Tutorial:

Scalable Infrastructures for Compute-Intensive Cognitive Neuroscience

Workshop Materials:

tinyurl.com/CogSci-ScalableComputing

Please complete the Pre-Workshop Survey!

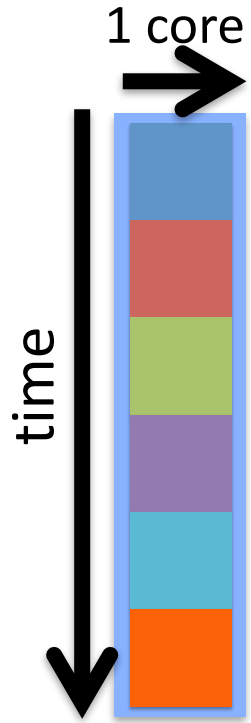
What is “large-scale” computing?

larger than a single computer

Computer Component:	Disk	Memory	Cores
Role of Component:	“long-term memory”	quick-access “working memory”	“math processing”
When You’ve Outgrown:	**I don’t have room for all of the data.**	**The computer crashes.**	**It takes too long.**

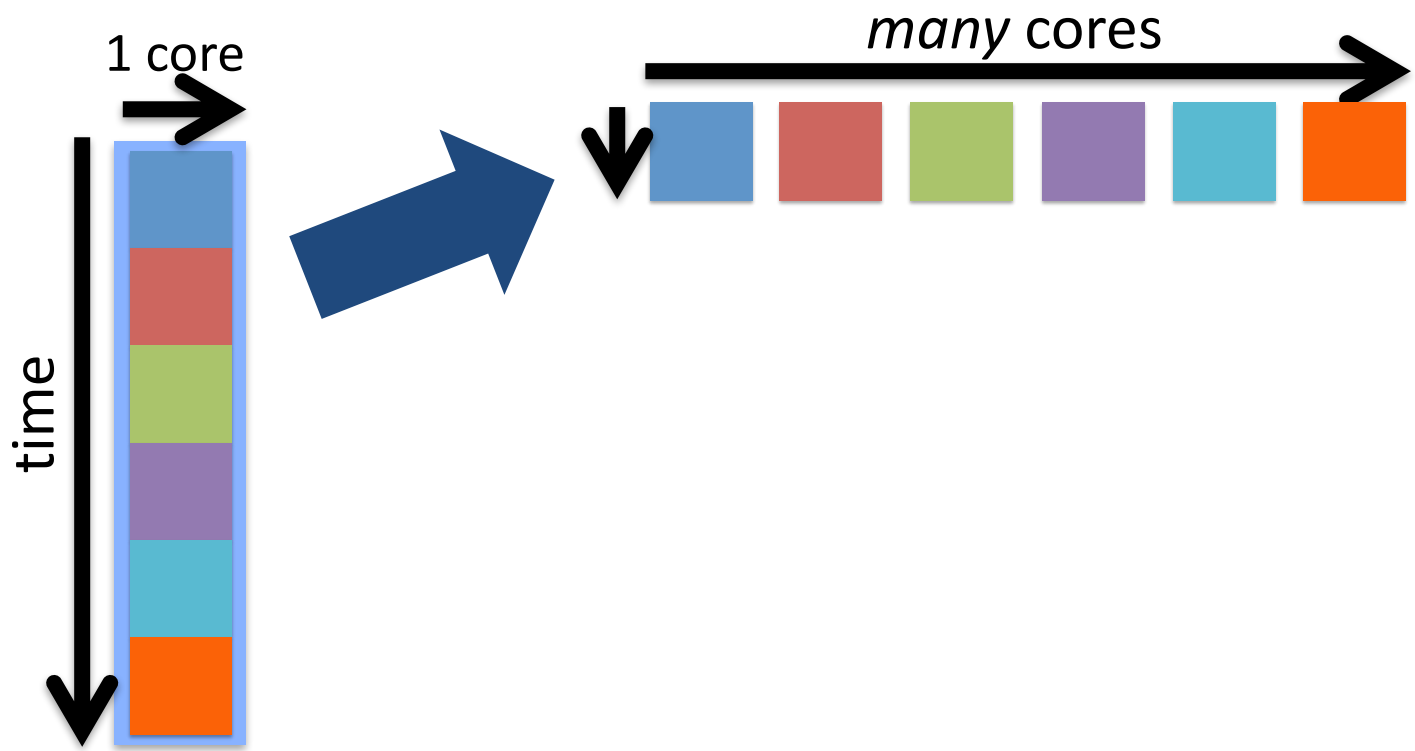
“It takes too long …”

