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Employing a Software-Driven Approach to Scalable HPC System Management

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FRONTIER



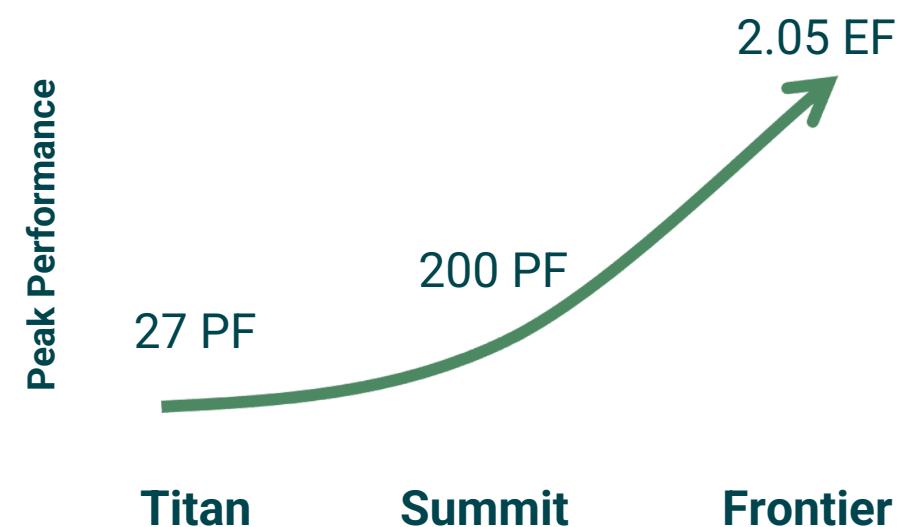
HPC System Management is Challenging

HPC Scale & Complexity

- Multi HPC system management
 - Over 30 allocatable HPE and non-HPE systems
- Thousands of users & research projects
- Massive resource allocations and enforcement
- Filesystem and permission management
- Identity and access management
 - Multi-system authentication (LDAP, OneID, XCAMS)

Operational Scale Challenges

- Manual processes don't scale & admin burden increases as systems and capabilities grow
- Our software supports the business of running HPC systems at our scale and complexity



System Management Progression

Line-by-Line Configuration

```
ilorest createuser "my_new_user" "password123" --role  
  Login,RemoteConsole  
useradd -m my_new_user  
passwd my_new_user  
groupadd user_group  
usermod -aG user_group my_new_user  
groupadd project123  
# Additional group commands here  
usermod -aG project007 my_new_user  
mkdir -p /gpfs/project123/my_new_user  
chown my_new_user:project123  
/gpfs/project123/my_new_user  
...
```

Abstracting with Bash Scripts

```
bash ./create_user.sh \  
  --username "my_new_user" \  
  --password "password123" \  
  --groups "user_group,project123,project007" \  
  --directories  
  "/gpfs/project123/my_new_user,/hpss/project007  
  /my_new_user" \  
  --with-filesystem \  
  --with-home-directory \  
  --with-directory-permissions
```

Problems with Manual System Configuration

1. Inconsistent Configuration Across Clusters

- Repeated manual setup across HPC systems is error-prone, time consuming, and leads to drift

2. Configuration Complexity

- UNIX users, UNIX groups, filesystems, sudo rules, and scheduler configurations (SLURM and LSF)

3. Slow Policy Enforcement

- Manual enforcement delays urgent changes such as ending compute allocations and user access

4. No Audit Trail

OLCF Solution

RATS CRM

- Handle operations of multiple large-scale HPC systems from a single application
- Authoritative source of truth that defines state of HPC systems via API endpoints



