XSEDE Service Provider
Software and Services Baseline

September 24, 2015

Version 1.2
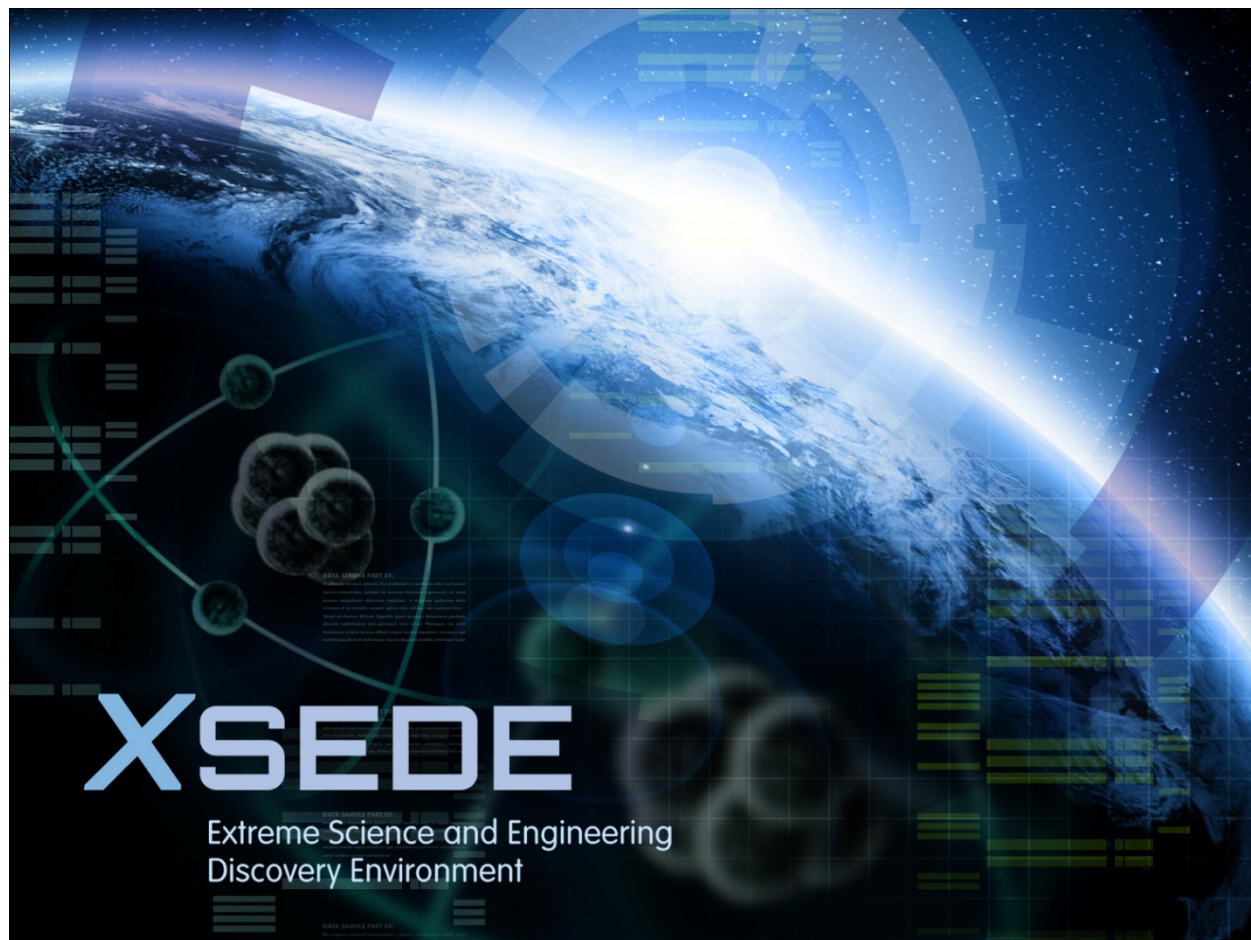

i

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

A. Document History

Document Section	Version	Date	Changes	Author
XSEDE Production Baseline: Service Provider Software and Services	1.0	02/20/2012	Baseline	J.P. Navarro V. Hazlewood K. Wallnau
	1.1	5/9/2013	Add xdusage and UNICORE. Made updates to remove deprecated items. Rearranged Science Gateway	V. Hazlewood
Most sections	1.2	9/24/2015	Updated based on current software and services as of 9/24/15	V.Hazlewood T.Samuel

B. Introduction

The term "XSEDE Production System" denotes the full suite of software and software-implemented services that XSEDE operates or makes available to its stakeholders, including, but not limited to, software developers, computational scientists, and registered XSEDE Service Providers (SP).

