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Integrated Rule-Oriented Data System (iRODS) and High Performance Computing (HPC) Architecture Design

Kevin D. Winters, Mark A. Cowan, Glover E. George, Megan E. Gonzalez, Brian Priest, Omar Morris, and Jonathan Landrum

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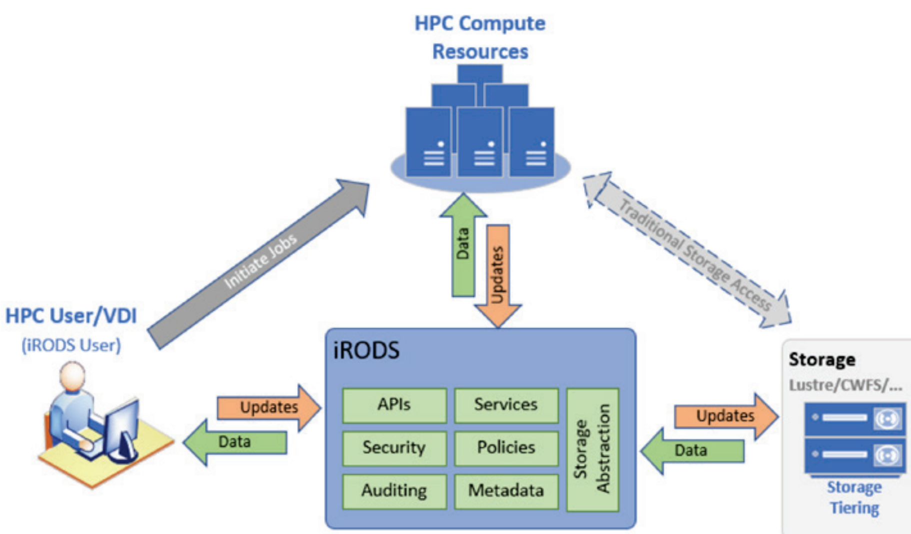

Integrated Rule-Oriented Data System (iRODS) and High Performance Computing (HPC) Architecture Design

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Abstract

The Integrated Rule-Oriented Data System (iRODS) proof-of-concept will be deployed within the existing U.S. Army Engineer Research and Development Center (ERDC) Department of Defense Supercomputing Resource Center (DSRC) to test additional capabilities and features for high performance computing (HPC) users. iRODS is a data-grid middleware that virtualizes access to data, regardless of which physical storage device the data resides within. Users, and HPC jobs on behalf of users, can leverage the various application programming interfaces (APIs) within iRODS to search and retrieve data using metadata and a unified data namespace. In addition to facilitating data discovery and retrieval, iRODS has a robust security system to implement fine-grained access control and auditing rules.

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Preface

This is a deliverable product under the Engineered Resilient Systems (ERS) Program, Data Analytics Work Package, Collaborative Tradespace Analytics Work Unit 92L5D8. Dr. Owen J. Eslinger was the Program Manager, and Dr. Robert M. Wallace was the Technical Director of the ERS program.

The work was performed by the Computational Analysis Branch (CAB) of the Computational Science and Engineering Division (CSED), U.S. Army Engineer Research and Development Center (ERDC), Information Technology Laboratory (ITL), Vicksburg, MS. At the time of publication, Dr. Jeffrey L. Hensley was Chief, CAB; Dr. Jerrell R. Ballard, Jr. was the Chief, CSED; Ms. Patti S. Duett was the Deputy Director of ITL and the Director was Dr. David A. Horner.