parallel computing approaches



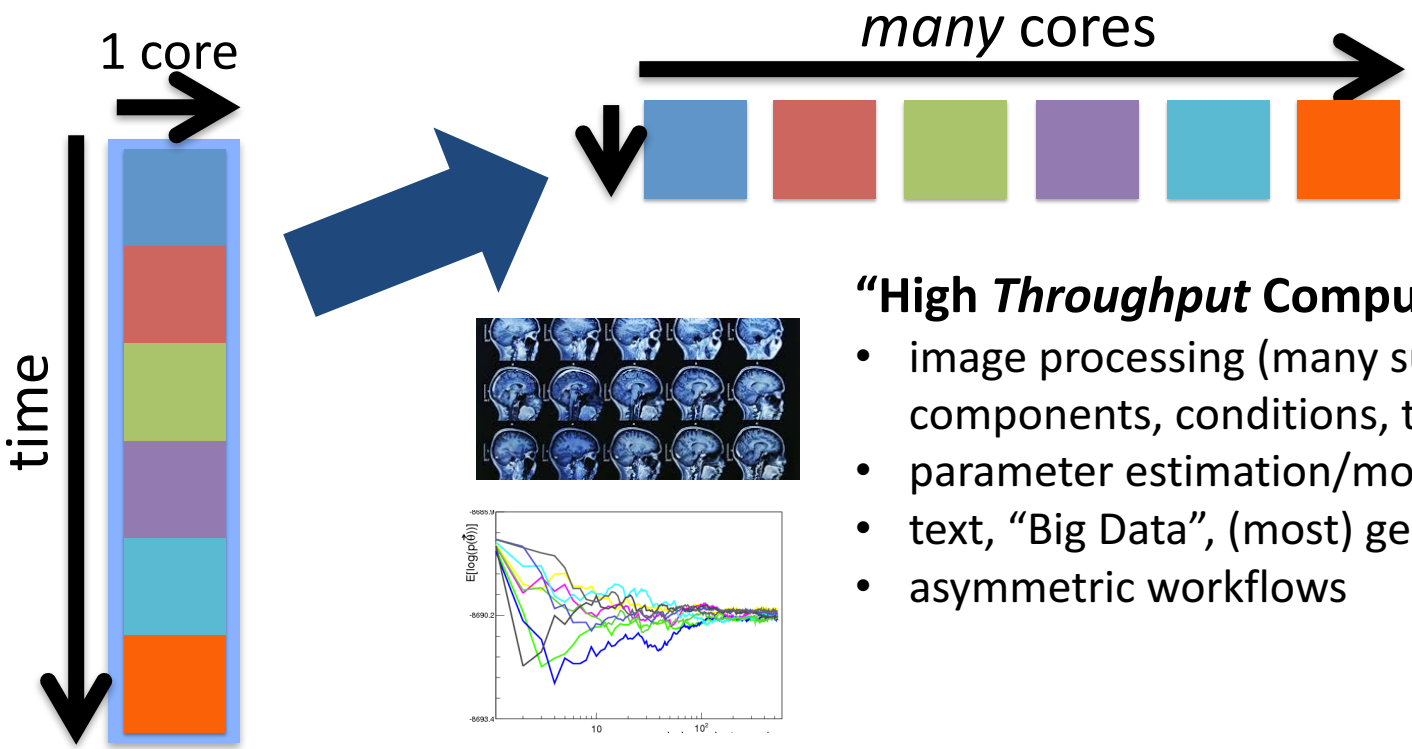
If order doesn't matter…

natural parallelization



If order doesn't matter…

natural parallelization



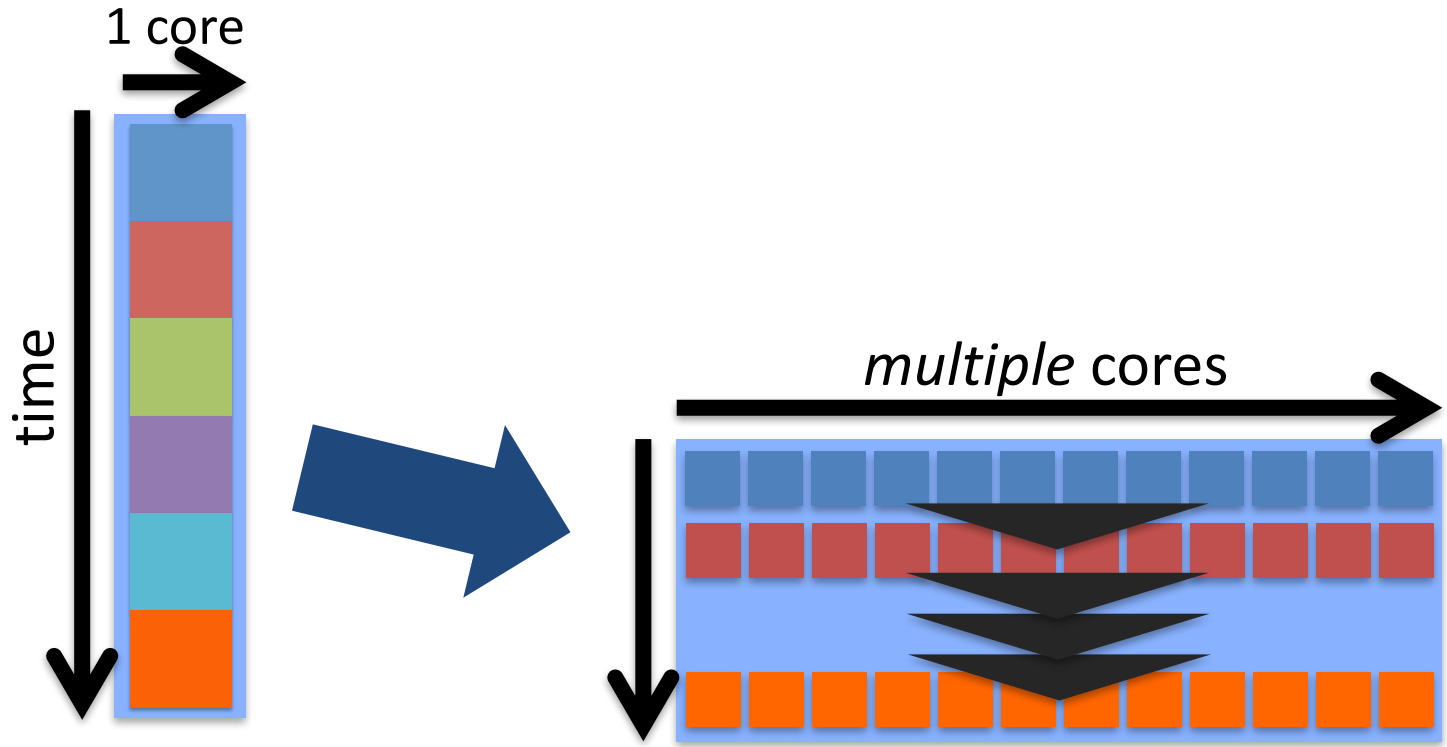
"High *Throughput* Computing (HTC)"

