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Introduction

The Geodise Toolboxes provide a collection of functions that provide Grid client functionality to the Jython scripting environment. The Geodise Compute, Database and XML toolboxes contain routines that facilitate many aspects of Grid computing and data management including:

- The submission and management of computational jobs on remote compute resources via the Globus GRAM service.
- File transfer and remote directory management using the GridFTP protocol.
- Single sign-on to the Grid with Globus proxy certificates.
- Storage and grouping of files and variables, annotated with user defined metadata, in an archive.
- Graphical and programmatic interfaces for querying the metadata to easily locate stored files and variables.
- Sharing and reuse of data among distributed users. Users may grant access to their data to other members of a Virtual Organisation.
- Conversion of Jython variables into a non-proprietary, plain text format (XML) which can be stored and used by other tools.

Grid computing provides the infrastructure for the collaborative use of computers, networks, data, storage and applications across distributed organisations. A computational job can be run on the Grid to make use of resources unavailable on the user’s desktop, for example to exploit software licenses or greater computational power. The Geodise Compute Toolbox provides Python functions for submitting and monitoring jobs on the Grid, transferring files to and from remote compute resources, and managing the certificates used to identify users and authorise use of the resources.

Compute intensive applications often use and produce many data files and data structures. It can become difficult to find, reuse and share data from various applications that have been run repeatedly with different parameters. The Geodise Database Toolbox can be used to store additional user-defined information (called metadata) describing files and Jython variables, so that they can be located and retrieved more easily with metadata queries. Files and variables can also be grouped together, and data can be shared with other users by granting access permissions.
XML is a flexible standard data format that is widely used to structure and store information, and to exchange data between various computer applications. The XML Toolbox functions convert and store Jython variables and structures from the internal format into XML and vice versa. This allows parameter structures, variables and results from computational applications to be stored in a non-proprietary file format, or in XML-capable databases, and can be used to transfer Jython variables across the Grid. The XML toolbox also enables the transparent exchange of data between the Jython scripting environment and the Matlab technical computing environment.

This user guide introduces the reader to the Compute, Database and XML toolboxes, with tutorials that give an overview of the functionality provided by each of the toolboxes. The function reference for each toolbox contains detailed information about the syntax of its functions.

**What is Jython?**

Jython is an implementation of the powerful object-oriented Python scripting language written in Java. The Python language is a high-level programming language has a clean syntax which allows scientists and engineers to rapidly develop scripts and workflows. The Jython environment also allows the developer to exploit the capabilities of extensive built-in and third party Java libraries. The Jython interpreter is freely available for both commercial and non-commercial use from [http://www.jython.org/](http://www.jython.org/).

Throughout this manual the term *Python* refers to the Python scripting language, and the term *Jython* refers to the Jython scripting environment.

**Use Cases**

The GeodiseLab toolboxes have applications in a wide range of scenarios. Here we will outline three use cases that describe the potential benefits of Grid computing to the daily practice of the scientist or engineer.

The use cases that we will discuss are:

- Engineering Design Search and Optimisation
- Data management in computational electromagnetics
- Transparent collaboration between Problem Solving Environments
Engineering Design Search and Optimisation

Engineering Design Search and Optimisation (EDSO) is a compute and data intensive task which is well matched to Grid computing. Optimisation algorithms are used to search the parameter space of an engineering problem to discover an optimal design subject to certain criteria. During EDSO the optimisation algorithm must repeatedly evaluate some measure of the quality of a design; this may involve one or more lengthy numerical calculations. For example, an engineer wishing to improve the aerodynamic performance of a wing design may configure an optimiser to vary key design parameters, whilst invoking simulations of Computational Fluid Dynamics (CFD) to determine the quality of alternative geometries.

Depending upon the complexity of the numerical calculations and the number of evaluations required to determine the optimum design, EDSO may be a lengthy and computationally intensive task. When the evaluation of the objective function involves complex simulations (i.e. CFD) numerous large data files may be required, or produced, by the numerous calculations. The Grid client functionality makes it straightforward for the engineer to leverage computational resources available on the Grid to perform EDSO.

When undertaking EDSO in the Jython scripting environment the engineer may use the Geodesic Compute toolbox to automate the transfer of files, and the submission and management of computational jobs required during the evaluation of a design. By exploiting Grid resources not only is the engineer able to leverage the greater computational power available, but he can also drive any applications that he requires on a multitude of platforms from the comfort of his desktop PSE.

Data management in computational electromagnetics

Data management is an issue in a number of scientific and engineering application domains, including that of computational electromagnetics. For example, when performing simulations of electromagnetic phenomena a large volume of data may be generated, typically in the form of the input and output files. It is a non-trivial problem for the researcher to store, manage and reuse this data. The investment associated with the computationally expensive Finite Difference Time Domain modelling technique used to explore the properties of electromagnetic devices require that simulation results are suitably managed for reuse at a later data.

At present the most common solution for this problem is to store these flat files within a hierarchical directory structure on a local file system. As the volume of data grows
over time this solution is frequently inadequate for long term storage since it may become increasingly difficult to locate and reuse data within the collection. The Geodise Database toolbox provides a solution as a client to a managed data archive on the Grid.

The Geodise Database Toolbox allows the researcher to archive data files to a managed repository from Jython and annotate these files with metadata. In addition to standard metadata the user may define custom metadata specific to the problem. The researcher can then query the metadata to find these files using a straightforward syntax within the Jython scripting environment. In addition the Geodise Database Toolbox supports the archiving of variables from Jython. Items in stored the repository can be associated together into datagroups, allowing the creation of annotated hierarchies within which the user's results can be organised.

**Transparent collaboration between Problem Solving Environments**
The Geodise XML toolbox provides a collection of straight-forward functions which convert variables in the Jython scripting environment to and from the external XML format. Variables in the Jython workspace can be saved to and loaded from an XML file with minimal effort on the part of the researcher. XML is a structured format that can be interpreted by third party applications. By encoding the Jython variables in the XML format there are a number of benefits.

The provision of the Geodise XML toolbox for Matlab allows the transparent exchange of variables between the Matlab technical computing environment and Jython scripting environment. Variables are mapped to the appropriate built-in datatypes in the two languages. This allows researchers working with these two Problem Solving Environments to collaborate on shared datasets.

The Geodise XML toolbox is also leveraged by the Geodise Database Toolbox to store variables and metadata in a database. The contents of variables and metadata in the database can then be queried and searched across. The Geodise Database toolbox may be used to share variables stored in the managed repository between members of a virtual organisation because researchers can authorise other users to access their data. When variables are retrieved from the repository they will be transparently converted into the built-in datatypes of that PSE.
**Function Arguments**

The input and output arguments used by all of the functions of the Geodise toolboxes are summarised below.