MyOLCF

- Reduce administrative burden through management and usage insight



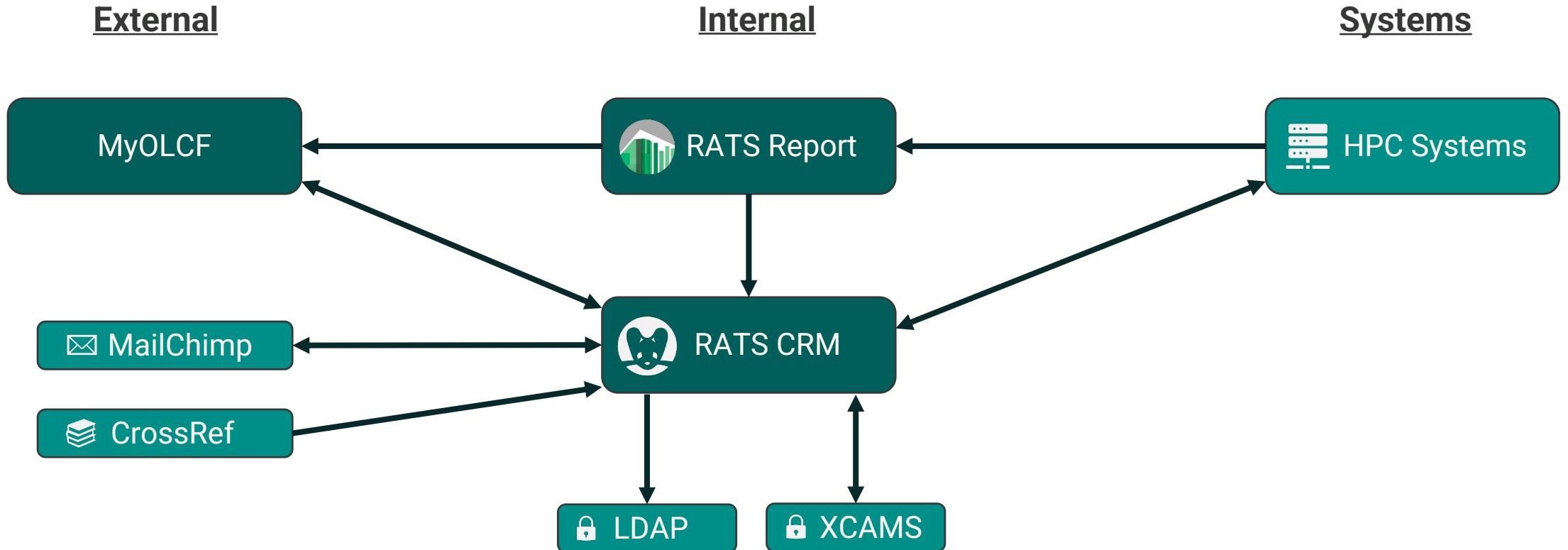
RATS Report

- Near real-time analytics & reporting of system compute & filesystem usage



* **RATS** stands for Resource Allocation Tracking System
* **CRM** stands for Customer Relationship Management

High-Level RATS CRM, MyOLCF, and HPC Integration



Arrows denote information flow direction

System Architecture Overview

RATS CRM

1. Built With

- Ruby (Rails framework)
- MariaDB

2. DevOps & Deployment

- GitLab Runners (CI/CD)
- Kustomize for declarative infrastructure

3. History

- Created in 2012
- Replaced legacy C++ and Bash scripts

RATS Report

1. Built With

- Ruby (Rails framework)
- MariaDB

2. DevOps & Deployment

- GitLab Runners (CI/CD)
- Kustomize for declarative infrastructure

3. History

- Created in 2015

MyOLCF

1. Built With

- JavaScript
- Vue framework

2. DevOps & Deployment

- GitLab Runners (CI/CD)
- Kustomize for declarative infrastructure

3. History

- Created in 2020

RATS CRM: Centralizing HPC Operations Management

1. Core HPC Management

- Job scheduler configurations
- Filesystem directories
- Node and core allocations
- Identity & security access
- User and system access
- Enforces & automates governance policies