- image processing (many subjects, components, conditions, time frames)
- parameter estimation/model fitting
- text, "Big Data", (most) genomics
- asymmetric workflows

***Future Directions for NSF Advanced Computing Infrastructure … 2017-2020*. NAP, 2016.**

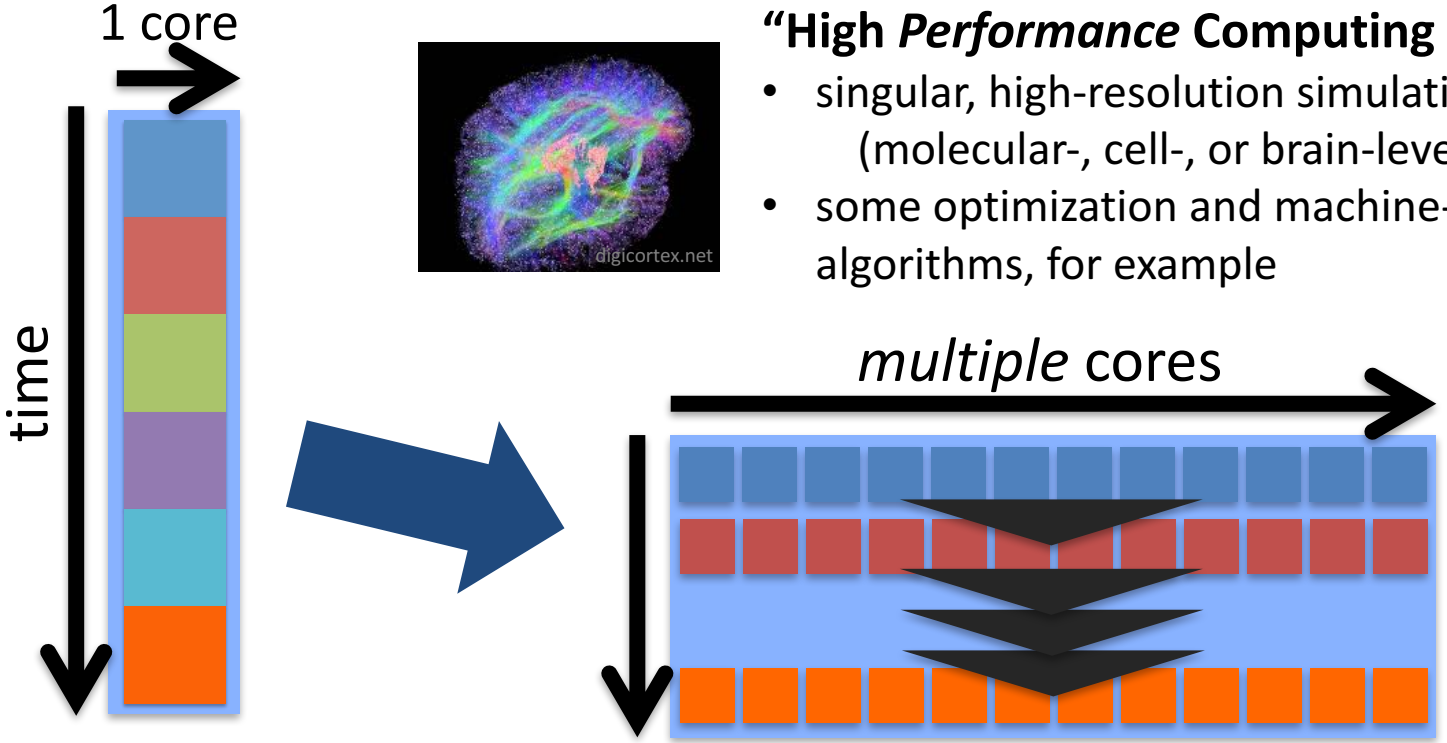
If order matters…

internal/interdependent parallelization



If order matters…

internal/interdependent parallelization



"High *Performance* Computing (HPC)"