### Input Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
<th>Used by Functions</th>
</tr>
</thead>
<tbody>
<tr>
<td>attswitch</td>
<td>A string specifying whether to use attributes (‘on’ = use attributes, ‘off’ = no attributes).</td>
<td>xml_format xml_load xml_parse xml_save</td>
</tr>
<tr>
<td>accesstype</td>
<td>A string specifying whether to add access permission for ‘users’ or ‘groups’.</td>
<td>gd_addusers</td>
</tr>
<tr>
<td>command</td>
<td>The absolute path of the chmod command on the Globus resource.</td>
<td>gd_chmod</td>
</tr>
<tr>
<td>datagroupID</td>
<td>The unique identifier of a datagroup.</td>
<td>gd_addusers gd_archive gd_datagroupadd</td>
</tr>
<tr>
<td>datagroupname</td>
<td>A user defined name for a datagroup.</td>
<td>gd_datagroup</td>
</tr>
<tr>
<td>datagrouptype</td>
<td>Set to ‘monitor’ if datagroup is to be monitored.</td>
<td>gd_datagroup</td>
</tr>
<tr>
<td>datatype</td>
<td>Used to override automatic data type selection for archive (‘var’) or retrieve (‘metadata’).</td>
<td>gd_archive gd_retrieve</td>
</tr>
<tr>
<td>datasource</td>
<td>Specifies what type of metadata or data to query (‘file’, ‘datagroup’, ‘varmeta’, ‘var’ or ‘monitor’).</td>
<td>gd_query gd_querydeleted</td>
</tr>
<tr>
<td>directory</td>
<td>The path of a local directory.</td>
<td>gd_retrieve</td>
</tr>
<tr>
<td>filename</td>
<td>The path of a local file.</td>
<td>gd_archive</td>
</tr>
<tr>
<td>Argument</td>
<td>Description</td>
<td>Used by Functions</td>
</tr>
<tr>
<td>------------</td>
<td>-----------------------------------------------------------------------------</td>
<td>-----------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>files</td>
<td>A cell array of filenames.</td>
<td>gd_submittunique</td>
</tr>
<tr>
<td>filetype</td>
<td>A string specifying the GridFTP transfer type (‘ASCII’ or ‘binary’).</td>
<td>gd_getfile, gd_putfile, gd_transferfile</td>
</tr>
<tr>
<td>groups</td>
<td>A user group ID string or list of user group IDs.</td>
<td>gd_addusers</td>
</tr>
<tr>
<td>host</td>
<td>A string specifying the Globus server to be used.</td>
<td>gd chmod, gd_fileexists, gd_getfile, gd_jobsubmit, gd_listdir, gd_makedir, gd_putfile, gd_rmdir, gd_rmfile, gd_rmuniquedir, gd_submittunique, gd_testauthentication, gd_testfiletransfer, gd_testjobsubmission, gd_timeauthentication, gd_timefiletransfer, gd_timejobsubmission</td>
</tr>
<tr>
<td>host1</td>
<td>The Globus server that sends the file.</td>
<td>gd_transferfile</td>
</tr>
<tr>
<td>host2</td>
<td>The Globus server that receives the file.</td>
<td>gd_transferfile</td>
</tr>
<tr>
<td>hostprompt</td>
<td>Indicates whether to prompt user for file host configuration during setup (1=true, 0=false).</td>
<td>gd_dbsetup</td>
</tr>
<tr>
<td>Argument</td>
<td>Description</td>
<td>Used by Functions</td>
</tr>
<tr>
<td>----------</td>
<td>-------------</td>
<td>-------------------</td>
</tr>
<tr>
<td>ID</td>
<td>The unique identifier of a file or variable.</td>
<td>gd_addusers, gd_datagroupsadd, gd_retrieve</td>
</tr>
<tr>
<td>IDs</td>
<td>A cell array which may contain the unique identifiers of files, variables and datagroups.</td>
<td>gd_markfordeletion, gd_unmarkfordeletion</td>
</tr>
<tr>
<td>interval</td>
<td>Interval (in seconds) at which the status of the job is polled.</td>
<td>gd_jobpoll</td>
</tr>
<tr>
<td>jobhandle</td>
<td>A Globus GRAM job handle.</td>
<td>gd_jobkill, gd_jobpoll, gd_jobstatus</td>
</tr>
<tr>
<td>listhidden</td>
<td>Indicates whether hidden files should be listed (1 = true, false otherwise).</td>
<td>gd_listdir</td>
</tr>
<tr>
<td>localfile</td>
<td>A filename on the local machine.</td>
<td>gd_getfile, gd_putfile</td>
</tr>
<tr>
<td>localpath</td>
<td>The path of a local file or directory.</td>
<td>gd_retrieve</td>
</tr>
<tr>
<td>maxtime</td>
<td>Upper limit (in seconds) for the period over which the job is polled.</td>
<td>gd_jobpoll</td>
</tr>
<tr>
<td>metadata</td>
<td>A metadata dictionary containing information about a file, variable or datagroup.</td>
<td>gd_archive, gd_datagroup</td>
</tr>
<tr>
<td>minvalue</td>
<td>The minimum acceptable value for the property of the proxy certificate examined (in hours or bits).</td>
<td>gd_proxyquery</td>
</tr>
<tr>
<td>mode</td>
<td>Permissions to set on the file.</td>
<td>gd_chmod</td>
</tr>
<tr>
<td>name</td>
<td>Name to use for the root element.</td>
<td>xml_format</td>
</tr>
<tr>
<td>prompt</td>
<td>Indicates whether to overwrite an existing file without prompting</td>
<td>gd_retrieve</td>
</tr>
<tr>
<td>Argument</td>
<td>Description</td>
<td>Used by Functions</td>
</tr>
<tr>
<td>----------------</td>
<td>-----------------------------------------------------------------------------</td>
<td>---------------------------------</td>
</tr>
<tr>
<td></td>
<td>(‘overwrite’) or prompt the user (default).</td>
<td></td>
</tr>
<tr>
<td>proxyattrib</td>
<td>A string specifying the property of the proxy certificate to be examined (‘time’ or ‘strength’).</td>
<td>gd_proxyquery</td>
</tr>
<tr>
<td>qresults</td>
<td>List of dictionaries containing results returned from a query.</td>
<td>gd_display</td>
</tr>
<tr>
<td>query</td>
<td>A query string which compares fields (dictionary keys) with values.</td>
<td>gd_query gd_querydeleted</td>
</tr>
<tr>
<td>remotedir</td>
<td>The path of a directory on a Globus server.</td>
<td>gd_listdir gd_makedir gd_rmdir gd_rmuniquedir gd_submitunique gd_testfiletransfer gd_testjobsubmission gd_timefiletransfer gd_timejobsubmission</td>
</tr>
<tr>
<td>remotefile</td>
<td>A filename on the remote server.</td>
<td>gd_chmod gd_fileexists gd_getfile gd_putfile gd_rmfile</td>
</tr>
<tr>
<td>remotefile1</td>
<td>The path of the file to be sent.</td>
<td>gd_transferfile</td>
</tr>
<tr>
<td>remotefile2</td>
<td>The path of the file to be received.</td>
<td>gd_transferfile</td>
</tr>
<tr>
<td>resultfields</td>
<td>A string specifying selected fields (dictionary keys) to return from a query.</td>
<td>gd_query gd_querydeleted</td>
</tr>
<tr>
<td>rsl</td>
<td>A string specifying the properties of a Globus GRAM job.</td>
<td>gd_jobsubmit gd_submitunique</td>
</tr>
<tr>
<td>subdatagroupID</td>
<td>The unique identifier of a</td>
<td>gd_datagroupadd</td>
</tr>
<tr>
<td>Argument</td>
<td>Description</td>
<td>Used by Functions</td>
</tr>
<tr>
<td>----------</td>
<td>-------------</td>
<td>------------------</td>
</tr>
<tr>
<td>users</td>
<td>A user ID string or list of user IDs.</td>
<td>gd_addusers</td>
</tr>
</tbody>
</table>
| v        | A generic structure or variable. | gd_archive  
xml_format  
xml_save |
| xmlstr   | An XML string. | xml_parse |
## Output Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
<th>Used by Functions</th>
</tr>
</thead>
<tbody>
<tr>
<td>datagroupID</td>
<td>The unique identifier of a datagroup.</td>
<td>gd_datagroup</td>
</tr>
<tr>
<td>exists</td>
<td>The existence of the file on the Globus server (1 = exists, 0 = does not exist).</td>
<td>gd_fileexists</td>
</tr>
<tr>
<td>filename</td>
<td>The path of a local file.</td>
<td>gd_retrieve</td>
</tr>
<tr>
<td>filedetails</td>
<td>A list containing structures that describe the details of the files and directories contained in the remote directory.</td>
<td>gd_listdir</td>
</tr>
<tr>
<td>files</td>
<td>A list of filenames.</td>
<td>gd_listdir</td>
</tr>
<tr>
<td>ID</td>
<td>The unique identifier of a file or variable.</td>
<td>gd_archive</td>
</tr>
<tr>
<td>isdone</td>
<td>Indicates whether the job complete successfully (1 = done, 0 = not done).</td>
<td>gd_jobpoll</td>
</tr>
<tr>
<td>isValid</td>
<td>Indicates whether the proxy certificate is valid (1 = valid, 0 = not valid).</td>
<td>gd_proxyinfo,</td>
</tr>
<tr>
<td></td>
<td></td>
<td>gd_proxyquery</td>
</tr>
<tr>
<td>jobhandle</td>
<td>A Globus GRAM job handle.</td>
<td>gd_jobsubmit</td>
</tr>
<tr>
<td></td>
<td></td>
<td>gd_submitunique</td>
</tr>
<tr>
<td>marktotal</td>
<td>Total number of IDs successfully marked for deletion.</td>
<td>gd_markfordeletion</td>
</tr>
<tr>
<td>metadata</td>
<td>A metadata structure containing information about a file, variable or datagroup.</td>
<td>gd_retrieve</td>
</tr>
<tr>
<td>qresults</td>
<td>List of dictionaries containing results returned from a query.</td>
<td>gd_query,</td>
</tr>
<tr>
<td></td>
<td></td>
<td>gd_querydeleted</td>
</tr>
<tr>
<td>status</td>
<td>The status of the Globus GRAM job.</td>
<td>gd_jobstatus</td>
</tr>
<tr>
<td>Argument</td>
<td>Description</td>
<td>Used by Functions</td>
</tr>
<tr>
<td>-------------</td>
<td>-----------------------------------------------------------------------------</td>
<td>-----------------------------------------------</td>
</tr>
<tr>
<td>subject</td>
<td>The certificate subject line in the Globus format.</td>
<td>gd_proxyinfo, gd_certinfo</td>
</tr>
<tr>
<td>success</td>
<td>The result of the operation or test (1 = success, 0 = failure).</td>
<td>gd_addusers, gd_datagroupadd, gd_testauthentication, gd_testfiletransfer, gd_testjobsubmission</td>
</tr>
<tr>
<td>time</td>
<td>The elapsed time in milliseconds or -1 if failed.</td>
<td>gd_timeauthentication, gd_timefiletransfer, gd_timejobsubmission</td>
</tr>
<tr>
<td>uniquedir</td>
<td>The path of the unique working directory created on the server.</td>
<td>gd_submitunique</td>
</tr>
<tr>
<td>unmarktotal</td>
<td>Total number of IDs successfully unmarked for deletion.</td>
<td>gd_unmarkfordeletion</td>
</tr>
<tr>
<td>v</td>
<td>A generic structure or variable.</td>
<td>gd_retrieve, xml_parse, xml_load</td>
</tr>
<tr>
<td>version</td>
<td>Version of the Database, XML or Compute toolbox.</td>
<td>gd_compute_version, gd_db_version, gd_xml_version</td>
</tr>
<tr>
<td>xmlstr</td>
<td>An XML string.</td>
<td>xml_format</td>
</tr>
</tbody>
</table>
Geodise Compute Toolbox

