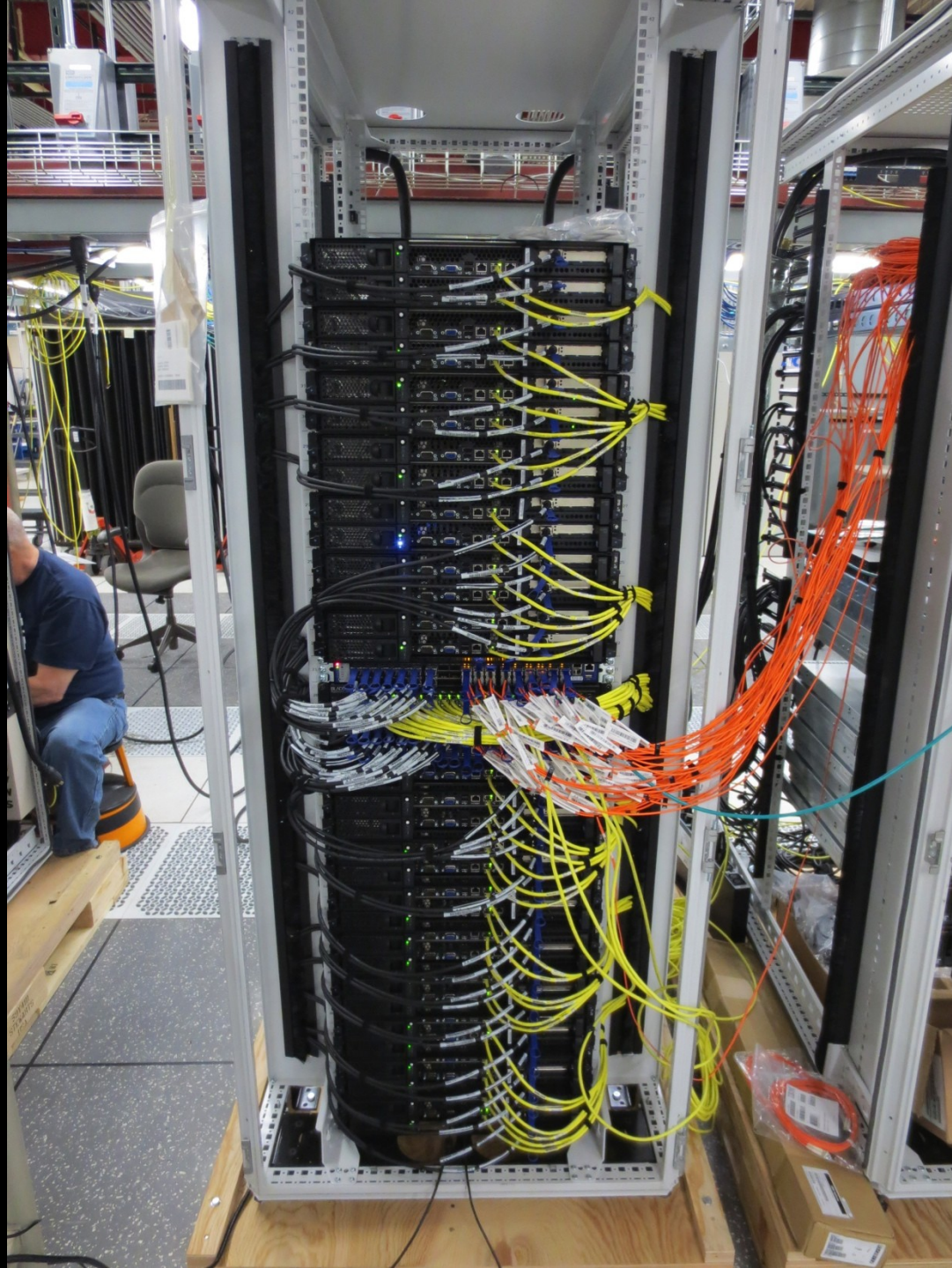
- **Tape Backup**

 - **900 TB** of tapes











Getting an Account

- ECON 41904 has a class account
 - All students in this class are eligible for an account during Spring 2015 quarter
- All PI-Eligible Uchicago faculty can obtain a PI account
 - Non pi-eligible Uchicago users can get an account via an RCC PI Account

Getting Help

- Email: help@rcc.uchicago.edu
- Docs: <https://docs.rcc.uchicago.edu>