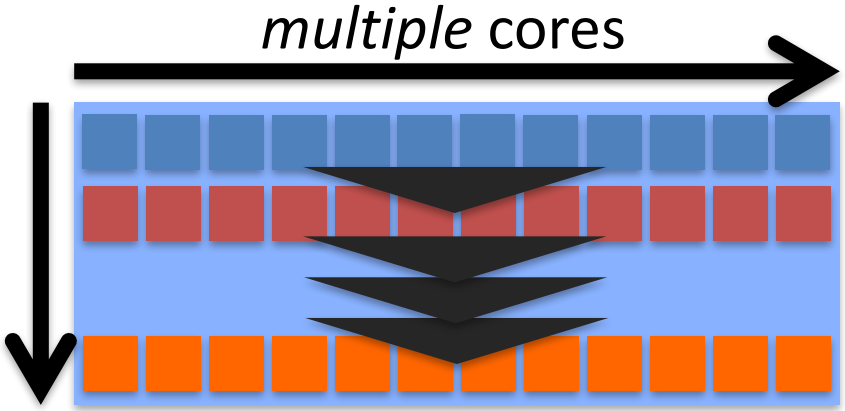
- singular, high-resolution simulations (molecular-, cell-, or brain-level)
- some optimization and machine-learning algorithms, for example

What is “large-scale” computing?

larger than a single computer

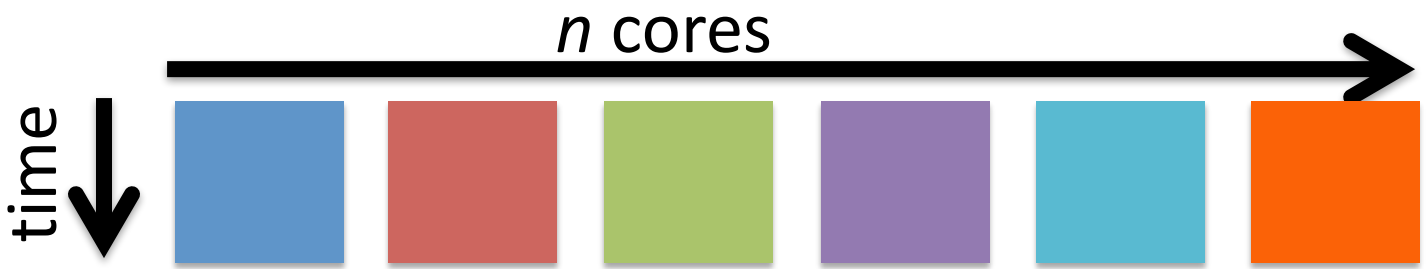
Computer Component:	Disk	Memory	Cores
Role of Component:	“long-term memory”	quick-access “working memory”	“math processing”
When You’ve Outgrown:	**I don’t have room for all of the data.**	**The computer crashes.**	**It takes too long.**

High Performance Computing (HPC)



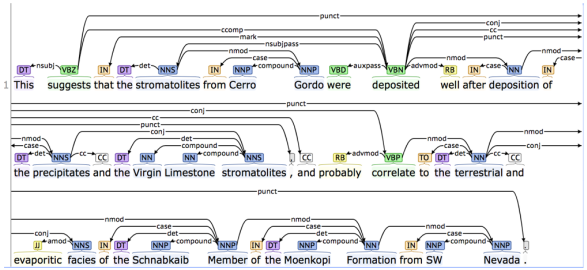
- Benefits greatly from:
  - CPU speed + homogeneity
  - Shared filesystems
  - Fast, expensive networking and servers co-located
- Scheduling: **Must wait until all processors are available**, *at the same time* and *for the full duration*
- Requires special programming (MP/MPI)
- ***What happens if one core or server fails or runs slower than the others?***

High Throughput Computing (HTC)

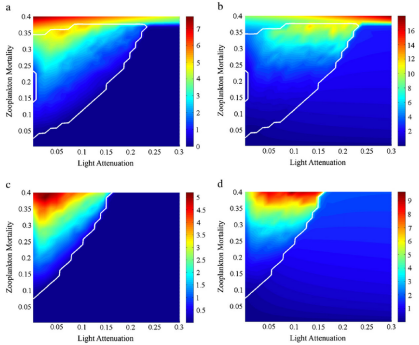


- Scheduling: only need **1 CPU core for each** (shorter wait)
- Easier recovery from failure
- No special programming required
- Number of concurrently running jobs is *more* important
- CPU speed and homogeneity are *less* important