Introduction

The Geodise Compute Toolbox exposes the power of the Grid to the Jython scripting environment. With this toolbox the engineer can programatically access Globus GT2 resources which provide the backbone of many computational Grids. In this manner the Geodise Compute Toolbox promotes the integration of Grid resources into the complex engineering workflows which can be described in the Python scripting language.

The Geodise Compute Toolbox provides Python functions which support the job submission, file transfer and certificate management in a familiar and intuitive syntax.

- Globus GRAM jobs can be submitted, queried and terminated.
- File transfer and remote directory management is supported using the GridFTP protocol.
- Single sign-on to the Grid is supported with Globus proxy certificates.

The Geodise Compute Toolbox functions for certificate management are listed in Table 1. Table 2 lists functions for the submission the computational jobs to a Globus GRAM service, and Table 3 lists the functions for GridFTP file transfer.

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>gd_certinfo</td>
<td>Returns information about the user's certificate.</td>
</tr>
<tr>
<td>gd_createproxy</td>
<td>Creates a Globus proxy certificate.</td>
</tr>
<tr>
<td>gd_proxyinfo</td>
<td>Returns information about the user's proxy certificate.</td>
</tr>
<tr>
<td>gd_proxyquery</td>
<td>Queries whether a valid proxy certificate exists.</td>
</tr>
<tr>
<td>gd_destroyproxy</td>
<td>Destroys the local copy of the user's Globus proxy certificate.</td>
</tr>
</tbody>
</table>

Table 1 Certificate management functions

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>gd_jobstatus</td>
<td>Gets the status of a Globus GRAM job.</td>
</tr>
<tr>
<td>gd_jobssubmit</td>
<td>Submits a compute job to a Globus service.</td>
</tr>
<tr>
<td>Function</td>
<td>Description</td>
</tr>
<tr>
<td>--------------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td>gd_jobpoll</td>
<td>Queries the status of a Globus GRAM job until complete.</td>
</tr>
<tr>
<td>gd_jobkill</td>
<td>Kills a Globus GRAM job specified by a job handle.</td>
</tr>
<tr>
<td>gd_chmod</td>
<td>Changes file permissions of a file on a Globus resource.</td>
</tr>
<tr>
<td>gd_submitunique</td>
<td>Submits a GRAM job to a unique working directory.</td>
</tr>
</tbody>
</table>

**Table 2 GRAM job submission functions**

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>gd_getfile</td>
<td>Retrieves a remote file using GridFTP.</td>
</tr>
<tr>
<td>gd_putfile</td>
<td>Puts a file on a remote server using GridFTP.</td>
</tr>
<tr>
<td>gd_transferfile</td>
<td>Performs a third-party file transfer using GridFTP.</td>
</tr>
<tr>
<td>gd_makedir</td>
<td>Creates a remote directory using GridFTP.</td>
</tr>
<tr>
<td>gd_listdir</td>
<td>Lists the contents of a directory on a GridFTP server.</td>
</tr>
<tr>
<td>gd_fileexists</td>
<td>Tests the existence of files and directories on a Globus resource.</td>
</tr>
<tr>
<td>gd_rmdir</td>
<td>Deletes a remote directory using GridFTP.</td>
</tr>
<tr>
<td>gd_rmfile</td>
<td>Deletes a remote file using GridFTP.</td>
</tr>
<tr>
<td>gd_rmuniquedir</td>
<td>Deletes a remote directory and its contents.</td>
</tr>
</tbody>
</table>

**Table 3 GridFTP file transfer functions**
Tutorial

Grid Certificates
To access Globus compute resources all users must be authenticated, and must also be authorised to access the resource. Authentication under the Globus toolkit is based upon X.509 certificates. X.509 certificates are digital tokens that have been cryptographically signed by a trusted third party, the Certificate Authority (CA), see Figure 1. Using X.509 certificates the identity of a user or server can be verified.