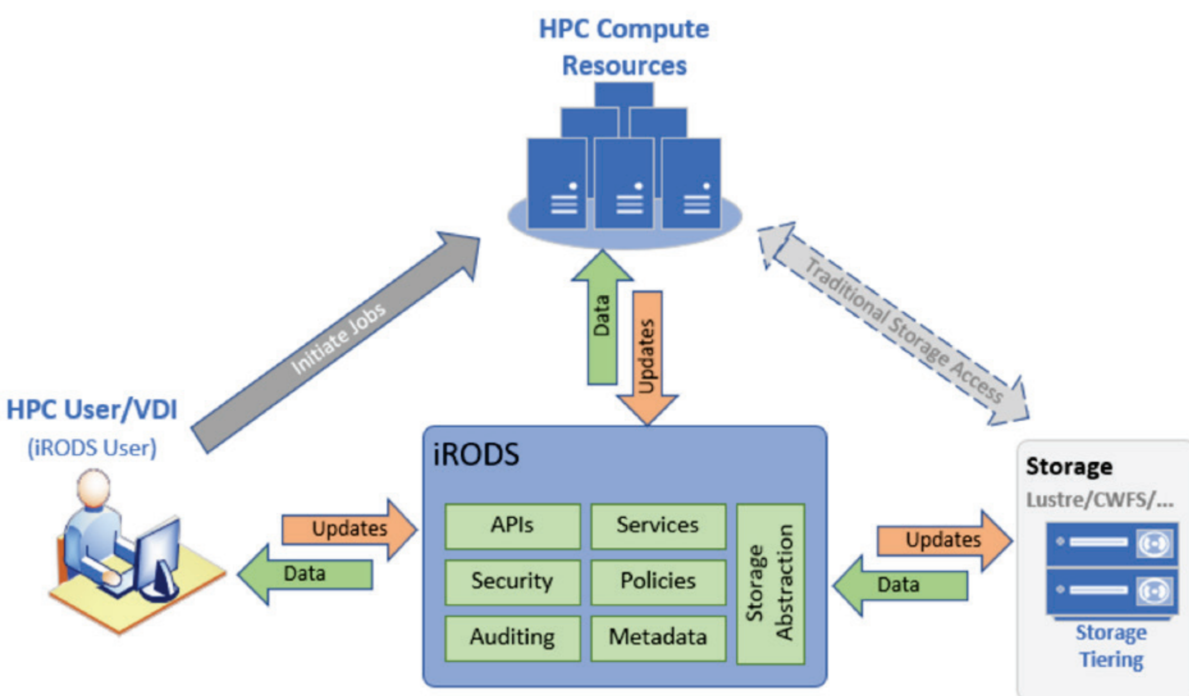
COL Teresa A. Schlosser was the Commander of ERDC, and Dr. David W. Pittman was the Director.

1 Introduction

1.1 Background

The Integrated Rule-Oriented Data System (iRODS) proof-of-concept will be deployed within the existing U.S. Army Engineer Research and Development Center (ERDC) Department of Defense Supercomputing Resource Center (DSRC) to test additional capabilities and features for high performance computing (HPC) users. iRODS (as seen in Figure 1-1) is a data-grid middleware that virtualizes access to data, regardless of which physical storage device the data resides within. Users, and HPC jobs on behalf of users, can leverage the various application programming interfaces (APIs) within iRODS to search and retrieve data using metadata and a unified data namespace. In addition to facilitating data discovery and retrieval, iRODS has a robust security system to implement fine-grained access control and auditing rules.

Figure 1-1. iRODS proof-of-concept conceptual diagram.



1.2 Objectives and approach

This report will outline the architectural design for the implementation of iRODS within the HPC system. To do this, the technical details of the operating environment, the iRODS architecture, the associated hardware, software, and the servers required will be outlined.

1.3 Project scope

The architecture design presented within this report is the result of the research phase conducted for the ERDC iRODS project with requirements input from multiple Engineered Resilient Systems (ERS) teams. Specifically, the Data Analytics Team, the Environmental Simulation Team, the Sensor Systems Research Team, and the HPC/Scientific computing group, representing the “general HPC user,” all contributed use cases and requirements that lead to the proposed architecture design for the iRODS proof-of-concept phase.

