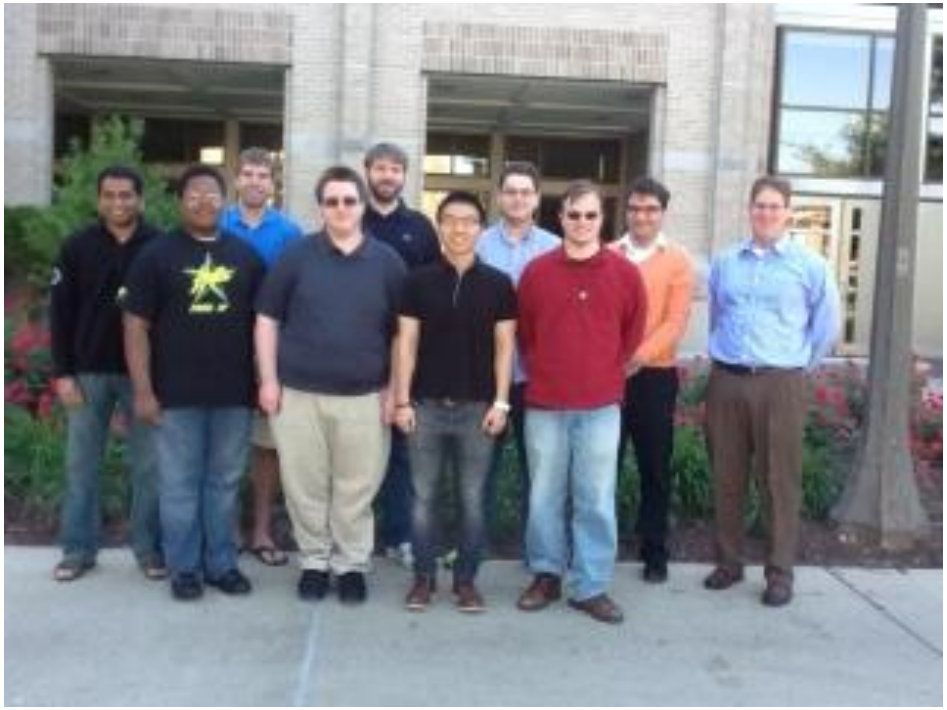
Welcome to Notre Dame!

CCL Workshop 2013

www.nd.edu/~ccl/workshop/2013

The Cooperative Computing Lab

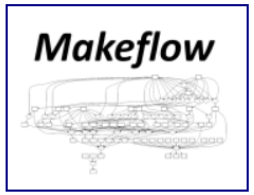
University of Notre Dame



http://www.nd.edu/~ccl

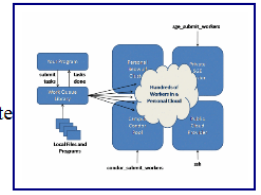
Makeflow

Makeflow is a workflow system for parallel and distributed computing that uses a language very similar to Make. Using Makeflow, you can write simple scripts that easily execute on hundreds or thousands of machines.



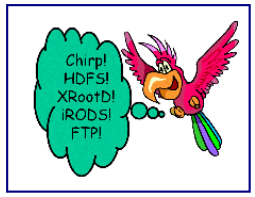
Work Queue

Work Queue is a system and library for creating and managing scalable master-worker style programs that scale up to thousands machines on clusters, clouds, and grids. Work Queue programs are easy to write in C, Python or Perl.



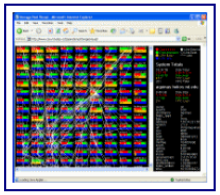
Parrot

Parrot is a transparent user-level virtual filesystem that allows any ordinary program to be attached to many different remote storage systems, including HDFS, iRODS, Chirp, and FTP.



Chirp

Chirp is a personal user-level distributed filesystem that allows unprivileged users to share space securely, efficiently, and conveniently. When combined with Parrot, Chirp allows users to create custom wide-area distributed filesystems.



Our goal:

Make it easy to scale up
real applications
from a single laptop
to national infrastructure,
enabling new discoveries.

The Cooperative Computing Lab

- We *collaborate with people* who have large scale computing problems in science, engineering, and other fields.
- We *operate computer systems* on the O(10,000) cores: clusters, clouds, grids.
- We *conduct computer science* research in the context of real people and problems.
- We *release open source software* for large scale distributed computing.