It is necessary to obtain a Grid certificate from a Certificate Authority that is acceptable to the administrators of the Globus resources that you wish to use. For step-by-step instructions about how to apply for an X.509 certificate, and how to export it into the format required by Compute Toolbox, a tutorial is available from the Geodise web-site (http://www.geodise.org/files/tutorials/Obtaining_Certificates.pdf).

![Figure 1 - Hierarchy of trust for user credentials](image)

The Globus toolkit authorises users to access resources by mapping their certificate to a user account on the resource. Therefore to use a Globus resource to run computational jobs you must be in possession of an X.509 certificate signed by a CA that is trusted by the administrators of the resource that you wish to access. You must then apply for permission to access the resource by having the subject line of your certificate mapped to a user account on that machine.

To enable users to delegate their identity, allowing Grid processes to submit jobs and transfer files on their behalf, the Globus toolkit also uses a technology called ‘proxy
certificates’. Proxy certificates are temporarily limited credentials that can be used to devolve the user’s identity across the Grid. In practice proxy certificates also provide a convenient single sign-on to the Grid; users enter the passphrase to the private key of their X.509 certificate just once when generating the proxy certificate.

Before accessing a Globus resource you should generate a valid proxy certificate, which will typically expire after 12 hours. The Geodise Compute Toolbox provides Python functions that allow the user to create, examine and destroy Globus proxy certificates within the Jython scripting environment.

Before using the Geodise Compute Toolbox you should configure the location of the credentials on your machine. Your X.509 certificate and corresponding private key should be separately encoded in PEM format (see the obtaining certificates tutorial for details). To do this create a file called ‘cog.properties’ located in a directory ‘.globus’ of the home directory on your workstation. Then configure the location of your X.509 certificate and private key, in addition to the certificates of trusted CAs.

For example the ‘cog.properties’ file on a Windows PC would contain the following lines:

```
cacert=C:\Documents and Settings\<USER>\.globus\01621954.0
proxy=C:\\DOCUME~1\<USER>\LOCALS~1\Temp\509up_u_<USER>
usercert=C:\\Documents and Settings\<USER>\.globus\usercert.pem
userkey=C:\\Documents and Settings\<USER>\.globus\userkey.pem
proxy.strength=512
proxy.lifetime=12
```

Please note that throughout this manual the term <USER> represents your username on any given machine.

The properties ‘usercert’ and ‘userkey’ refer to locations of the PEM encoded user certificate and corresponding private key. The file ‘cacert’ contains the certificate of the CA which signed the user’s X.509 certificate (in PEM format). Where ‘proxy’ will be the location of the user’s proxy certificate once it has been generated by `gd_createproxy`. The properties ‘proxy.strength’ and ‘proxy.lifetime’ contain default settings for the cryptographic strength and lifetime of the proxy certificate. Note that the file separator on a Windows PC must be defined with double backslashes, “\\”.
Once the user’s credentials have been configured in the ‘cog.properties’ file they are accessible to the Geodise Compute Toolbox. To verify the configuration from the interactive Jython prompt query the X.509 certificate:

```python
>>> from gdcompute import *
>>> subject = gd_certinfo()
>>> print subject
subject: C=UK,O=eScience,OU=Southampton,L=SeSC,CN=some user
issuer: C=UK,O=eScience,OU=Authority,CN=CA,E=ca-operator@grid-support.ac.uk
start date: Tue Oct 07 13:00:31 BST 2003
end date: Wed Oct 06 13:00:31 BST 2004
/C=UK/O=eScience/OU=Southampton/L=SeSC/CN=some user
```

The details of the user’s certificate are printed to the screen. The subject line returned by `gd_certinfo` is in the Globus format and can be used to apply for access to a Globus resource. By supplying this subject line to the administrator of a Globus resource your credentials can be mapped to a user account on that machine.

To create a proxy certificate the `gd_createproxy` command is used:

```python
>>> gd_createproxy()
```

When this command is entered a GUI will prompt the user for the passphrase to their private key. The details of the proxy certificate can be configured using the 'Options' button. The proxy certificate is generated by pressing the 'Create' button. After the proxy has been generated, click 'Cancel' to dismiss the GUI.

Now you may query the details of the proxy certificate:

```python
>>> (exists, subject) = gd_proxyinfo()
```
The details printed to the screen indicate that the proxy certificate will remain valid for almost 12 hours. We may also query the validity of the proxy certificate programmatically, for example:

```python
>>> isvalid = gd_proxyquery('time',11)
>>> print isvalid
1
```

This indicates that our proxy certificate will remain valid for at least 11 hours.

**Job submission and file transfer**

The primary services offered by Globus GT2 resources are GRAM job submission and GridFTP file transfer. Typically Globus resources can simply be specified by the machine name, for example:

```python
>>> host = 'server1.domain.com'
```

However some Globus computational resources may offer GRAM job submission to a number of alternative job managers or non-default ports. These can be specified as follows:

```python
>>> GRAM1 = 'server1.domain.com/jobmanager-fork'
>>> GRAM2 = 'server1.domain.com/jobmanager-pbs'
>>> GRAM3 = 'server1.domain.com:2119/jobmanager'
```

Globus resources offering GridFTP will typically listen on the default port (2811), however a non-default port can be specified as follows:

```python
>>> GridFTP1 = 'server1.domain.com:2812'
```
For all examples in this tutorial we will assume that a single Globus resource (host) is used offering GRAM and GridFTP services on default ports, and using the default job manager.

To submit a job to a computational resource via a Globus GRAM service you must describe the attributes of the job using a Resource Specification Language (RSL) string. An RSL string is a list of property/values pairs each enclosed by brackets (see the example below). The most frequently used GRAM RSL parameters are listed in Table 4, these and other GRAM RSL parameters are further documented on the Globus website (http://www.globus.org/).