2. Data Dissemination

- 224 API endpoints used by HPC systems and services

The screenshot displays the RATS CRM application interface. At the top, a navigation bar includes the RATS CRM logo, Home, Project Applications, User Applications, Projects, UNIX Users, Host Accesses, Employers, All, My RATS Account, Help, and Logout. The main content area features a 'Welcome to RATS CRM' message with a house icon. Below this are four main sections: 'Check UNIX User Status' (showing 'jameson' as the user, 'sydh' as the user, 'Full Name: Ms. Sydny Herman', 'User Status: ✘ Disabled', and 'Active Accesses:'), 'Upcoming Downtimes' (listing two entries: '19317 ace 2025-04-18 12:08:00 -0400 48.00' and '19318 frontier 2025-04-18 12:08:00 -0400 48.00'), 'My Public Staff Profile' (showing 'Last Updated: Never' and a 'View My Public Staff Profile' link), and 'My RATS Account' (showing 'RATS Username: allmon', 'Name: aroswift (Mr. Aaron Barlow)', 'Email: 14220@fake.ccs.ornl.gov', 'RATS Roles: 6', and 'RATS API Keys: 0').

RATS CRM: first look with anonymized data

RATS CRM: Project-Centric Approach

1. Simplifies management
2. Definitive configuration source
3. Enables life-cycle automation

 RATS CRM Home Project Applications User Applications Projects UNIX Users Host Accesses Employers All ▾

Projects

 TST001  OLCF  Moderate  OLCF Director's Discretionary Program

 General  Subprojects  Project Applications  Mirrors  Status  Host Accesses  Resources  Allocations  Fundings  Points of Contact  IP Allow Lists  Quantum Backends  Custom Fields  UNIX Users  Scheduler Configurations  Automation Users  Sudo Rules  UNIX Groups  Directories  Primary / Default Filesystems Auto Email Settings

Science Project

 TST001  Enabled until Apr 22, 2025  Part of the OLCF organization  Part of the Moderate security enclave  (Not tagged)  (No staff comments)

Principal Investigator

 Dr. Gali Keplier  23312_person@fake.com  Has (2) UNIX Users in  Currently a Postdoctoral

Classifications

Research Area: Astrophysics  Export Control Classification

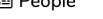
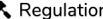
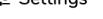
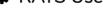
Science Category: Physics  Export Control Classification

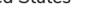
Allocation Programs

Allocation Program (Current): OLCF DIRECTOR'S DISCRETIONARY PROGRAM

Allocation Programs/Cycles (All): DD 2023

History

OLCF APPLICATIONS  AUDITING  Project Applications  Allocations  User Applications  Downtimes  Employers  Funders  People  Sent Mail  RATS Logs  Regulations  Tags  Video Conferences  Office Hours  Streams  PUBLIC WEB PROFILES  Settings  RATS Users  RATS Roles  Emails

United States 

 LEADERSHIP COMPUTING FACILITY

RATS CRM: From Proposal to Access

1. Proposal Submission

- Researcher submits proposal via MyOLCF

2. Review & Approval

- Admin reviews and applies policy

3. Automated Setup

1. Project-level setup

- Scheduler configuration & filesystem creation
- Sub-projects enable delegation and subdivision

2. User-level setup

- UNIX user & group creation, filesystem creation, identity access sync, myOLCF access
- Cascaded resource & filesystem access

NFS Home Areas

ID	Path	Policy/Template	Owner/UID	Group/GID	User	Project	Permissions	Quota	State
65665	/fake/directory/path	OLCF Moderate Project Home (nccs_mod_filer_proj) project home area	root / 0	gen110 / 27121	--	GEN110	0770	50 🖊	✓ RECONCILED

GPFS Filesystems

ID	Path	Policy/Template	Owner/UID	Group/GID	User	Project	Permissions	Quota	State
54190	/gpfs/alpine2/gen110	Alpine2	root / 0	gen110 / 27121	--	GEN110	2755	0 🚧	PENDING
54191	/gpfs/alpine2/gen110/scratch	Alpine2	root / 0	gen110 / 27121	--	GEN110	2750	0 🚧	PENDING
54193	/gpfs/alpine2/gen110/proj-shared symlink: /gpfs/alpine2/project-shared/gen110	Alpine2	root / 0	gen110 / 27121	--	GEN110	2770	0 🚧	PENDING
54194	/gpfs/alpine2/gen110/world-shared symlink: /gpfs/alpine2/world-shared/gen110	Alpine2	root / 0	gen110 / 27121	--	GEN110	2775	0 🚧	PENDING

