Harnessing the Power of Distributed HTC

Miron Livny
John P. Morgridge Professor of Computer Science
UW Center for High Throughput Computing
Morgridge Institute for Research
Why am I here today?

Because we believe in the power of distributed HTC to advance scientific discovery and because we are eager to work with you on exploring the value distributed HTC can bring to your research and because we have the distributed HTC knowhow, technologies and services to translate this potential into impact on your research!
INVIDIA CEO keynote @ SC19

The Largest Cloud Simulation in History - 7% of Annual IceCube Simulation in Two Hours!

Saturday morning before SC19 we bought all GPU capacity that was for sale in Amazon Web Services, Microsoft Azure, and Google Cloud Platform worldwide.

Overview of the IceCube Cloud runs is at the Internet2 October 2021 event: “TechEXtra21: Running a 380PFLOP32s GPU burst for Multi-Messenger Astrophysics with IceCube”
https://internet2.edu/past-events/
80,000 jobs, 40 billion base pairs, and 20 bats — all in 4 weeks

An evolutionary biologist at the AMNH used HTC services provided by the OSG to unlock a genomic basis for convergent evolution in bats.

AMNH – American Museum of Natural History

opensciencegrid.org/news/2021/10/26/bat-genomics.html
PATH project - a Partnership launched by the NSF in 2020 between UW-Madison Center for High Throughput Computing (CHTC) and the OSG Consortium to advance Throughput Computing.

HTCondor Software Suite (HTCSS) manages High Throughput workloads across all forms of research computing resources from campus clusters to commercial clouds and HPC facilities.

OSG services enable science collaborations and campuses to build and operate private distributed high throughput computing environments across >300 sites.

Aligned with NSF CI Eco-system
NSF’s Vision for a National CI Ecosystem

Computational Ecosystem: Elements

- **Leadership Class Systems**
  - Frontera
  - LCCF Phase II (MREFC PDR)

- **Innovative Capacity Capabilities**
  - Expanse
  - Bridges II
  - Jetstream II
  - Delta
  - Anvil

- **Federated Resources**
  - OAKAMI
  - Neocortex
  - Voyager

- **PATH (OSG)**

**HT CENTER FOR HIGH THROUGHPUT COMPUTING**

**OSG**

**PATH PARTNERSHIP TO ADVANCE THROUGHPUT COMPUTING**
Proposals are required to commit to a minimum of 20% shared time on the cluster and describe their approach to making the cluster available as a shared resource external to the campus, with access and authorization according to local administrative policy. Conversely, the proposal should describe the approach to providing on-demand access to additional external computing resources for its targeted on-campus users and projects. One possible approach to implementing such a federated distributed computing solution is joining a multi-campus or national federated system such as the Open Science Grid. Whatever opportunistic, federated, scalable, distributed computing platform is
Following a summer of 2021 NSF investment, the PATh project is in the process of establishing a pool of dedicated computing (CPUs, GPUs and Storage) at five sites (ETA end of Q1 2022) that will support accounts of “PATH Credits” to be assigned to PIs by the NSF as part of an award.

- ~20K CPU cores (170M core hours annually)
- 44 A100 GPU
PROGRAM SOLICITATION
NSF 21-617

REPLACES DOCUMENT(S):
NSF 20-592

National Science Foundation
Directorate for Computer and Information Science and Engineering
Office of Advanced Cyberinfrastructure
Division of Computing and Communication Foundations
Division of Information and Intelligent Systems

High-Throughput Computing Resources

Proposals may request high-throughput computing (HTC) resources through the Partnership to Advance Throughput Computing (PATH) project supported by NSF.

Proposers should describe the request in a Supplementary Document no longer than two pages with a technical description of, and justification for, the requested HTC resources that includes (a) the expected number of self-contained tasks per ensemble – note that each task can be packaged into one or more batch job; (b) the resource requirements for each task type in the ensemble – for example, requirements for cores, memory, wall-time, and scratch space; (c) the expected number of ensembles; (d) the expected input and output data requirements for each task type; and (e) the expected number and size of shared input files within an ensemble – expected number of times each file is read per ensemble.
vision – Distributed High Throughput Computing and Research Computing Facilitation are powerful enablers of scientific discovery.

“... many fields today rely on high-throughput computing for discovery.”