At the top level, the XSEDE Production System includes:

- *XSEDE Service Provider Software and Services*. Software and services that XSEDE service providers may, and in some cases must, deploy in their computational environments. This part of the baseline includes GridFTP, for example.
- *XSEDE Security Software and Services*. Software and services that XSEDE uses to provide security to its diverse community of stakeholders. This part of the baseline includes GSISSH, for example.
- *XSEDE Enterprise Software and Services*. Software and services operated by XSEDE to support and manage and integrate the entire XSEDE ecosystem. This part of the baseline includes the Kerberos and AMIE, for example.

A "Baseline" is a term in software and system engineering that refers to a version of a system or system component that is significant in some way. This document describes the *Service Provider Software and Services* of the XSEDE Production System Baseline (version 1.2). The objective of this document is therefore twofold:

1. To describe the software and services which XSEDE service providers (SPs) may, and in some cases must deploy into their own environments; and,
2. To obtain community feedback on the suitability for purpose of these software and services, and in the manner of their description.

B.1   Production Baseline

The components described in this document are mostly derived from the first four years of XSEDE. All the components that are thought to be in use are listed as required or optional. Those components that are known to be obsolete have been listed separately because they may still be installed on some SP resources. As a consequence, there is a non-trivial possibility that one or more SPs still offer obsolete components.

The XSEDE Architecture specifies[1] a collection of interfaces as well as a collection of software components that conform to and implement these interfaces. SPs are *required* to support some interfaces; SP support of the remaining interfaces is optional. In all cases, SPs may choose to support one or more required or optional interfaces using XSEDE-supplied components.

B.2   Terminology

Capabilities are groupings of related components that provide a user-meaningful related set of abilities, and that services providers can elect to support on individual resources. Capabilities are the service provider's menu of high-level abilities made available to users. Capabilities definitions and implementations can be owned by different support groups, internal or external, and can include whatever combination of optional and required components the capability owner defines as necessary to support the abilities and uses cases documented for that capability.

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[1] As proposed in the XSEDE Proposal and Revision Narrative.

Examples include *Remote Login*, *Remote Job Execution*, *Data Movement Servers*, *Workflow Support*, etc. More specifically, the *Remote Login* Capability combines components enabling users to remotely login using XSEDE issued credentials (single sign-on) PLUS the Common User Environment "CUE" standard set of environment variables and standard XSEDE shell utilities such as the xdusage utility. Since XSEDE's definition of the *Remote Login* capability included both of these, an SP cannot claim to support the XSEDE defined *Remote Login* capability unless they support both required elements of the capability. Capabilities can be defined to include alternate implementations and optional components.

In this document the term ***Capability*** refers to this bundling of related components.

B.3   Document Structure

Section C specifies XSEDE's *required* capabilities derived from minimal *required* capabilities necessary for basic operational integration.

Section D describes the large set of optional capabilities that XSEDE SPs may optionally support.

C. Required Capabilities

This section describes which capabilities must be supported by SPs integrating at the different XSEDE SP integration levels. A brief description of these levels is:

Level 1: Tightest integration; Offers one more digital services that satisfy all XSEDE interface requirements; Significant resources shared with and allocated by XSEDE.

Level 2: Medium integration; Offers one or more digital services through at least one XSEDE interface; Less significant sharing with XSEDE users. Can be XSEDE allocated or not.

Level 3: Minimum integration; Offers one or more digital services through non-XSEDE interfaces; Local users and with no sharing required with XSEDE. Participation in XSEDE information services registration is the only required service for this level.

A service provider "level" description is defined in the latest Service Provider Forum Charter, Membership and Governance document found on the project documents page of the XSEDE website.

Requirements vary by integration level and type of resource (HPC, HTC, Viz, Storage) as summarized in the following table.