2 Proposed iRODS Architecture

2.1 Operating environment

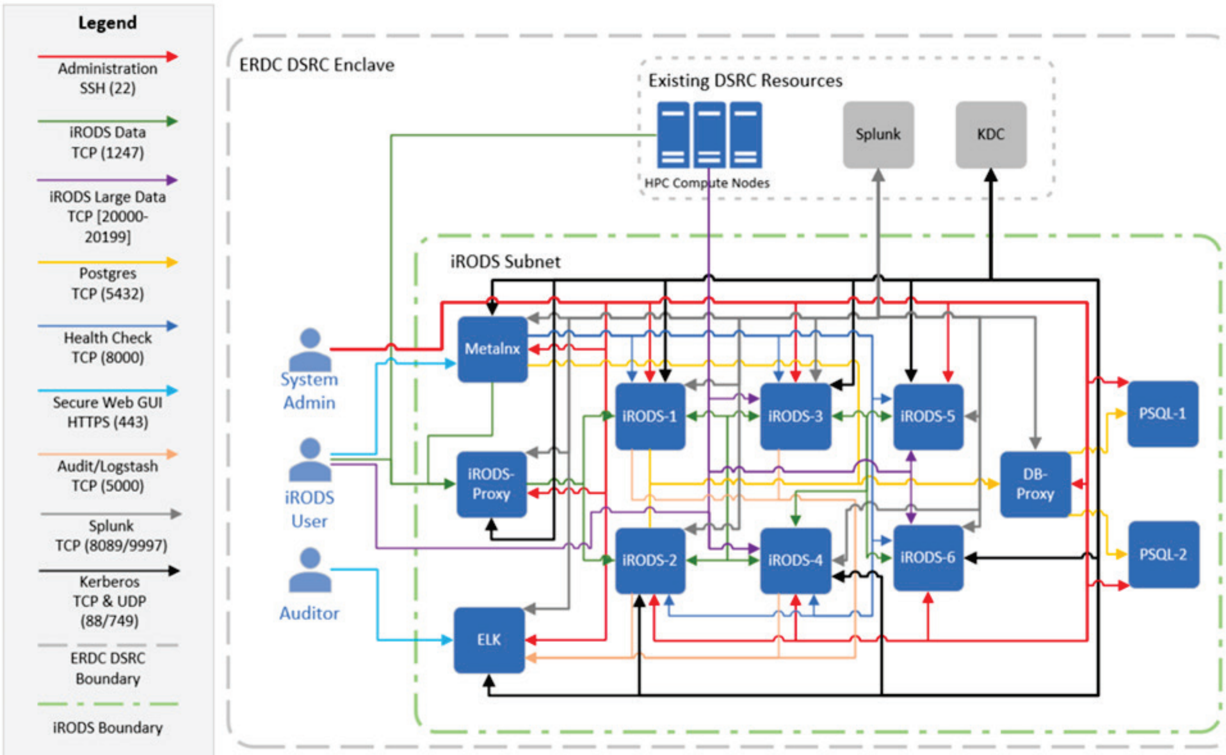
Initially, the iRODS prototype will be built and configured within a test network to ensure all software is configured correctly, applicable security technical implementation guides (STIGs) are applied, and functional testing of available components is complete. During this testing phase, iRODS-5 and iRODS-6, which leverage storage from ONYX Lustre and the center-wide file system (CWFS), respectively, will not be tested. Once the security assessment is complete, the iRODS prototype will be moved to production and testing of iRODS-5 and iRODS-6. Figure 2-1 shows the production architecture diagram of the iRODS prototype.

2.2 iRODS architecture

The individual host components (i.e., virtual machines) for iRODS and the required ports and protocols within and across the iRODS test subnet (i.e., iRODS boundary) are shown in Figure 2-1.

Network access control lists (ACLs) will be implemented so communication across the iRODS test subnet is strictly controlled and within the bounds of the testing required for the iRODS proof-of-concept test event. Users, and HPC resources running jobs (e.g., scripts to retrieve data), will be able to query and retrieve data from iRODS, however, iRODS components will not be able to initiate communication outside of the iRODS test subnet.

Figure 2-1. iRODS prototype architecture diagram.



2.3 Hardware

The identified hosts and specifications for the iRODS virtual machine prototype are listed in Table 2-1.

Table 2-1. iRODS prototype hosts.

Server Name	Server Role	CPUs	RAM	Disk Storage
iRODS-Proxy	Load Balancer	16	16 GB	50 GB
iRODS-1	iCAT Server	8	8 GB	50 GB
iRODS-2	iCAT Server	8	8 GB	50 GB
iRODS-3	Resource Server	16	16 GB	50 TB
iRODS-4	Resource Server	16	16 GB	50 TB
iRODS-5	Resource Server	16	16 GB	500 TB*
iRODS-6	Resource Server	16	16 GB	500 TB**
ELK	Elastic Stack	16	32 GB	500 GB
Metalnx	iRODS GUI	8	8 GB	50 GB
DB-Proxy	DB Load Balancer	32	16 GB	50 GB
PSQL-1	Database Server	32	128 GB	500 GB
PSQL-2	Database Server	32	128 GB	500 GB

* iRODS-5 storage must be provided by ONYX Lustre filesystem (i.e., iRODS vault on ONYX).

** iRODS-6 storage must be provided by CWFS (i.e., iRODS vault on CWFS).

2.4 Software

The software and version for each identified host for the iRODS prototype is listed in Table 2-2.

Table 2-2. System software per host.