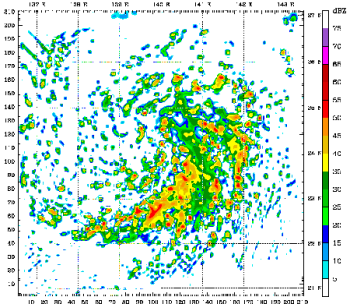
HTC-able Research Examples



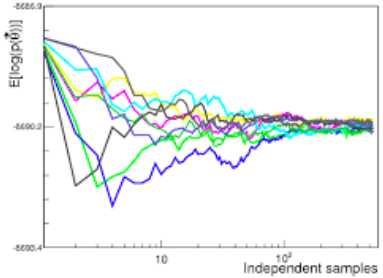
text analysis (most genomics …)



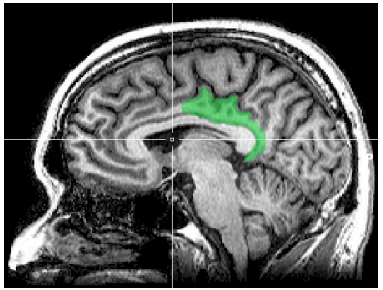
parameter sweeps



multi-start simulations



statistical model optimization
(MCMC, numerical methods, etc.)



multi-image and
mulit-sample analysis

Scope of Computing Infrastructures

Accessibility and Scale

- **per research group, per institution, national, or commercial**
- free, by-proposal, or fee-based

Supported computing modes

- HTC- vs. HPC-optimized; availability of specialized hardware: GPUs, high-memory, etc.

Interface graphical/pipeline (specialized) or command-line (generalizable)

Human Support

- local vs. remote personnel; domain-specificity?
- learning materials

National-Scale Resources

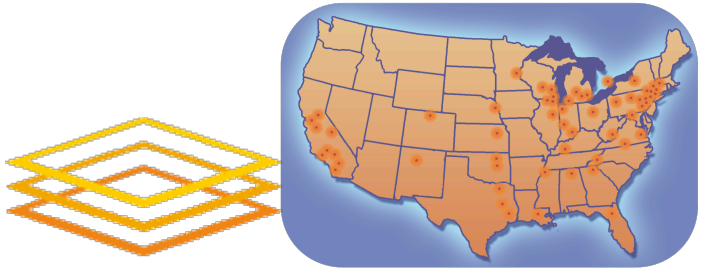
XSEDE (HPC)

- multiple, large HPC-style clusters
- proposal-based allocations

XSEDE
Extreme Science and Engineering Discovery Environment

Open Science Grid (HTC)

- extreme-scale HTC sharing
- **OSG Connect**: free for academic, govt., and non-profit researchers



Other HPC Clusters via Funding or Collaboration: U.S. DEPARTMENT OF ENERGY, NASA, DEPARTMENT OF DEFENSE

Commercial Cloud Providers

Computation

- run your own HPC or HTC (more frequently) system
- some ready-to-use tools (map-reduce, machine-learning, visualization, workflows, genomics, etc.)
- some free, proposal-based allocations via NIH, NSF, etc.