Capability	Level 1	Level 2	Level 3
Information Services Registration	Yes	Yes	Yes
Monitoring	Yes	Yes (a)	Optional
Account Management and Information Exchange – AMIE	Yes	Yes (b)	Optional
Data Movement Servers (All)	Yes	Optional	Optional
Data Movement Clients (On HPC, HTC, Viz)	Yes	Optional	Optional
Local Compute (On HPC, Viz)	Yes	Optional	Optional
Single Sign-on / Remote Login (On HPC, Viz)	Yes	Optional	Optional
Visualization Software Support (On Viz)	Yes	Optional	Optional

Table 1 – Capability Requirements for SP levels

Notes:

a) Only XSEDE specified interfaces (see 1.2 above) are verified and validated.
b) Only if the resource is allocated through XSEDE.

C.1   Information Services Registration

XSEDE users, the XSEDE program and SPs need an authoritative catalog of capabilities, software and services supported by SPs.

XSEDE Information Services provides this authoritative catalog for use by the XSEDE User Portal (XUP) to produce component availability documentation, by the Inca verification/validation system for runtime and operational monitoring, by Science Gateways to enable resource and component discovery, and by any other software, services, or applications. Figure 1 shows the components and connectors that implement capability registration. Each service provider operates a local service with a Information Services registration component, and multiple other capability registration components. The information published by all SP local services is aggregated and made available by an XSEDE wide central service,

a.k.a. Integrated Information Services (IIS) located at http://info.xsede.org/. The XUP, Inca, Science Gateways, and other software can query the central information service for information from all SPs. Arrows show information flowing from the source to the services using it and presenting it to users.
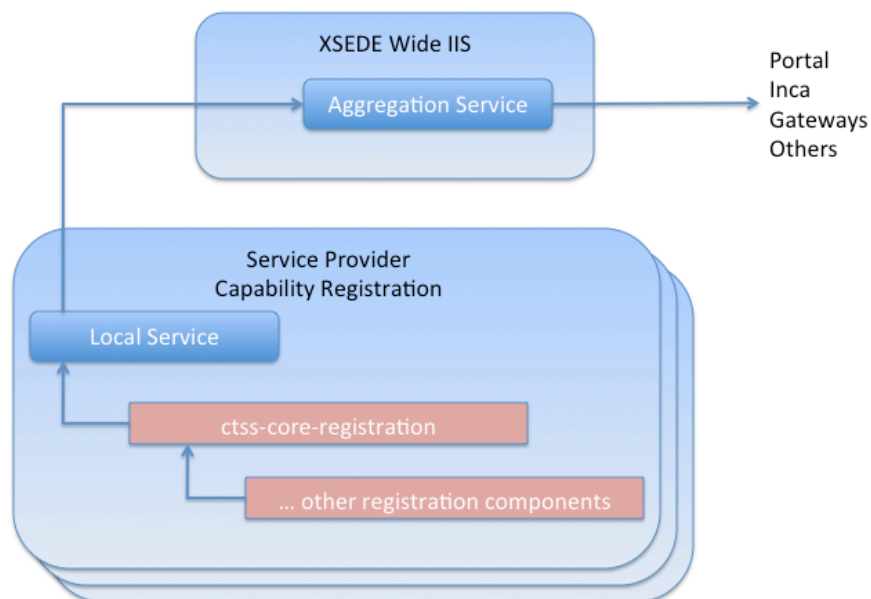
Figure 1 – Capability Registration and XSEDE Wide IIS

SPs implement Information Services Registration by installing the Core Integration Capability Kit version 5.0.x, which includes:

1

Name	**MDS Stopgap**
Version	1
Description	Information service capable of publishing generic XML content. Use this until Glue2 is available. Note: XSEDE Operations will provide an MDS Stopgap service for all SPs who do not want to implement the MDS Stopgap locally until Glue2 is available.
Availability	http://software.xsede.org/production/mds-stopgap/

2

Name	**Glue2**
Version	2
Description	Information publishing for SPs to deploy that publishes to the information service
Availability	Glue2 for Job and Load information will be available 4Q2015. Glue2 for all other information services is expected first quarter 2016. See http://software.xsede.org/production/glue2

C.2   Monitoring

Level 1 and Level 2 SPs with allocated resources must support Inca validation and verification of their XSEDE capabilities. Because the Inca system is designed to verify and validate user functionality it can be installed and operate as a normal user. The INCA team is responsible for deploying and operating the INCA components that implements verification and validation on SP systems in coordination with SP site staff. SPs should contact the Inca team (e-mail help@xsede.org) and provide access and assistance as needed to implement verification and validation of their resource.