Server Name	Software	Version
PSQL-1	RHEL	7
	PostgreSQL	10.3
	Splunk Universal Forwarder	7.2.3
	HPCMP Kerberos Kit	Latest Version
PSQL-2	RHEL	7
	PostgreSQL	10.3
	Splunk Universal Forwarder	7.2.3
	HPCMP Kerberos Kit	Latest Version
iRODS-1	RHEL	7
	iRODS	4.2.4
	irods-rule-engine-plugin-audit-amqp	4.2.4
	irods-externals-qpid-with-proton0.34	4.2.4
	Python	3.7.2
	python-irodsclient	4.2.4
	irods-rule-engine-plugin-python	4.2.4
	irods-database-plugin-postgres	4.2.4
	irods-rule-engine-plugin-storage-tiering	4.2.4
	Metalnx Remote Monitor Daemon	2.0-0
	Splunk Universal Forwarder	7.2.3
	HPCMP Kerberos Kit	Latest Version
iRODS-2	RHEL	7
	iRODS	4.2.4
	irods-rule-engine-plugin-audit-amqp	4.24
	irods-externals-qpid-with-proton0.34	4.2.4
	Python	3.7.2
	python-irodsclient	4.2.4
	irods-rule-engine-plugin-python	4.2.4
	irods-database-plugin-postgres	4.2.4
	irods-rule-engine-plugin-storage-tiering	4.2.4
	Metalnx Remote Monitor Daemon	2.0-0
	Splunk Universal Forwarder	7.2.3
	HPCMP Kerberos Kit	Latest Version

Server Name	Software	Version
iRODS-3	RHEL	7
	iRODS	4.2.4
	irods-rule-engine-plugin-audit-amqp	4.2.4
	Python	3.7.2
	python-irodsclient	4.2.4
	irods-rule-engine-plugin-python	4.2.4
	irods-database-plugin-postgres	4.2.4
	irods-rule-engine-plugin-storage-tiering	4.2.4
	Metalnx Remote Monitor Daemon	2.0-0
	Redis	5.0.3
	Pip	8.1.1
	irods-capability-automated-ingest	0.3.4
	Splunk Universal Forwarder	7.2.3
	HPCMP Kerberos Kit	Latest Version
iRODS-4	RHEL	7
	iRODS	4.2.4
	irods-rule-engine-plugin-audit-amqp	4.2.4
	Python	3.7.2
	python-irodsclient	4.2.4
	irods-rule-engine-plugin-python	4.2.4
	irods-database-plugin-postgres	4.2.4
	irods-rule-engine-plugin-storage-tiering	4.2.4
	Metalnx Remote Monitor Daemon	2.0-0
	Redis	5.0.3
	Pip	8.1.1
	irods-capability-automated-ingest	0.3.4
	Splunk Universal Forwarder	7.2.3
	HPCMP Kerberos Kit	Latest Version
iRODS-5	RHEL	7
	iRODS	4.2.4
	irods-rule-engine-plugin-audit-amqp	4.2.4
	Python	3.7.2
	python-irodsclient	4.2.4
	irods-rule-engine-plugin-python	4.2.4
	irods-database-plugin-postgres	4.2.4
	irods-rule-engine-plugin-storage-tiering	4.2.4
	Metalnx Remote Monitor Daemon	2.0-0
	Redis	5.0.3
	Pip	8.1.1
	irods-capability-automated-ingest	0.3.4

Server Name	Software	Version
	Splunk Universal Forwarder	7.2.3
	HPCMP Kerberos Kit	Latest Version
iRODS-6	RHEL	7
	iRODS	4.2.4
	irods-rule-engine-plugin-audit-amqp	4.2.4
	Python	3.7.2
	python-irodsclient	4.2.4
	irods-rule-engine-plugin-python	4.2.4
	irods-database-plugin-postgres	4.2.4
	irods-rule-engine-plugin-storage-tiering	4.2.4
	Metalnx Remote Monitor Daemon	2.0-0
	Redis	5.0.3
	Pip	8.1.1
	irods-capability-automated-ingest	0.3.4
	Splunk Universal Forwarder	7.2.3
	HPCMP Kerberos Kit	Latest Version
iRODS-Proxy	RHEL	7
	HAProxy	1.7
	Splunk Universal Forwarder	7.2.3
	HPCMP Kerberos Kit	Latest Version
Metalnx	RHEL	7
	Metalnx	2.0.0
	Java	1.8
	Tomcat	9.0.14
	Splunk Universal Forwarder	7.2.3
	HPCMP Kerberos Kit	Latest Version
DB-Proxy	RHEL	7
	HAProxy	1.7
	Splunk Universal Forwarder	7.2.3
	HPCMP Kerberos Kit	Latest Version
ELK	RHEL	7
	Java	1.8
	Active MQ	5.15.8
	Elastic Search	6.5.4
	Logstash	6.5.4
	Kibana	6.5.4
	Stomp-plugin	3.0.8
	Splunk Universal Forwarder	7.2.3
	HPCMP Kerberos Kit	Latest Version

2.5 Ports and protocols

The required ports and protocols utilized by the iRODS proof-of-concept architecture are listed in Table 2-3.