<table>
<thead>
<tr>
<th>executable</th>
<th>The name of the executable file to be run. This is the only required parameter.</th>
</tr>
</thead>
<tbody>
<tr>
<td>directory</td>
<td>The name of the default working directory.</td>
</tr>
<tr>
<td>arguments</td>
<td>The arguments to be passed to the executable.</td>
</tr>
<tr>
<td>stdin</td>
<td>The name of the file containing the standard input for the executable.</td>
</tr>
<tr>
<td>stdout</td>
<td>The name of the file that will contain the standard output from the executable.</td>
</tr>
<tr>
<td>stderr</td>
<td>The name of the file that will contain the standard error from the executable.</td>
</tr>
<tr>
<td>count</td>
<td>The number of times that the executable should be executed.</td>
</tr>
<tr>
<td>environment</td>
<td>The environment variables to be set. A list of name/value pairs each enclosed by brackets.</td>
</tr>
<tr>
<td>maxTime</td>
<td>The maximum execution time in minutes.</td>
</tr>
<tr>
<td>jobType</td>
<td>A string specifying the job types. Possible values include “single”, “multiple”, “mpi” and “condor”.</td>
</tr>
</tbody>
</table>

Table 4 GRAM RSL parameters

This example demonstrates the submission of a simple job to the Globus GRAM service on host. The first argument to gd_jobsubmit is an RSL string that specifies the file name of the executable to be run, ‘sleep’, and the argument to be passed to that executable which specifies that the process will sleep for 1 minute.
$$\begin{align*}
&\text{>>> rsl = '\&(executable="/bin/sleep")\(arguments="1m")'}
&\text{>>> jobhandle = gd_jobsubmit(rsl,host)}
&\text{>>> print jobhandle}
&\text{https://server1.domain.com:30001/27531/1096385757/}
\end{align*}$$

The function \texttt{gd\_jobsubmit} returns a GRAM job handle that can be used to check the status of the job, and if necessary to kill the job. In the following example we use the job handle returned by \texttt{gd\_jobsubmit} to query the status of the job. The integer returned by \texttt{gd\_jobstatus} indicates the state of the job, where “2” indicates that the job is active and “3” indicates that the job has completed.

$$\begin{align*}
&\text{>>> status = gd\_jobstatus(jobhandle)}
&\text{>>> print status}
&\text{2}
\end{align*}$$

We can also poll the status of the job until the job has completed.

$$\begin{align*}
&\text{>>> isdone = gd\_jobpoll(jobhandle)}
\end{align*}$$

In addition to high-performance, high-volume file transfer GridFTP offers all of the standard FTP file operations. We can use GridFTP to create a working directory on the Globus resource.

$$\begin{align*}
&\text{>>> gd\_makedir(host,'/home/</USER>/demo')}
\end{align*}$$

We will now run a second job, piping the output to a file ‘date.out’ in our working directory on \texttt{host}. We will then use the GridFTP command \texttt{gd\_getfile} to retrieve the output to a temporary file on the local machine, and print the results.

$$\begin{align*}
&\text{>>> import tempfile}
&\text{>>> rsl = '\&(executable="/bin/date")\(arguments="-u")}
&\text{(directory="/home/</USER>/demo")\(stdout="date.out")'}
&\text{>>> jobhandle = gd\_jobsubmit(rsl,host)}
&\text{>>> print jobhandle}
\end{align*}$$
We can now use the GridFTP commands `gd_rmfile` and `gd_rmdir` to clean-up the file and directory on the server:

```python
>>> gd_rmfile(host,'/home/<USER>/demo/date.out')
>>> gd_rmdir(host,'/home/<USER>/demo/')
```

Frequently an engineer may wish to submit and run several jobs independently upon a Globus resource, for example when conducting a parameter sweep. To prevent conflicts between the input and output parameters of the different jobs it is convenient to run the jobs in separate directories. The function `gd_submitunique` handles the submission of compute jobs into unique directories, returning a job handle and the path of the unique directory. In the following example we use the function `gd_submitunique` to submit two concurrent jobs, we will then retrieve the results and delete unique directories and their contents using `gd_rmuniquedir`.

```python
>>> rsl = '&(executable="/bin/date"){arguments="-u")
(stdout="date.out")'
>>> (jobhandle1,uniquedir1) = gd_submitunique(rsl,host, remotedir='/home/<USER>/')
>>> (jobhandle2,uniquedir2) = gd_submitunique(rsl,host, remotedir='/home/<USER>/')
>>> print jobhandle1; print uniquedir1
>>> print jobhandle2; print uniquedir2
```
Scripting the Grid
The Geodise Compute Toolbox allows engineers to script Grid processes in the Jython scripting environment. Unfortunately due to the dynamic nature of the Grid the resources that you wish to use may become unavailable, or may be more or less reliable. In these situations, when a function in the Geodise Compute Toolbox is unable to complete its operation, the function will typically throw an exception with a diagnostic message.

```python
>>> gd_getfile(host, '\tmp\fileDoesNotExist.txt', 'demo.txt')
```
If a Python function throws an error that is not suitably handled, this will cause the Python script or function which invoked it to stop executing. Therefore it is important if you wish to write a robust Python script or function that communicates with the Grid that you use Python exception handling to deal with errors appropriately if and when they occur.

Python exception handling is based upon `try`, `except` statements. Placing a block of code between a pair of `try`, `except` statements means that if an exception occurs when Jython evaluates this code the script will not stop executing. Instead the code inside the `except` block is evaluated and the script continues. This behaviour is demonstrated by the example below.

```python
>>> try:
...      gd_getfile(host,'\tmp\fileDoesNotExist.txt','demo.txt')
... except Exception, e:
...      print 'An error has occurred with the following message:'
...      print e
...```

In this way errors that occur when communicating with the Grid can be ‘caught’ by the script and dealt with appropriately. Exceptions can be classified depending upon their type, and if appropriate the script can continue, or stopped by throwing another exception (using `raise`).
We recommend that when writing a script or function that communicates with the Grid that you enclose all Grid functions with `try, except` statements. You should also consider how the script should behave if an error occurs; should it tidy up and exit, or should it continue? This way you will be prepared for the unexpected, and your Python scripts and functions will be more robust as a result.
**Function Reference**

**gd_certinfo**

Returns information about the user's certificate.

**Syntax**

```python
subject = gd_certinfo(filename=None)
```

**Description**

This command prints information about the user's certificate to the screen. The command also returns the certificate subject line in a format which is suitable for use in a Globus gridmap file. The default location of the user's certificate is specified by the cog.properties file.

```python
subject = gd_certinfo() where subject is the certificate subject in the Globus format.
```