1	Name	Inca
	Version	2.5
	Description	Inca validation and verification system
	Availability	http://software.xsede.org/production/inca

C.3   Account Management Information Exchange - AMIE

Account, allocation, and accounting information is exchanged between XSEDE's central database XDCDB and SPs so that 1) XSEDE can inform SPs that XSEDE users need accounts and have allocations on SP resources, and 2) SPs can report back to XSEDE allocation usage accounting information.

SP resources that users can access using XSEDE credentials must install and support AMIE in order to receive account create, modify, delete, and other requests. Additionally, AMIE is also necessary if an SP needs to receive allocation information from XSEDE and then report accounting usage against that allocation.

1	Name	AMIE
	Version	Latest
	Description	Account and accounting SP transaction integration
	Availability	http://software.xsede.org/production/amie

C.4   Data Movement Servers

To enable remote access to High-performance computing (HPC), High-throughput computing (HTC), Visualization, or Storage file-systems, SPs must deploy data-movement-servers registration and GridFTP.

1	Name	Data Movement Registration
	Version	4.2.0
	Description	Adaptors and data files that control what is published/registered about the CTSS Data Movement Servers Capability kit and associated user facing components. This will be implemented in the MDS StopGap capability. Use until Glue2 is available.

Availability	http://software.xsede.org/production/mds-stopgap/

2

Name	**Globus GridFTP**
Version	5.2.5
Description	GridFTP server
Availability	http://software.xsede.org/production/gridftp/

3

Name	**GSI OpenSSH SCP w/ HPN**
Version	5.7
Description	GSI OpenSSH SCP service with the HPN patch (provides scp service)
Availability	http://grid.ncsa.illinois.edu/ssh/ or Globus 5.2.5 GSI-OpenSSH metapackages until SDIACT-152 is available. http://software.xsede.org/production/gsissh when an XSEDE version is available.

C.5   Data Movement Clients

This capability provides users with data movement client components.

1

Name	**ctss-data-movement-clients-registration**
Version	4.2.0
Description	Adaptors and data files that control what is published/registered about the CTSS Data Movement Clients capability kit and associated user facing components. This will be implemented in the MDS StopGap capability. Use until Glue2 is available.
Availability	http://software.xsede.org/production/mds-stopgap/

2

Name	**Globus Toolkit** **(provides myproxy client and globus-url-copy client commands)**
Version	6.0
Description	GridFTP command line client
Availability	http://software.xsede.org/production/globus-toolkit/

3

Name	**GSI OpenSSH SCP w/ HPN**
Version	5.7
Description	GSI OpenSSH scp command line client with HPN patch.
Availability	http://grid.ncsa.illinois.edu/ssh/ or Globus 5.2.5 GSI-OpenSSH metapackages until SDIACT-152 is available.

	http://software.xsede.org/production/gsissh when an XSEDE version is available.

C.6   Local Compute

This capability provides users with access to HPC/HTC batch job execution. It is also used to advertise Resource Description Repository "RDR" information.

1

Name	**ctss-local-compute-registration**
Version	4.2.2
Description	Adaptors and data files that control what is published/registered about the Local Compute capability kit and associated user facing components. Use until Glue2 is available. This will be implemented in the MDS StopGap capability.
Availability	http://software.xsede.org/production/mds-stopgap/

2

Name	**Local resource management system**
Version	Various
Description	Local resource management system such as Slurm, Cobalt, Condor, LSF, Load Leveler, PBS Pro, PBS Torque, etc.
Availability	SP dependent

C.7   Single Sign-On / Remote Login

This capability provides users the ability to remotely login using XSEDE credentials (a.k.a. single sign-on), and to access a shell that conforms to the Common User Environment "CUE". The CUE is considered part of the Remote Login capability in order to provide the ability to remotely login and access a CUE compliant shell environment as a bundled SP ability. The GSI OpenSSH server below must be configured to accept XSEDE issues X.509 user credentials, and credentials issued by other certificate authorities (CAs) accepted by XSEDE.

1

Name	**ctss-login-registration**
Version	4.0.3
Description	Adaptors and data files that control what is published/registered about the Remote Login capability kit and associated user facing components. Use until Glue2 is available. This will be implemented in the MDS StopGap capability.
Availability	http://software.xsede.org/production/mds-stopgap/

2

Name	**GSI OpenSSH server and client**
Version	5.7

Description	Remote login shell service using SSH protocol with GSI authentication
Availability	http://grid.ncsa.illinois.edu/ssh/ or Globus 5.2.5 GSI-OpenSSH metapackages until SDIACT-152 is available. http://software.xsede.org/production/gsissh when XSEDE version available.