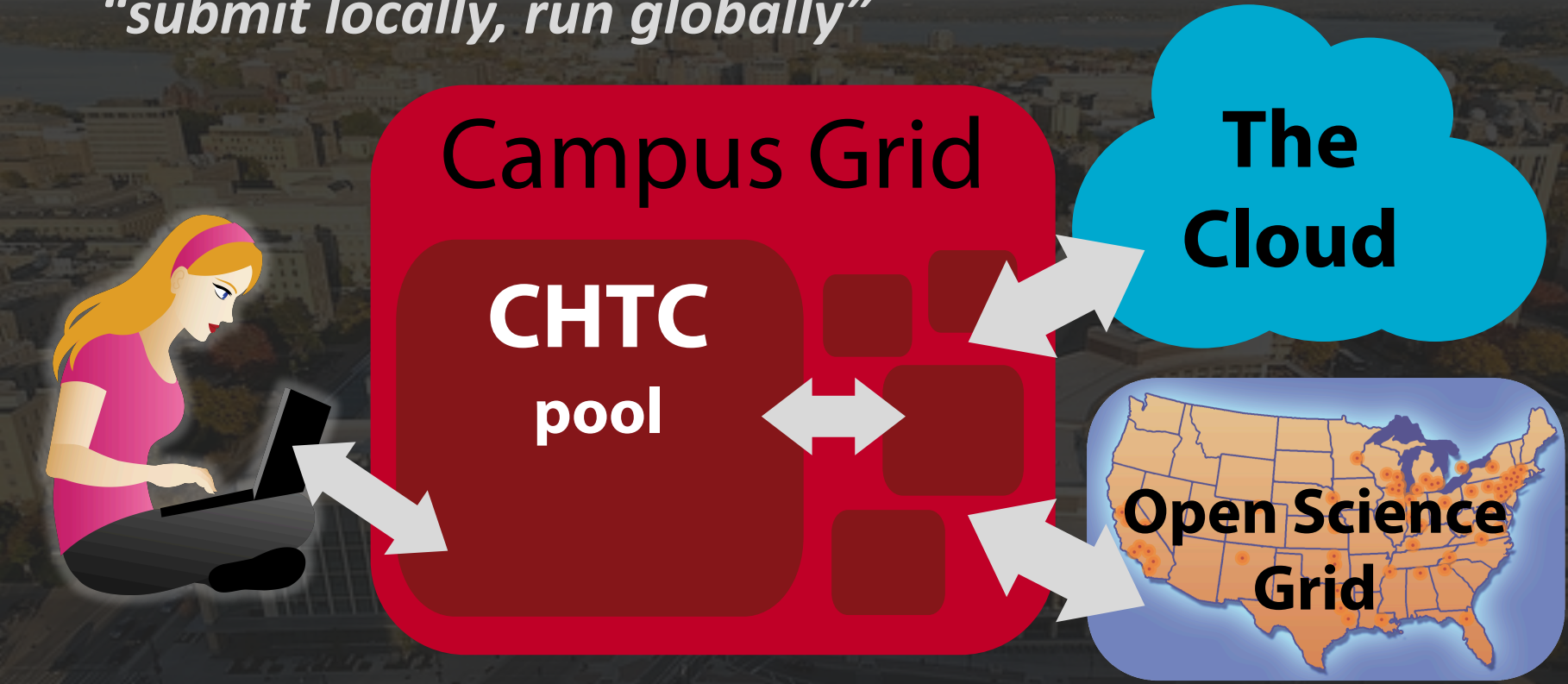
Data Management

- GoogleDrive, Box, databases, etc.
- Large-scale data transfer

ECAR-CCI Working Group. ***"Research Computing in the Cloud: Functional Considerations for Research,"*** *Research bulletin, ECAR, July 15, 2015*

Agile, Shared Compute Systems

"submit locally, run globally"



Science Gateways

Easy-to-use, Method-/Domain-Specific Computing

Scope of Computing Infrastructures

Accessibility and Scale

- **per research group, per institution, national, or commercial**
- free, by-proposal, or fee-based

Supported computing modes

- HTC- vs. HPC-optimized; availability of specialized hardware: GPUs, high-memory, etc.

Interface graphical/pipeline (specialized) or command-line (generalizable)