Table 2-3. Ports and protocols per host.

Source	Destination	Protocol	Port	Notes
<Sys Admin>	ELK iRODS-Proxy iRODS-1 iRODS-2 iRODS-3 iRODS-4 iRODS-5 iRODS-6 MetaInx DB-Proxy PSQL-1 PSQL-2	SSH	22	Remote system administration via command line
iRODS-1 iRODS-2 iRODS-3 iRODS-4 iRODS-5 iRODS-6	iRODS-1 iRODS-2 iRODS-3 iRODS-4 iRODS-5 iRODS-6	TCP	1247	Inter-sever communication
<iRODS User>	iRODS-Proxy	TCP	1247	Load balancing (iCommands, MetaInx GUI)
iRODS-Proxy	iRODS-1 iRODS-2	TCP	1247	Load balancing (iCommands, MetaInx GUI)
<iRODS Admin>	iRODS-1 iRODS-2 iRODS-3 iRODS-4 iRODS-5 iRODS-6	TCP	1248	iRODS Data grid tasks (ex: status, pause, resume, shutdown)
iRODS-1 iRODS-2	DB-Proxy	TCP	5432	iCAT Database communication
DB-Proxy	PSQL-1 PSQL-2	TCP	5432	Database communication
<iRODS User>	iRODS-3 iRODS-4 iRODS-5 iRODS-6	TCP	20000 - 20199	Port range for files > 32MB multiple thread parallel transfer
MetaInx	iRODS-Proxy	TCP	1247	iCAT Load balancing
MetaInx	DB-Proxy	TCP	5432	MetaInx Database communication

Source	Destination	Protocol	Port	Notes
MetaInx	iRODS-1 iRODS-2 iRODS-3 iRODS-4 iRODS-5 iRODS-6	TCP	8000	Remote Monitoring Daemon communication
<iRODS User>	MetaInx	HTTPS	443	iRODS Web interface
<Auditor>	ELK	HTTPS	443	Kibana Web Interface
iRODS-1 iRODS-2 iRODS-3 iRODS-4 iRODS-5 iRODS-6	ELK	TCP	5000	Logstash
ELK HA-Proxy iRODS-1 iRODS-2 iRODS-3 iRODS-4 iRODS-5 iRODS-6 MetaInx DB-Proxy PSQL-1 PSQL-2	Splunk Server	TCP	8089 9997	Splunkd Splunk indexer
ELK HA-Proxy iRODS-1 iRODS-2 iRODS-3 iRODS-4 iRODS-5 iRODS-6 MetaInx PSQL	Kerberos Server	TCP/UPD TCP/UDP	88 749	Kerberos KDC Kerberos KDC

2.6 Security technical implementation guides (STIGS)

The following STIG or Security Requirements Guides (SRG) will be implemented for each host server containing the associated software components:

- Application Security and Development STIG - Ver 4, Rel 9
- Application Server SRG - Ver 2, Rel 5
- Oracle JRE 8 UNIX STIG - Ver 1, Rel 3
- PostgreSQL 9.x STIG- Ver 1, Rel 4
- Red Hat 6 STIG - Ver 1, Rel 21
- Web Server Security Requirements Guide (SRG) - Ver 2, Rel 2.

3 Conclusion

This report presents the integrated iRODS and HPC architecture design. This includes the technical details of the operating environment, the iRODS architecture, the associated hardware, software, and the minimum servers required.

Acronyms and Abbreviations

Acronym	Meaning
ACL	Access Control Lists
APIs	Application Programming Interfaces
CWFS	Center-Wide File System
DoD	Department of Defense
DSRC	Defense Supercomputing Resource Center
ERDC	Engineer Research and Development Center
ERS	Engineered Resilient Systems
HPC	High-Performance Computing
IA	Information Assurance
iRODS	Integrated Rule-Oriented Data System
SRG	Security Requirements Guides
STIGS	Security Technical Implementation Guide
USACE	U.S. Army Corps of Engineers

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14. ABSTRACT

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