RATS CRM: A Closer Look at Scheduler Configurations

1. Centralized policy control for each HPC system:

- Queues / partitions
- Job size limits & default wall times
- QOS policies

2. Defined once, applied everywhere:

- System-wide defaults
- Project and user specific overrides
- Supports cascading rules by project, group, or user

3. Simplifies multi-scheduler environments:

- Abstracts SLURM, LSF, KUBE, MOAB config differences

Defaults

ID	Context	Granularity	Target	Perpetual?	Precedence
1915	Resource: Summit	Per User	User: All Users	✓ Yes	50 / 100
310	Resource: Summit	Per Project	Project: All Projects	✓ Yes	0 / 100
311	Resource: Summit	Per User	User: All Users	✓ Yes	0 / 100

Overallocation Auto-Penalties

Showing 1 to 10 of 303 entries

ID	Context	Granularity	Target	Perpetual?	Precedence
2048	Resource: Summit	Per Project	Project: TST001	✓ Yes	75 / 100
5632	Resource: Summit	Per Project	Project: TST002	✓ Yes	75 / 100
2052	Resource: Summit	Per Project	Project: TST003RSCH	✓ Yes	75 / 100
5380	Resource: Summit	Per Project	Project: TST004	✓ Yes	75 / 100

RATS CRM: HPC scheduler configurations with anonymized data

RATS CRM: A Closer Look at Scheduler Configurations Cont.

RATS CRM: Individual Scheduler Configuration

SLURM Scheduler Configuration '1077' on Dtn

Basics	
ID:	1077
Config Type:	default
Context:	Resource: Dtn
Granularity:	per_project
Target:	<input checked="" type="checkbox"/> Project: All Projects
Precedence:	50 / 100
Status:	✓ Enabled
Valid From:	2019-09-10 16:10:00 -0400
Valid Until:	
Description:	

Constraints		
Name	Value	Description
minsize	1	Minimum jobsize constraint for this configuration
maxsize		
maxsize	4	Maximum jobsize constraint for this configuration

Priorities & Limits		
Name	Value	Description
Priority	0	Scheduling priority for eligible batch jobs per this scheduler scope.
MaxWallDurationPerJob	24	Maximum allowable walltime hours for running batch jobs per this scheduler scope.

Equivalent Scheduler Configuration via API

```
"config_type": "default",
"resource": "dtn",
"source_id": 1077,
"description": "",
"precedence": 50,
"primary_scope": {
  "id": 52,
  "type": "Resource",
  "name": "Dtn"
},
"secondary_scope": {
  "id": 9,
  "type": "SchedulerCredential",
  "name": "All Projects"
},
"granularity": "per_project",
"constraints": [
  {
    "type": "minsize",
    "value": 1
  }
]
```

Managing HPC Systems via API: Scheduler Configurations

Retrieving Scheduler Configuration Data

Request

```
GET /api/scheduler_configurations
```

Response

```
[{ ...,
  "attributes": {
    "config_type": "default",
    "resource": "frontier",
    "precedence": 50,
    "primary_scope": { ... },
    ...
  },
  ...
}]
```

HPC Systems Enforcement

```
# Assume API response parsing above
for entry in "${config_lines[@]}"; do
  read -r part min_n max_n wall_h <<< "$entry"
  for host in "${SLURM_HOSTS[@]}"; do
    ssh admin@"$host" "sacctmgr --immediate update
      partition name=$part \
      set MinNodes=$min_n MaxNodes=$max_n \
      MaxWall=${wall_h}:00:00 \
      || sacctmgr --immediate add partition name=$part \
      default=NO target=ALL MinNodes=$min_n \
      MaxNodes=$max_n MaxWall=${wall_h}:00:00"
  ...
}
```

Managing HPC Systems via API: UNIX Groups

Retrieving UNIX Group Data

Request

```
GET /api/groups?filter[system]=frontier
```

Response

```
[  
  "data": {  
    "type": "groups",  
    "id": 1,  
    "attributes": {  
      "name": "testgroup",  
      "gid": 10000,  
      "organization": "olcf",  
      "security_enclave": "moderate"  
    }, ...  
  }]
```