3

Name	**XSEDE-ca-certificates**
Version	1.0
Description	Utility to download and maintain the CRLs,
Availability	http://software.xsede.org/production/CA/

4

Name	**Globus Toolkit (client commands and myproxy credential tool)**
Version	6.0-3
Description	Globus Toolkit with MyProxy command line client tool
Availability	http://software.xsede.org/production/globus-toolkit/

Other Tools

1

Name	**xdusage**
Version	1.1-2
Description	View XSEDE allocation usage command line client
Availability	http://software.xsede.org/production/xdusage/

2

Name	**Modules**
Version	Latest version
Description	The XSEDE standard environment management tool
Availability	http://modules.sourceforge.net/

3

Name	**xdresourceid**
Version	1.0-2
Description	XSEDE Resource ID command line display tool
Availability	http://software.xsede.org/production/xdresourceid/

4

Name	**Common User Environment (CUE)**
Version	1.0
Description	XSEDE standardized user environment

Availability	https://www.ideals.illinois.edu/handle/2142/75910
	XSEDE CUE Variable definition document

C.8   Visualization Software Support

This capability provides users with visualization software.

Components:

1	Name	vtss-registration
	Version	4.2.0
	Description	Adaptors and data files that control what is published/registered about the Visualization capability kit and associated user facing components. This will be implemented in the MDS StopGap capability. Use until Glue2 is available.
	Availability	http://software.xsede.org/production/mds-stopgap/

SPs will obtain visualization software from providers of their choice and advertise availability of each component through this Visualization software registration component. There is no required or optional XSEDE visualization software.

D. Optional Capabilities

While the following capabilities are all optional, they are important to many XSEDE users. SPs may install and support a subset of these depending both on appropriateness for their type of resource and on what their allocated users need.

Capability \ Resource Type	HPC/HTC	Storage	Visualization
Application Development and Runtime Support	Recommended	No	Recommended
Distributed Programming Systems	As needed	No	As needed
Local HPC Software Advertising	Recommended	No	Recommended
Meta-Scheduling Support	As needed	No	As needed
Co-Scheduling Support	As needed	No	As needed
Parallel Application Support	Recommended	No	As needed
Remote Compute	Recommended	No	As needed
Science Gateway Support	Recommended	No	As needed
Wide Area File System	Recommended	As needed	Recommended
Workflow Support	As needed	No	As needed
End User Two Factor Authentication	Recommended	No	Recommended

Table 2 -- Capability support by resource type

The following subsections describe each of these capabilities in more detail, along with components that comprise the capability.

D.1   Application Development and Runtime Support

This capability provides users with application development and runtime support software components. XSEDE distributes a small subset, with the vast majority to be obtained by the SP from a software provider of their choice. The components in this capability distributed by XSEDE are:

	Name	ctss-app-support-registration
1	Version	4.2.0
	Description	Adaptors and data files that control what is published/registered about the CTSS Application Development and Runtime Support capability kit and associated user facing components. This will be implemented in the MDS StopGap capability. Use until Glue2 is available.
	Availability	http://software.xsede.org/production/mds-stopgap/

SPs may obtain the application development and runtime support components from a software provider of their choice and advertise them through the above app-support-registration component. XSEDE supports the mechanism for advertising information about these components. Support for the components

themselves is from the vendors that SPs obtain the components from. SPs may deploy and advertise any version of these components. Examples include, but are not limited to:

1) Apache Ant, Java
2) BLAS, Intel MKL
3) C/C++/Fortran compilers
4) GNU Make
5) HDF
6) Python, TCL

D.2   Distributed Programming Systems

This capability provides users with access to SAGA software.

1	Name	**ctss-distributed-programming-systems-registration**
	Version	4.2.0
	Description	Adaptors and data files that control what is published/registered about the Distributed Programming Systems capability kit and associated user facing components. This will be implemented in the MDS StopGap capability. Use until Glue2 is available.
	Availability	http://software.xsede.org/production/mds-stopgap/

D.3   Local HPC Software

This capability provides users with information about locally installed and supported HPC application libraries, tools, and scientific software.