```python
subject = gd_certinfo(filename) as above, where filename is the filename of the certificate to be queried. The certificate must be encoded in pem format.
```

**See also**

[gd_proxyinfo](#), [gd_createproxy](#), [gd_destroyproxy](#)
gd_chmod

Changes file permissions of a file on a Globus resource.

Syntax

    gd_chmod(host, remotefile, mode, command='/bin/chmod')

Description

    gd_chmod(host, remotefile, mode) where host is a string describing
the resource. It could be in one of the following formats:
    - hostname
    - hostname:port
    - hostname/service
    - hostname:port/service

The second argument remotefile is a string describing the full name of the file
starting from root '/'. The final argument mode is a string describing the permissions
of the file. The permission of a file can be either a symbolic representation of changes
to make, or an octal number representing the bit pattern for the new permissions (see
below).

    gd_chmod(host, remotefile, mode, command) as above, except the
argument command is a string specifying the absolute path of the chmod command on
the Globus resource.

Input arguments

    mode

The argument mode may have two alternative forms:

1. Symbolic representation:

   A combination of the letters 'ugoa' controls which users' access to the
file will be changed: the user who owns it (u), other users in the file's
group (g), other users not in the file's group (o), or all users (a).

   The operator '+' causes the permissions selected to be added to the
existing permissions of each file; '-' causes them to be removed; and '='
causes them to be the only permissions that the file has.

   The letters 'rwxXstugo' select the new permissions for the affected
users: read (r), write (w), execute (or access for directories) (x),

execute only if the file is a directory or already has execute permission for some user (X), set user or group ID on execution (s), sticky (t), the permissions granted to the user who owns the file (u), the permissions granted to other users who are members of the file's group (g), and the permissions granted to users that are in neither of the two preceding categories (o).

2. Octal number representation:
A numeric mode is from one to four octal digits (0-7), derived by adding up the bits with values 4, 2, and 1. Any omitted digits are assumed to be leading zeros. The first digit selects the set user ID (4) and set group ID (2) and sticky (1) attributes. The second digit selects permissions for the user who owns the file: read (4), write (2), and execute (1); the third selects permissions for other users in the file's group, with the same values; and the fourth for other users not in the file's group, with the same values.

For example, 0750 gives rwx permissions to the owner and rx permissions to the group.

Examples
To give read/write/execute permissions to the owner and read/execute permissions to the group of a file named '/tmp/foo' which is on a Globus resource called 'server.domain.com', you can use:

```python
from gdcompute import *
gd_chmod('server.domain.com','/tmp/foo','0750')
```

To remove group execute permissions from the same file you can use:

```python
gd_chmod('server.domain.com','/tmp/foo','g-x')
```

Notes
A valid proxy certificate is required to use this function.

See also
**gd_fileexists**, **gd_listdir**
gd_compute_version

Returns the current version of the Geodise Compute Toolbox.

Syntax

    version = gd_compute_version()

Description

    version = gd_compute_version() returns the version of the current
Geodise Compute Toolbox release as a string of the form MAJOR.MINOR.POINT.

See also

README.txt
gd_createproxy

Creates a Globus proxy certificate.

Syntax

    gd_createproxy()

Description

This command creates a Globus proxy certificate for the user's credentials at the location specified by the cog.properties file. The user is queried for the passphrase to their private key by a pop-up window.

Notes

A valid proxy certificate is required to use this function.

See also

    gd_proxyinfo, gd_proxyquery, gd_certinfo, gd_destroyproxy
**gd_destroyproxy**

Destroys the local copy of the user's Globus proxy certificate.

Syntax

```
    gd_destroyproxy()
```

Description

This command deletes the local copy of the Globus proxy certificate for the user's credentials at the location specified by the cog.properties file. Returns 1 if proxy successfully destroyed, otherwise 0.

See also

* gd_createproxy, gd_proxyinfo, gd_certinfo
**gd_fileexists**

Tests the existence of files and directories on a Globus resource.

**Syntax**

```python
exists = gd_fileexists(host, remotefile)
```

**Description**

`exists = gd_fileexists(host, remotefile)` returns an integer `exists` indicating whether the file or directory specified by `remotefile` exists on the GridFTP server specified by the string `host`.

**Example**

```python
from gdcompute import *
exists = gd_fileexists('server.domain.com', '/tmp/test.dat')
```

**Notes**

A valid proxy certificate is required to use this function.

**See also**

`gd_listdir`
\textbf{gd\_getfile}

Retrieves a remote file using GridFTP.

\textbf{Syntax}

\begin{verbatim}
gd_getfile(host, remotefile, localfile, filetype='ASCII')
\end{verbatim}

\textbf{Description}

This command retrieves a file from a remote server using GridFTP. The user must specify the remote file location on a remote server and the local destination for the file. The user can also specify the file type.

\texttt{gd\_getfile(host, remotefile, localfile)} transfers the remote ASCII file \texttt{remotefile} from the machine \texttt{host}. The file is saved to the path and file specified by the string \texttt{localfile}.

\texttt{gd\_getfile(host, remotefile, localfile, filetype)} as above except the string \texttt{filetype} sets the file transfer type. When \texttt{filetype} = 'ASCII' the file transfer type will be ASCII (this is the default setting), alternatively when \texttt{filetype} = 'binary' the file transfer type is set to binary.

\textbf{Examples}

The following command copies the file 'data2.dat' from the users home directory on the remote host 'server' to the local file 'C:/data1.dat'. The file is transferred as a binary file type.

\begin{verbatim}
from gdcompute import *
gd_getfile('server.domain.com','data2.dat','C:/data1.dat',
'binary')
\end{verbatim}

This example behaves as above except the file is copied from the subdirectory 'tmp' in the users home directory.

\begin{verbatim}
gd_getfile('server.domain.com','tmp/data2.dat','C:/data1.dat',
'binary')
\end{verbatim}

The following example is similar to the first example except the file is copied from the subdirectory 'tmp' of the root directory on the remote machine.
gd_getfile('server.domain.com','/tmp/data2.dat','C:/data1.dat','binary')

Notes
A valid proxy certificate is required to use GridFTP. Suitable credentials may be required to transfer files from a remote server.

See also
gd_putfile, gd_createproxy
**gd_jobkill**

Kills a Globus GRAM job specified by a job handle.

**Syntax**

```
gd_jobkill(jobhandle)
```

**Description**

`gd_jobkill(jobhandle)` terminates the Globus job specified by the Globus job handle.

**Notes**

A valid proxy certificate for the correct user credentials is required to kill a GRAM job.

**See also**

`gd_createproxy, gd_jobsubmit, gd_jobstatus`
**gd_jobpoll**

Queries the status of a Globus GRAM job until complete.

**Syntax**

```python
isdone = gd_jobpoll(jobhandle, interval=5, maxtime=Infinity)
```

**Description**

This command polls the status of a Globus GRAM job specified by the job handle until the job is complete. This function can be used to block the process of a Python script until a job has finished. If the job fails an error is thrown.

```python
isdone = gd_jobpoll(jobhandle) where jobhandle is the handle to a Globus GRAM job. The return value isdone indicates whether the job handle returned the DONE state (1), or whether polling was aborted (0).
```

```python
isdone = gd_jobpoll(jobhandle, interval) where jobhandle is the handle to a Globus GRAM job and interval is the interval (in seconds) between polling the job handle.
```

```python
isdone = gd_jobpoll(jobhandle, interval, maxtime) as above. The argument maxtime allows an upper limit (in seconds) to be placed on the period over which the job is polled.
```

**Notes**

The state DONE returned by job handle does not necessarily indicate that the job completed successfully. A valid proxy certificate is required to query a GRAM job.

**See also**

`gd_jobstatus`, `gd_jobsubmit`, `gd_jobkill`
### gd_jobstatus

Gets the status of a Globus GRAM job.

**Syntax**

```python
status = gd_jobstatus(jobhandle)
```

**Description**

The `status = gd_jobstatus(jobhandle)` function returns an integer value indicating the status of a Globus GRAM job, where `status`:

-1 is UNKNOWN
1 is PENDING
2 is ACTIVE
3 is DONE
4 is FAILED
5 is SUSPENDED
6 is UNSUBMITTED

**Notes**

A valid proxy certificate is required to query a GRAM job.

**See also**

`gd_createproxy`, `gd_jobsubmit`, `gd_jobkill`
**gd_jobsubmit**

Submits a compute job to a Globus GRAM job manager.

**Syntax**

```python
jobhandle = gd_jobsubmit(rsl, host)
```

**Description**

This command submits the compute job described by a Resource Specification Language (RSL) string to a Globus server running a GRAM job manager. Upon a successful submission the command returns a job handle that may be used to query the status of, or terminate, the job.