HPC Systems Enforcement

```
#!/bin/bash  
# Triggered via cronjob every 30 minutes:  
# */30 * * * * /opt/scripts/group_enforcement.sh  
  
groups_json=$(curl -s -H "Authorization: Bearer  
$API_TOKEN" "$BASE_URL")  
  
echo "$groups_json" | jq -r '.[] | .data.attributes | "\(.name)  
\(.gid)"'  
  
while read -r group gid; do  
  for system in "${HPE_SYSTEMS[@]}"; do  
    ssh admin@"$system" "sudo groupadd -g $gid $group"  
  done  
done
```

RATS Report: HPC Analytics & Reporting

- **Key capabilities:**

1. Extracts, transforms, and loads (ETL) HPC data
2. Monitoring of compute resource consumption
3. Allocation burn-down analysis
4. Custom queries for job and storage analytics
5. Aid in auditing

- 4 API endpoints with filtering to disseminate information

The screenshot shows the RATS Report homepage with a navigation bar at the top. The navigation bar includes icons for RATS REPORT, Compute Usage, Filesystems, and Job Search, along with links for Resources, Resources/Programs, Resources/Users, Programs, Programs/Projects, Projects, Project Groups, Science, Allocations, and Custom Query. On the right side of the navigation bar are links for Help and a user profile (aroswift).

The main content area is divided into four sections:

- By Resource**: Explore utilization and availability stats per resource including Summit, Titan, Eos, Rhea, Cumulus, and others.
 - Resources - Overall Utilization and Availability
 - Resources/Programs - Usage Breakdown by Program
 - Resources/Users - Usage Breakdown by Project and User
- By Program**: Compare burn rates and usage breakdowns for all allocation programs including INCITE, ALCC, DD, ECP, and Early Science.
 - Programs - Burn Rates
 - Programs/Projects - Usage Breakdown by Project
- By Project**: Search for project allocations by name, PI, year, etc. and see burn rates and daily usage.
 - Projects - Burn Rates and Daily Usage
 - Project Groups - Usage and Utilization across Resources and Allocations
- Custom Queries**: Get GPU usage and capability stats for any combination of user, project, program, cycle, and resource.
 - Custom Query

MyOLCF: Public Self-Service Application

- Publicly available application that extends management capabilities and provides insights into available resources for users
 - my.olcf.ornl.gov
- Some key features:
 - Apply for and renew projects and accounts on HPC systems
 - Check the status of their applications
 - Monitor their submitted issues
 - Allocation usage monitoring
 - Compute usage report generation
 - Schedule office hours for help

The screenshot shows the MyOLCF GUI interface. At the top, there is a header with the Oak Ridge National Laboratory logo and the text "LEADERSHIP COMPUTING FACILITY" and "myOLCF". On the right side of the header, there are "MY PROJECTS" and "MODERATE ACCOUNT" buttons. A user profile for "aswift" is shown, including an email address "avery@fake.ccs.ornl.gov". The main content area is divided into sections: "Project Profile" for "TST001: 'Science Project'", "General" (Project ID: TST001, Name: Science Project, Organization: OLCF - Oak Ridge Leadership Computing Facility, Security Enclave: Moderate, Research Summary: --), "Points of Contact" (Account manager: Sarah Swift, Principal Investigator: Aaron Barlow), and a sidebar with links for "MY PROFILE", "FOR MY APPROVAL", "MY ACCOUNT APPLICATIONS", "NEW PROJECT APPLICATION", "JOIN ANOTHER PROJECT", "TICKETS", "FAQ", and "LOG OUT". At the bottom, there are logos for the U.S. Department of Energy, Office of Science, Oak Ridge National Laboratory, and Oak Ridge Leadership Computing Facility, along with a "LIKE US ON FACEBOOK" button.

OLCF Acknowledgement

This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

An aerial photograph of the Oak Ridge National Laboratory (ORNL) complex. The facility is a large cluster of buildings with red brick and white trim, surrounded by green lawns and trees. In the background, a range of green mountains is visible under a bright blue sky with scattered white clouds. The text "Questions?" is overlaid in the upper portion of the image.

Questions?