1	Name	**local-hpc-software-registration**
	Version	4.2.2
	Description	Adaptors and data files that control what is published/registered about the Local HPC Software Publishing capability kit and associated user facing components. This will be implemented in the MDS StopGap capability. Use until Glue2 is available.
	Availability	http://software.xsede.org/production/mds-stopgap/

An SP will obtain HPC software from providers of their choice and advertise its availability through the above local-hpc-software registration component. Service providers generally support these components locally.

D.4   Meta-scheduling Support

This capability provides users the ability to meta-schedule jobs. If SPs support metascheduling then they can make this known to users via metascheduling registration.

Components:

1	Name	ctss-metascheduling-registration
	Version	4.2.1
	Description	Adaptors and data files that control what is published/registered about the Meta-scheduling Support capability kit and associated user facing components. This will be implemented in the MDS StopGap capability. Use until Glue2 is available.
	Availability	http://software.xsede.org/production/mds-stopgap/

D.5   Co-scheduling Support

This capability provides users information on an SP providing a service for the ability to co-schedule jobs.

Components:

1	Name	ctss-coscheduling-registration
	Version	1.0.0
	Description	Adaptors and data files that control what is published/registered about the Co-Scheduling Support capability kit and associated user facing components. This will be implemented in the MDS StopGap capability. Use until Glue2 is available.
	Availability	http://software.xsede.org/production/mds-stopgap/

D.6   Parallel Application Support

Enables users to compile and run parallel (MPI) applications.

Components:

1	Name	ctss-parallel-app-registration
	Version	4.2.0
	Description	Adaptors and data files that control what is published/registered about the Parallel Application Support capability kit and associated user facing components. This will be implemented in the MDS StopGap capability. Use until Glue2 is available.
	Availability	http://software.xsede.org/production/mds-stopgap/

An SP may obtain from a provider of their choice any number of MPI libraries which can be advertised through the parallel-app registration component. Service providers generally support these components locally.

D.7   Remote Compute

This capability provides users the ability to remotely execute jobs. GRAM4 is deprecated and should not be installed unless there are specific allocated users that require it. In that case SPs should help users to migrate to the production GRAM5 or to the new BES/JSDL (UNICORE 6) as they are available.

Components:

1	Name	ctss-remote-compute-registration
	Version	5.0.1
	Description	Adaptors and data files that control what is published/registered about the Remote Compute capability kit and associated user facing components. This will be implemented in the MDS StopGap capability. Use until Glue2 is available.
	Availability	http://software.xsede.org/production/mds-stopgap/

2	Name	Globus Toolkit (client) and GRAM 5 (server)
	Version	5.0.4
	Description	Globus GRAM 5
	Availability	http://software.teragrid.org/pacman/ctss4/gram5/

3	Name	GSI OpenSSH server and client
	Version	5.7
	Description	Remote login shell service using SSH protocol with GSI authentication
	Availability	http://grid.ncsa.illinois.edu/ssh/ or Globus 5.2.5 GSI-OpenSSH metapackages until SDIACT-152 is available. http://software.xsede.org/production/gsissh when an XSEDE version is available.

4	Name	**UNICORE command-line client (UCC)** **UNICORE Rich Client (URC)** **UNICORE servers (UNICORE)**
	Version	6.6.0
	Description	UNICORE (Uniform Interface to Computing Resources) offers a ready-to-run Grid system including client and server software. UNICORE makes distributed computing and data resources available in a seamless and secure way
	Availability	http://software.xsede.org/production/UNICORE/ Server: xsede-unicore-servers-6.6.0-p3.tgz (6.6.0p3) Command line client: /ucc-client (6.6.0) GUI client: /urc-client (6.6.0)

5	Name	**Genesis II client and server**
	Version	2.7
	Description	Genesis II is an open source, standards based grid platform designed to support both high-throughput computing and secure data sharing with both client and server components.
	Availability	Information http://genesis2.virginia.edu/wiki/ Software: Clients: http://software.xsede.org/production/genesis2/genesis2-v2.7/genesis2_clients/ Server: http://software.xsede.org/production/genesis2/genesis2-v2.7/

D.8   Science Gateway Support

Science Gateway Support has all the items in D.7 Remote Compute as a prerequisite. This capability provides science gateways the ability to remotely execute jobs using a variety of tools and services.