http://www.nd.edu/~ccl

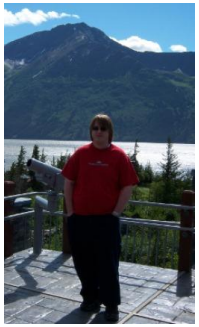
CCL Team Changes

Ben Tovar, Ph.D.
Principal Research
Software Engineer

Li Yu
Financial Software
Bloomberg

Principal
Hadoop Developer
AT&T Foundry

Dinesh Rajan



Patrick Donnelly

Peter Sempolinski

Casey Robinson

Peter Ivie

Haiyan Meng

Nick Hazekamp

Current Focus Areas

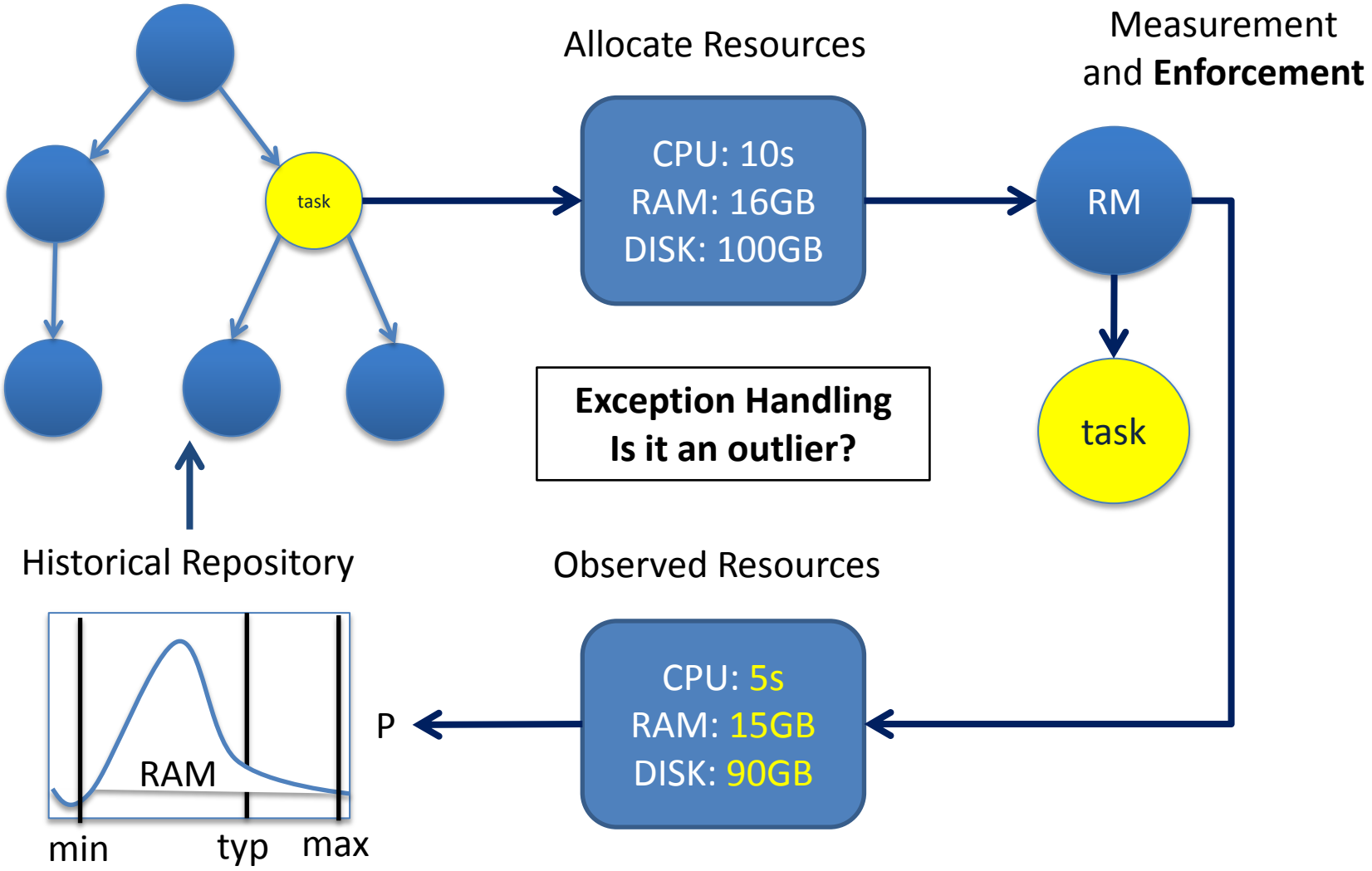
- Right Sizing Systems and Applications
  - I have this workload. How many machines (and what size) do I actually need to run it?
- Scaling Up without Blowing Up
  - 10M tasks on 10K workers?
- Data Intensive Applications
  - Move code to data and share across workers, across applications, across users….
- Evolving with Our Ecosystem:
  - Hadoop, Galaxy, GPUs, iRODS, OSG, XSEDE

dV/dt : **Accelerating the Rate of Progress Towards Extreme Scale Collaborative Science**

Miron Livny (UW), Ewa Deelman (USC/ISI), Douglas Thain (ND), Frank Wuerthwein (UCSD), Bill Allcock (ANL)

… make it easier for scientists to conduct large-scale computational tasks that use the power of computing resources they do not own to process data they did not collect with applications they did not develop …