```python
jobhandle = gd_jobsubmit(rsl, host) where rsl is a string describing the submitted job, and host is the name of the Globus server. Returns a GRAM job handle that may be used to query, poll or terminate the job. An error is thrown if job submission is unsuccessful.
```

**Example**

```python
from gdcompute import *
jobhandle =
gd_jobsubmit('&(executable=/bin/date)','server.domain.com')
```

**Notes**

A valid proxy certificate is required to submit a GRAM job. For more information about RSL see [http://www.globus.org/gram/](http://www.globus.org/gram/).

**See also**

`gd_createproxy, gd_jobkill, gd_jobstatus`
<table>
<thead>
<tr>
<th><strong>gd_listdir</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Lists the contents of a directory on a GridFTP server.</td>
</tr>
</tbody>
</table>

**Syntax**

```python
(files, details) = gd_listdir(host, remotedir=None,
                             listhidden=0)
```

**Description**

`(files, details) = gd_listdir(host)` returns a tuple containing `files`, a list of the names of files in `remotedir`, and `details`, a list containing dictionaries describing the details of these files in the user's home directory on the GridFTP server `host`.

`(files, details) = gd_listdir(host, remotedir)` where `files` is a list containing the filenames of files in the directory `remotedir` on the GridFTP server `host` (if `remotedir` is empty the contents of the user's home directory will be listed).

`(files, details) = gd_listdir(host, remotedir, listhidden)` the list of filenames will include hidden files if the argument `listhidden` is true (equal to 1). Otherwise the names of hidden files will not be returned (default behaviour).

**Notes**

A valid proxy certificate is required to use GridFTP.

**See also**

[gd_putfile](#), [gd_getfile](#), [gd_createproxy](#)
gd_makedir

Creates a remote directory using GridFTP.

Syntax

gd_makedir(host, directory)

Description

gd_makedir(host, directory) Creates a directory specified by the string directory on the GridFTP server specified by the string host.

Notes

A valid proxy certificate is required to use GridFTP. Suitable credentials will be required to create a directory on a GridFTP server.

See also

gd_getfile, gd_putfile, gd_rmdir, gd_rmfile
**gd_proxyinfo**

Returns information about the user's proxy certificate.

**Syntax**

\[(exists, subject) = gd_proxyinfo()\]

**Description**

This command checks the existence of the user's proxy certificate and prints information to the screen. The command also returns the subject line of the proxy certificate.

\[(exists, subject) = gd_proxyinfo()\] Returns a tuple containing `exists`, an integer indicating whether the proxy certificate exists at the default location (otherwise 0), and `subject`, the subject line of the proxy certificate.

**See also**

`gd_proxyquery`, `gd_certinfo`, `gd_createproxy`, `gd_destroyproxy`
gd_proxyquery

Queries whether a valid proxy certificate exists.

**Syntax**

```
isvalid = gd_proxyquery(proxyattrib=None,minvalue=-1)
```

**Description**

This command determines whether a valid proxy certificate exists for user's certificate. The strength or time remaining for the proxy certificate may also be queried. The location of the user's proxy certificate is specified by the cog.properties file.

```
isvalid = gd_proxyquery(proxyattrib,minvalue) returns 1 when the proxy certificate is valid, or meets the requirements of remaining lifetime or cryptographic strength specified by proxyattrib/minvalue, otherwise 0. If proxyattrib = 'time' the time remaining for the proxy certificate is queried against minvalue hours. If proxyattrib = 'strength' the cryptographic strength of the proxy certificate is queried against minvalue bits.
```

**Example**

The following example returns isvalid = 0 for a proxy certificate of strength 512.

```
from gdcompute import *
isvalid = gd_proxyquery('strength',1024)
```

0

**See also**

`gd_proxyinfo, gd_certinfo, gd_createproxy, gd_destroyproxy`
gd_putfile

Puts a file on a remote server using GridFTP.

**Syntax**
```
 gd_putfile(host, localfile, remotefile, filetype='ASCII')
```

**Description**
This command puts a local file upon a remote server using GridFTP. The user must specify the remote server name, the local file path, and the remote file path. The user can also specify the filetype.

```
 gd_putfile(host, localfile, remotefile) transfers the ASCII file localfile to the machine host. The file is saved to the path and file specified by the string remotefile.
```

```
 gd_putfile(host, localfile, remotefile, filetype) as above except the string filetype sets the file transfer type. When filetype = 'ASCII' the file transfer type will be ASCII (this is the default setting), alternatively when filetype = 'binary' the file transfer type is set to binary.
```

**Examples**
The following command places the local file 'C:/data1.dat' on the remote host 'server' in the users home directory with the file name 'data2.dat'. The file is transferred as a binary file type.

```
from gdcompute import *

gd_putfile('server.domain.com','C:/data1.dat','data2.dat', 'binary')
```

This example behaves as above except the file is placed in the existing subdirectory to the users home directory; 'tmp'.

```
 gd_putfile('server.domain.com','C:/data1.dat','tmp/data2.dat', 'binary')
```

This example is similar to the first example except the file is placed in the subdirectory to the root directory; 'tmp'.

45
gd_putfile('server.domain.com','C:/data1.dat','/tmp/data2.dat', 'binary')

Notes
A valid proxy certificate is required to use GridFTP. Suitable credentials may be required to transfer files to remote servers.

See also
gd_getfile, gd_createproxy
**gd_rmdir**

Deletes an empty remote directory using GridFTP.

**Syntax**