0   *All the items from D.7 Remote Compute PLUS:*

1	Name	**ctss-science-gateway-registration**
	Version	5.0.1
	Description	Adaptors and data files that control what is published/registered about the Science Gateway Support capability kit and associated user facing components. This will be implemented in the MDS StopGap capability. Use until Glue2 is available.
	Availability	http://software.xsede.org/production/mds-stopgap/

2	Name	CommSH
	Version	0.1.4
	Description	Community shell
	Availability	http://software.teragrid.org/pacman/ctss4/commsh/0.1.4-r1/

3	Name	Gateway User Count
	Version	1.0
	Description	Gateway submit attributes capability for use by SPs which have XSEDE Science Gateways which submit jobs via GSISSH
	Availability	http://software.xsede.org/production/gatewayUserCount/

D.9 Wide Area File System

This capability provides users with access to an XSEDE wide are file system capability. If an SP supports this capability they should register the service with XSEDE information services.

Components:

1	Name	ctss-wan-lustre-registration
	Version	5.0.0
	Description	Adaptors and data files that control what is published/registered about the WAN Lustre capability kit and associated user facing components and file-systems. This will be implemented in the MDS StopGap capability. Use until Glue2 is available.
	Availability	http://software.xsede.org/production/mds-stopgap/

D.10 Workflow Support

This capability can provide users with the ability to execute workflows.

Components:

1	Name	ctss-workflow-registration
	Version	4.2.0
	Description	Adaptors and data files that control what is published/registered about the Science Workflow Support capability kit and associated user facing components. This will be implemented in the MDS StopGap capability.
	Availability	http://software.xsede.org/production/mds-stopgap/

2	Name	Condor/Condor-G
	Version	7.4.4
	Description	Condor software and Condor-G service
	Availability	http://software.teragrid.org/pacman/ctss4/condor/condor-7.4.4-r1/README.install

D.11 XSEDE End User Two Factor Authentication

This two factor authentication is available for use as an XSEDE Service Providers' authentication service as an optional authentication method that can be used by all XSEDE users. If implemented by SPs it should be available on their SP resource login nodes. This two factor authentication service will be mandatory as one of the available authentication services for the XSEDE single sign on hub, login.xsede.org.

1	Name	XSEDE end user two factor authentication registration
	Version	1.0
	Description	Registration if the SP implements XSEDE end user two factor authentication. This will be implemented in the MDS StopGap capability.
	Availability	http://software.xsede.org/production/mds-stopgap/

2	Name	XSEDE end user two factor authentication
	Version	1.0
	Description	Two factor authentication service available for use as an XSEDE Service Providers' authentication service as an optional authentication method that can be used by all XSEDE users. Also, an authentication service for login.xsede.org.
	Availability	http://software.xsede.org/production/two-factor/

E. Retired Capabilities

This section contains all retired capabilities and components. SPs should not install these components, and if they are already installed may retire them.

Retired capabilities:

- ➢ Data Management/data-management.teragrid.org (SRB server)
- ➢ Data Movement/data-movement.teragrid.org (replaced by Data Movement Servers/data-movement-servers.teragrid.org)
- ➢ Distributed Parallel Application Support (mpich-g2, mpiG)
- ➢ TeraGrid Wide Area GPFS File Systems/wan-gpfs.teragrid.org
- ➢ Globus GRAM4
- ➢ GUR
- ➢ MCP

Components retired from older versions of required and optional capabilities (sections 2 and 3 above):

- ➢ PreWS-GRAM/GRAM2 service
- ➢ SoftEnv
- ➢ SRB Client
- ➢ MyCluster/gridshell
- ➢ Tg-policy
- ➢ tgusage
- ➢ tgresid
- ➢ tginfo

XSEDE

F. Obtaining Production Support

Production support of the components listed in this document is coordinated through the XSEDE ticket system. Support requests should be made using an XSEDE ticket. The XSEDE Operations Center (XOC), which is the Level 1 support, assigns XSEDE tickets. Tickets are assigned to the appropriate Level 2 supporter or support group – usually the Service Provider where the software or service is running. If the Level 2 supporter cannot solve the problem and needs configuration, customization or defect support then Level 3 supporter or support group would be consulting and assigned the ticket. Level 3 supporters can be in any group in XSEDE or an external organization that provides the software (the vendor). All support levels (1, 2, and 3) are coordinated by the XOC. Contact the XOC lead coordinator (currently Mike Pingleton) for help in identifying support staff for Level 2 and Level 3 support.