Human Support

- local vs. remote personnel; domain-specificity?
- learning materials

Research Computing Facilitators

accelerating research transformations

proactive engagement

personalized guidance

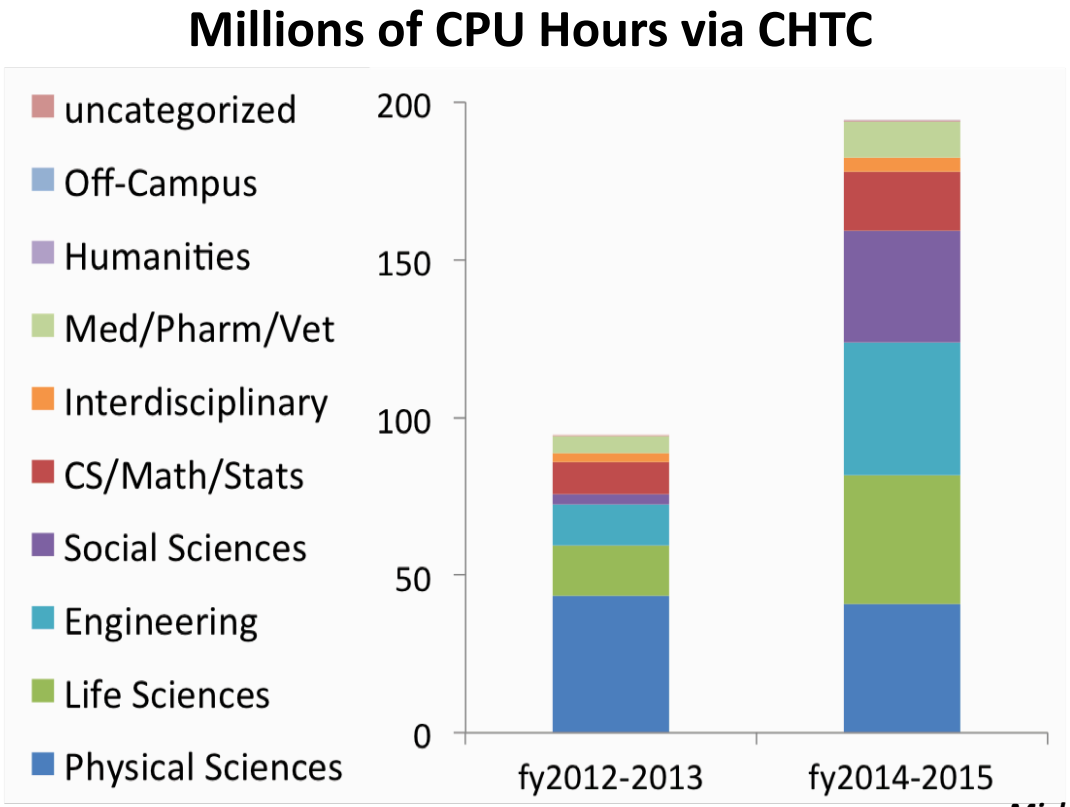
teach-to-fish training

technology agnostic

collaboration liaising

upward advocacy

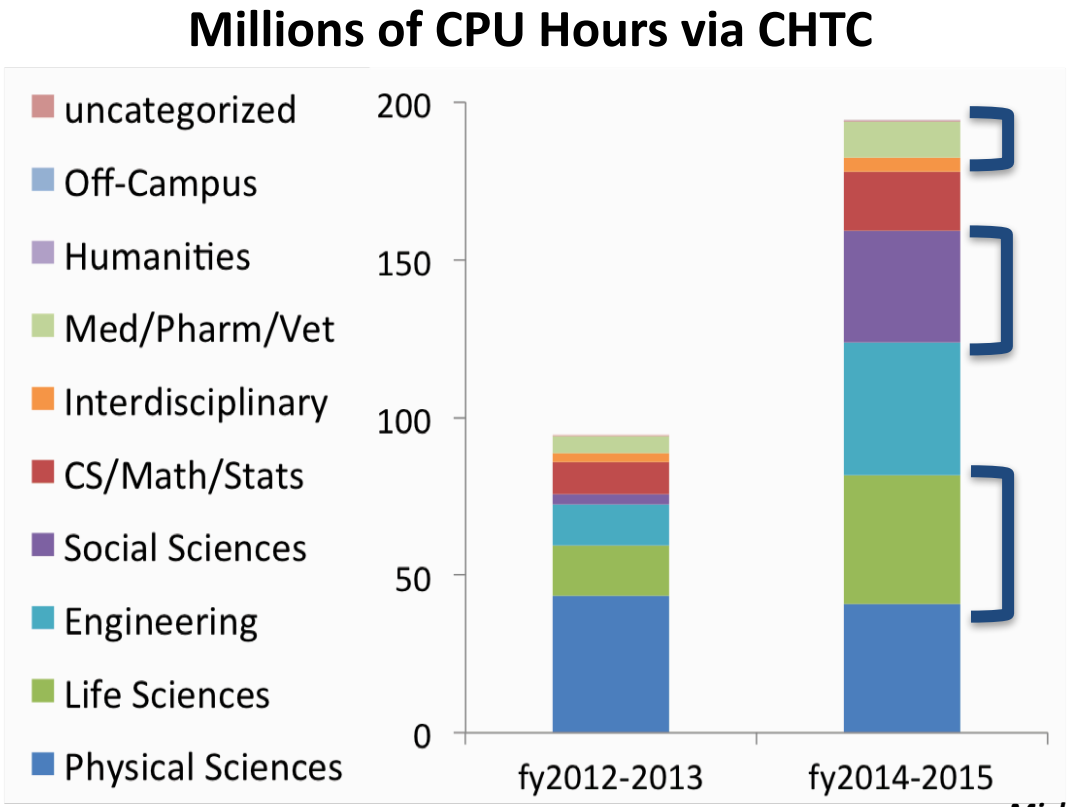
Impact Across Domains



Facilitators hired: Jan 2013, Nov 2014

Michael LA and Maas B. Research Bulletin. ECAR. May 16 2016.

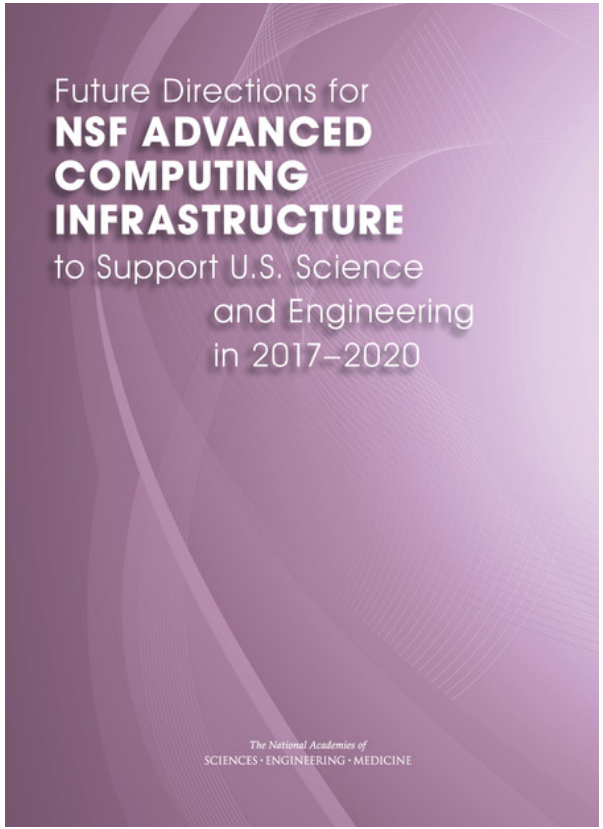
Impact Across Domains



>95% high *throughput* computing

Michael LA and Maas B. Research Bulletin. ECAR. May 16 2016.