Committee on Future Directions for NSF Advanced Computing Infrastructure to Support U.S. Science in 2017-2020; Computer Science and Telecommunications Board; Division on Engineering and Physical Sciences; National Academies of Sciences, Engineering, and Medicine.
OSG Statement of Purpose

OSG is a consortium dedicated to the advancement of open science via the practice of distributed High Throughput Computing (dHTC), and the advancement of its state of the art.
OSG Consortium

- Established in 2005, the OSG is a consortium governed by a council (IceCube and LIGO have a seat)
- Consortium Members (Stakeholder) include campuses, research collaborations, software providers and compute, storage, and networking providers
- The OSG provides a fabric of dHTC Services to the consortium members and to the broader Science and Engineering (S&E) community
- While members own and operate resources, the consortium does not own or operate any resources
- Council elects the OSG Executive Director who appoints an Executive team. Together they steer and manage available effort
Innovation and Services

The UW-Madison Center for High Throughput Computing (CHTC) was established in 2006 by the UW-Madison UAPC with a commitment to bring the power of High Throughput Computing (HTC) to all fields of research, and to allow the future of HTC to be shaped by insight from all fields of research

• Part of the recently formed Compute, Data and Information School (CDIS)
Technical Committee on Distributed Processing

2020 Outstanding Technical Achievement Award

Professor Miron Livny

For Influential Contributions of the Condor System to Distributed and High Throughput Computing
Claims for “benefits” provided by Distributed Processing Systems

P.H. Enslow “What is a Distributed Data Processing System?” IEEE Computer, January 1978

– High Availability and Reliability
– High System Performance
– Ease of Modular and Incremental Growth
– Automatic Load and Resource Sharing
– Good Response to Temporary Overloads
– Easy Expansion in Capacity and/or Function
Unity of Control

All the component of the system should be unified in their desire to achieve a common goal. This goal will determine the rules according to which each of these elements will be controlled.
Component autonomy

The components of the system, both the logical and physical, should be **autonomous** and are thus afforded the ability to refuse a request of service made by another element. However, in order to achieve the system’s goals they have to interact in a **cooperative** manner and thus adhere to a common set of policies. These policies should be carried out by the control schemes of each element.
In 1996 I introduced the distinction between High Performance Computing (HPC) and High Throughput Computing (HTC) in a seminar at the NASA Goddard Flight Center and a month later at the European Laboratory for Particle Physics (CERN).

In June of 1997 HPCWire published an interview on High Throughput Computing.

This month, NCSA's (National Center for Supercomputing Applications) Advanced Computing Group (ACG) will begin testing Condor, a software system developed at the University of Wisconsin that promises to expand computing capabilities through efficient capture of cycles on idle machines. The software, operating within an HTC (High Throughput Computing) rather than a traditional HPC (High Performance Computing) paradigm, organizes machines...
“I remember sitting on the couch with Miron Livny in my office when we made the decision to name this the National Technology Grid. The NSF-funded vBNS directly led to the formation of Internet2, which is now the dominant network connecting all the universities in the country,” said Smarr.
High Throughput Computing requires **automation** as it is a *24-7-365* activity that involves large numbers of jobs and distributed computing resources.

\[
\text{FLOPY} \neq (60 \times 60 \times 24 \times 7 \times 52) \times \text{FLOPS}
\]

\[
100\text{K Hours} \times 1 \text{ Job} \neq 1 \text{ H} \times 100\text{K J}
\]
Mechanisms hold the key

The most important lesson our HTC experience has taught us is that in order to deliver and sustain high throughput over long time intervals, a computing environment must build its resource management services on an integrated collection of robust, scalable and portable mechanisms. Robustness minimizes down time whereas scalability and portability increases the size of the resource pool the environment can draw upon to serve its customers. As will be argued

The Grid: Blueprint for a New Computing Infrastructure
Edited by Ian Foster and Carl Kesselman
OSG Fabric of Services

- Organized under three main thrusts – Community Building, Research Computing Facilitation, and Operation

- Designed and operated to assure, scalability, trustworthiness, reproducibility.

- OSG claims its services enabled in the past 12 month more than 2B core hours across clusters located at more than 300 sites and more than 200TB of data cached across 17 caches worldwide.
Who benefits from the OSG dHTC services?

- Organizations that want to build and operate a distributed HTC environment
- Organizations that want to share their resources with remote (external) researchers
- Researchers with High Throughput workloads access to local resources, remote resources, HPC allocations, or commercial cloud credit
PATH partitions the research computing eco-system into three main groups

• Campuses (researchers and Research Computing organizations)
• Multi institution research communities/collaborations/projects
• Large Hadron Collider (LHC) experiments
The Open Science Pool (OSPool)

An OSG service operated by PATH

- A means for campus/organization to make (following autonomous policies) capacity available to the US open science community
- A HTCondor pool that serves as a fair-share source of High Throughput Capacity (HTC) to researchers
- Integrated with the OS Data Federation
OSPool (typical) Weekly Numbers:

• move more than **100M** files to
• run more then **2M** jobs
• placed by more than **60** users
• from more than **40** projects
• at more than **10** Access Points
• on more than **40K** cores
• at more than **60** sites
• that consume more than **3M** core hours
OSPool is not the only pool!