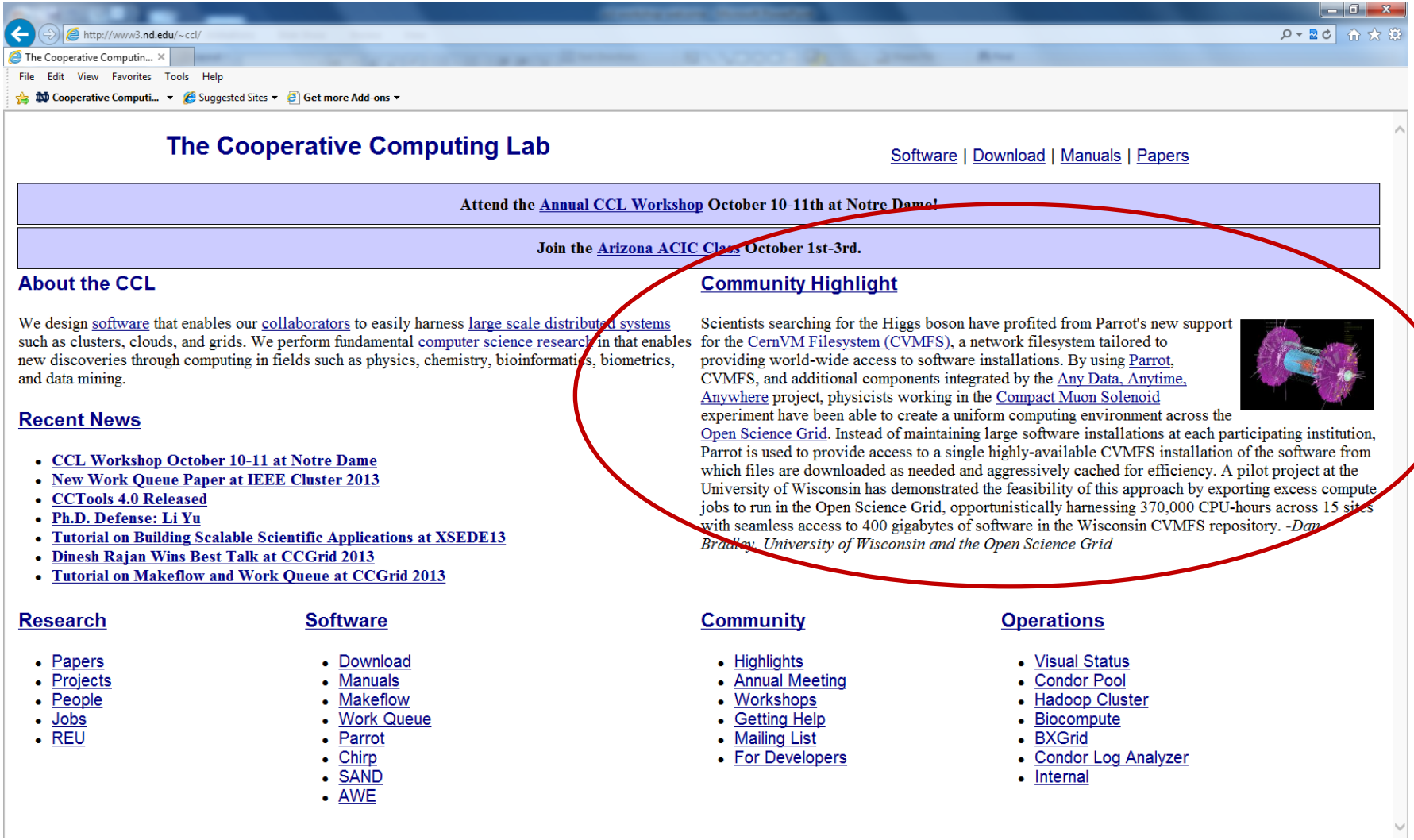
Resource Management Cycle



CCTools in Education

- UW – Eau Claire: IEEE Cluster 2013 Best Education Outreach and Training Paper:
  - Peter Bui, Travis Boettcher, Nicholas Jaeger, Jeffrey Westphal, “Using Clusters in Undergraduate Research”
- MF and WQ in University of Arizona Advanced Cyberinfrastructure Class (ACIC)
- WQ in Notre Dame Undergraduate Programming Paradigms Class

Your Highlight Here!



Agenda

- **9:00 Introduction**
  - Welcome and Introduction
  - What's new in the CCTools – CCL Team
- **10:15 Coffee Break**
  - Stash and Skeleton Key on the Open Science Grid, Rob Gardner, University of Chicago
  - Swift+Chirp for Synchrotron Beamline Data Analysis, Justin Wozniak, Argonne National Lab
  - Big Data and Data Science: The View from NIST, Geoffrey Fox, Indiana University
- **Noon - Lunch**
  - Scaling Up CMS Tier-3 Data Processing, Kevin Lannon
  - HotRAD: Harnessing distributed systems for population genetics sampling Scott Emrich
  - Data Management Challenges in the iPlant Collaboration, Nirav Merchant
  - Massively Parallel Molecular Dynamics Using Adaptive Weighted Ensemble, RJ Nowling
- **2:30 - Coffee Break**
  - Weather Data Processing with Makeflow and SLURM, Neil Best
  - Using Work Queue Inside and Outside the Classroom, Peter Bui
  - Systematic development of accurate model potentials using the Work Queue distributed computing environment, Lee-Ping Wang
  - Large Scale Image Processing for Biometrics, Joseph Thompson
- **4:00 Discussion and Adjourn**