Impact Across Domains



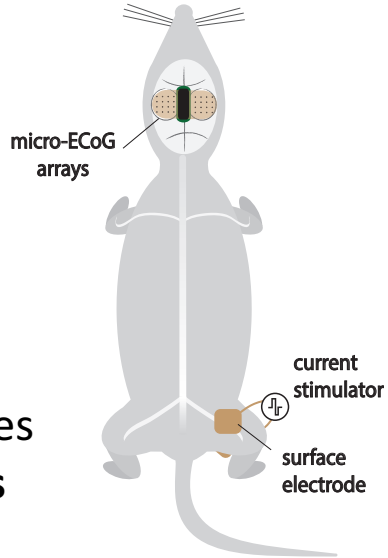
*"Increased advanced computing capability has historically enabled new science, and many fields today increasingly rely on **high-throughput computing** for discovery. Modeling and simulation, the historical focus of **high-performance computing**, is a well-established peer of theory and experiment. Data-driven research, a complementary "fourth paradigm" for scientific discovery, needs data-intensive computing capabilities and resources."* - p. S1 (Summary)

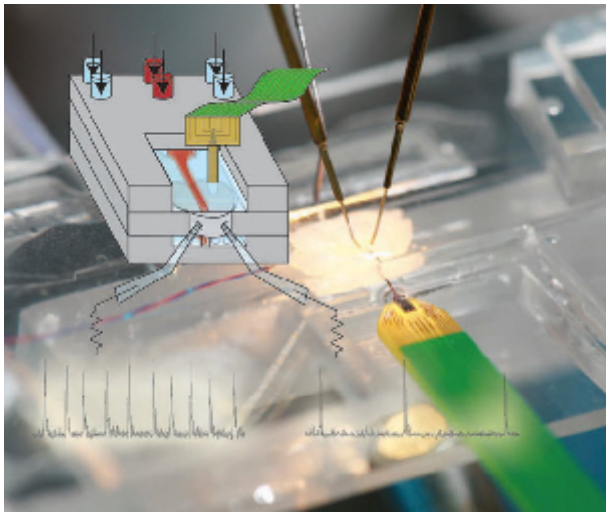
"For data-volume-driven workflows, scientific outcomes are best achieved when the advanced computing is configured for efficient, high-throughput processing, at scale …" - p. 5-3

Modeling Sensory Networks for the Design of Brain-Computer Interfaces

Surgically-implanted arrays record potentials from the sensory cortex for estimation of the neural connection between regions.

Ricardo Pizarro used a *Descriminatory Category Matching* (DCM) algorithm to calculate network likelihood and features for **10,000 independent parameter sets** across **hundreds of experiments**.





4.3 million HTC hours in one year, ~1 millennium

https://www.opensciencegrid.org/harnessing-the-osg-to-better-understand-the-brain/

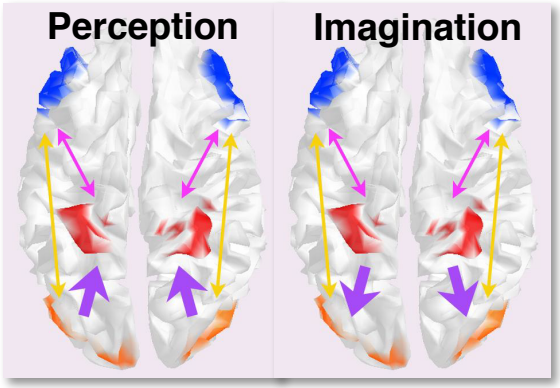
Elucidating Cognition Pathways

Expectation-maximization algorithm Barry Van Veen predicts neural connectivity from EEG data.

Used by numerous on-campus clinical projects examining:

- **short-term memory**
- **imagination vs perception**
- **sleep versus waking states**
- and others

EEG data collection



Brain Regions and Connectivity

Per subject, per condition, per time point:
***dozens trials* X *20,000* Monte Carlo iterations**

13 million CPU hours in one year, ~1.5 millennia

J.Y. Chang, *et al*, Front. Hum. Neurosci., vol. 6, no. 317, November 2012.
http://www.engr.wisc.edu/ece/faculty/vanveen_barry.html

See Also:

Saturday Symposium, 3pm:

Data-intensive brain imaging: The state of the art

also presenting insights from…

NeuroComp17 Workshop, Aug 2017

https://conferences.discovery.wisc.edu/neurocomp17/

What scalable computing modes and infrastructures are most important to major challenges in neuroscience?