Organizations like science collaborations (CMS, LIGO, IceCube) and campuses (UCSD, UNL, UW-Madison, JLab) leverage OSG services to deploy and operate private distributed HTCondor pools

- Deployment of Execution Points negotiated by the organization with sites
- Resource acquisition and allocation policies defined by the organization

* A site can contribute to several HTCondor pools
How do sites contribute to the OSPool?

When a site in the OS Compute Federation wants to contribute the capacity of one of its server to the OSPool, it runs an Execution Point on the server

- Site can start and stop the Execution Point at any time
- Execution Point needs to establish trust with HTCondor Pool
- OSG provides services to remotely activate Execution Points through a Compute EntryPoint (CE) that submits activation requests to the batch system of the cluster
- OSG provides services to automate remote activation of Execution Points
- Execution Point prefers to have out-going network connectivity
- Execution Point can Access the OS Data Federation
OpenStack Environment

The **Jetstream** cloud is an OpenStack, NSF-funded academic cloud operated by the Indiana University and TACC.

Operators decide when to start and terminate Virtual Machines (or containers) that run OSPool Execution Points.

750K core hours

Work with NSF funded **Chameleoon** is progressing nicely
k8s Cluster

The NSF funded Pacific Research Platform PRP operates a k8s cluster across more than 35 location worldwide. A PRP HTCondor pool grows and shrinks under the control of the k8S cluster pod scheduler. A CE submits requests to HTCondor to deploy Execution Points.

800K GPU hours

GPU Wall Hours by Project
Open Science Data Federation (OSDF)

An OSG service operated by PATH

- Provides a global file namespace for files stored and managed by autonomous Data Origins.
- Enables researchers to remotely access files placed in the namespace.
- Enables via a network of Data Caches effective, sustained remote access to files across large numbers of jobs.
OSG Data Federation

Data Origins from West to East:
- LIGO
- UNL x2
- CHTC
- FNAL
- U.Chicago x2
- JLab
- GlueX @ U.Connecticut
- Virgo

17 Caches … 6 of which are in R&E network backbone
10 Data Origins … one of which is for all open science
HTC Access Points (OSG-Connect)

An HTCSS Technology and OSG service provided and operated by PATh

• Manage High Throughput Computing workloads
• Can execute jobs on HTCondor pools
• Can delegate jobs to Batch Systems
• Supports Bring Your Own Resources (BYOR)
• Supports Workflow Management Systems
• Integrated with the Open Science Data Federation
• Can be dedicated to an organization
Deploy your Private Access Points

An HTCSS Technology and OSG service provided and operated by PATh

• Control the resources and policies of the AP
• Local Identity Management
• Interface to the OSPool and/or private HTCondor pools
• Support local/private Workflow Management Systems
• Integrated with the Open Science Data Federation
HTC Research Computing Facilitation

An OSG service provided and operated by PATh

- Work with single PI and large international research collaboration on maximizing the impact of the capabilities provided by Access Points on their science
- Work with campuses on maximizing the impact of the services provided by OSG on local research and education (includes CC* proposals)
- Continuous monitoring of how the services provided by OSG are utilized
- On going training via focused events and a weeklong summer school
Let’s work together!

- Understand your science and education computing needs
- Decide what CI is needed to address these needs
- Identify technologies and services PATH can provide
- Identify gaps in technologies and services that PATH can address
Each color is a different cloud region in US, EU, or Asia.

Total of 28 Regions in use.

Peaked at 51,500 GPUs

~380 Petaflops of fp32

Summary of stats at peak

<table>
<thead>
<tr>
<th></th>
<th>V100</th>
<th>P100</th>
<th>P40</th>
<th>P4</th>
<th>T4</th>
<th>M60</th>
<th>K80</th>
<th>K520</th>
</tr>
</thead>
<tbody>
<tr>
<td>GPUS</td>
<td>9.2k</td>
<td>7.2k</td>
<td>2.1k</td>
<td>0.5k</td>
<td>4.6k</td>
<td>10.1k</td>
<td>12.5k</td>
<td>5.4k</td>
</tr>
<tr>
<td>PFLOP32s</td>
<td>132.2</td>
<td>68.1</td>
<td>25.2</td>
<td>2.5</td>
<td>38.6</td>
<td>48.8</td>
<td>51.6</td>
<td>12.4</td>
</tr>
</tbody>
</table>

8 generations of NVIDIA GPUs used.
Archimedes of Syracuse was a Greek mathematician, philosopher, scientist and engineer.

Give me a place to run an Execution Point and I shall run your job.

Frank Würthwein is a Physics professor at UCSD and the Executive Director of the OSG.