```
gd_rmdir(host, remotedir)
```

**Description**

`gd_rmdir(host, remotedir)` Deletes an empty directory specified by the string `remotedir` on the GridFTP server specified by the string `host`.

**Notes**

A valid proxy certificate is required to use GridFTP. Suitable credentials will be required to delete a directory on a GridFTP server.

**See also**

`gd_getfile, gd_putfile, gd_makedir, gd_rmdir`
**gd_rmfile**

Deletes a remote file using GridFTP.

**Syntax**

`gd_rmfile(host, remotefile)`

**Description**

`gd_rmfile(host, remotefile)` Deletes the file specified by the string remotefile on the GridFTP server specified by the string host.

**Notes**

A valid proxy certificate is required to use GridFTP. Suitable credentials will be required to delete a file on a GridFTP server.

**See also**

`gd_getfile, gd_putfile, gd_makedir, gd_rmdir`
**gd_rmuniquedir**

Deletes a remote directory and its contents.

**Syntax**

\[ gd_rmuniquedir(host, remotedir) \]

**Description**

This function deletes a remote directory and the files that it contains using GridFTP. The function will not delete the remote directory specified (or any of its contents) if the remote directory contains any sub-directories. This is a safety feature which is intended to mitigate the risks of wildcard deletions on a remote machine.

If the specified directory contains sub-directories an error will be thrown. Errors will also be thrown if the directory does not exist or if permission is denied to delete the directory or its contents.

\[ gd_rmuniquedir(host, remotedir) \] where *host* is the name of the GridFTP server and *remotedir* is the name of the directory to be deleted.

**Notes**

A valid proxy certificate is required to use GridFTP. Suitable credentials may be required to delete files on remote servers.

**See Also**

* gd_rmdir, gd_rmfile, gd_submitunique
**gd_submitunique**

Submits a GRAM job to a unique working directory.

**Syntax**

\[
(jobhandle, uniquedir) = gd_submitunique(rsl, host, 
   files=None, remotedir=None)
\]

**Description**

This command creates a unique working directory on a Globus server, transferring files as required, and submits the compute job to the GRAM job manager. Upon a successful submission the command returns a job handle and the name of the unique directory.

\[
(jobhandle, uniquedir) = gd_submitunique(rsl, host)
\]

where \( rsl \) is a string describing the submitted job, and \( host \) is the name of the Globus server. Returns a tuple containing the GRAM job handle and the name of the unique working directory. Where \( jobhandle \) is the handle for a successfully submitted job and \( uniquedir \) is the location of the working directory created on \( host \).

\[
(jobhandle, uniquedir) = gd_submitunique(rsl, host, files) 
\]

as above, where \( files \) is a list of the files to be transferred to the working directory on the \( host \).

\[
(jobhandle, uniquedir) = gd_submitunique(rsl, host, files, 
   remotedir)
\]

as above, where \( remotedir \) is the directory on the \( host \) within which the unique working directory is created. \( files \) can be empty if no files are required.

**Example**

This command creates a directory ‘20040427T130607_643492’ in the user’s home directory on the machine \( host \). The working directory in the user supplied RSL string is set to the unique directory.

```python
from gdcompute import *

rsl = '&(executable=/bin/date) (stdout="test.out")'

(jobhandle, dirname) = gd_submitunique(rsl, host)

print jobhandle
print dirname
```
Notes
A valid proxy certificate is required to submit a GRAM job. For more information about RSL see http://www.globus.org/gram/.

See also
gd_jobsubmit, gd_createproxy, gd_jobkill, gd_jobstatus
**gd_transferfile**

Performs a third-party file transfer using GridFTP.

**Syntax**

```python
gd_transferfile(host1, host2, remotefile1, remotefile2, filetype='ASCII')
```

**Description**

`gd_transferfile(host1, host2, remotefile1, remotefile2)` transfers the file specified by the string `remotefile1` on the GridFTP server `host1` to the file specified by `remotefile2` on `host2`.

`gd_transferfile(host1, host2, remotefile1, remotefile2, filetype)` as above except the string `filetype` sets the file transfer type. When `filetype = 'ASCII'` the file transfer type will be ASCII (this is the default setting), alternatively when `filetype = 'binary'` the file transfer type is set to binary.

**Examples**

The following command will transfer a file called `/tmp/test1` from `server1` to a file called `/tmp/test2` on `server2` in ASCII mode:

```python
from gdcompute import *
gd_transferfile('server1.domain.com','server2.domain.com', '/tmp/test1','/tmp/test2')
```

**Notes**

A valid proxy certificate is required to use GridFTP. Suitable credentials may be required to transfer files to remote servers.

**See also**

`gd_putfile`, `gd_getfile`, `gd_createproxy`
Geodise Database Toolbox

Introduction

The Geodise Database Toolbox consists of client and server tools which enable distributed users to easily manage, share and reuse their data from within the Jython scripting environment. Users with no database experience can integrate data management into their applications by calling the archive, query and retrieve functions provided by the toolbox. Any data files or variables can be stored in the Geodise archive. User defined Python dictionaries specify additional descriptive information (metadata), which can be queried to easily locate data of interest. The Geodise Database Toolbox allows you to:

- Manage data from the local Jython environment or remotely in scripts.
- Store files and variables with customized descriptive metadata.
- Organise related data into datagroups.
- Query over metadata to easily locate required data using functions or a GUI.
- Retrieve data based on logical data identities, no need to remember file locations.
- Share data with other distributed users by granting them access permissions.

There are a separate set of server side tools for the Geodise Database Toolbox. Variables and metadata are stored in an Oracle 9i or 10g database as XML, converted using the XML Toolbox. The Geodise Database Toolbox functions call data management services which utilise Grid, Web Service and database technologies with certificate based authentication and authorisation. The server side tools are not described in any detail in this document.
Tutorial

Getting started
Before using the Geodise Database Toolbox you need to register your details in the database by providing your certificate subject to an administrator, who will then assign you a username. To get your certificate subject call `gd_certinfo` from the Compute Toolbox.

```python
>>> from gdcompute import *
>>> subject = gd_certinfo()
>>> print subject
```

```
subject: C=UK,O=eScience,OU=Southampton,L=SeSC,CN=some user
issuer: C=UK,O=eScience,OU=Authority,CN=CA,E=ca-operator@grid-support.ac.uk
start date: Tue Oct 07 13:00:31 BST 2003
end date: Wed Oct 06 13:00:31 BST 2004
```

To setup the Database Toolbox call `gd_dbsetup` which will create a .geodise directory in your home directory and copy the necessary configuration files into it.

```python
>>> from gddatabase import *
>>> gd_dbsetup()
```

You will be prompted for details of your file store host (where `gd_archive` will store your files). Set `hostname` to a Globus enabled server you have GridFTP permission on, and set `hostdir` to an existing directory on that server where files can be stored. These settings will be saved in `<home_dir>/geodise/ClientConfig.xml`.

A valid proxy certificate is required to use the Database Toolbox functions, and this can be created using the function `gd_createproxy` from the Compute Toolbox.

```python
>>> gd_createproxy()
```

A GUI will appear and prompt you for your certificate passphrase. Click the ‘Create’
button to generate the proxy certificate. When this is finished click ‘Cancel’ to close the GUI.

See the Compute Toolbox Tutorial for more information on certificates and proxy certificates.

**Archiving files**
To archive a file from the local filesystem, first create a metadata dictionary containing some information that describes your file. This can be any combination of numbers, strings, lists, tuples, complex numbers and subdictionaries.

```python
>>> m = {'product': 25.5431}
>>> m['model'] = {'name': 'test_design', 'params': [1, 4.7, 5.3]}
```

Add some standard information (localName, format, comment, version or tree) about the file.

```python
>>> m['standard'] = {'comment': 'Test design model file'}
>>> m['standard']['version'] = '1.2.0'
```

The file can then be archived with the metadata.

```python
>>> fileID = gd_archive('C:/file.dat', m)
>>> print fileID
```

```
file_dat_c6afa4b4-03cb-49a4-8c4e-008c38aae413
```

In addition to the optional metadata structure, gd_archive takes a string representing the path and filename of a local file. It stores this file on a remote file store (specified in `<user_home>/geodise/ClientConfig.xml`). An ID is returned which is a unique handle that can be used to retrieve the file.

The metadata is stored in a database and can be queried to help you find relevant files. When the file is archived some additional metadata is automatically generated and stored in the standard subdictionary, regardless of whether user defined metadata was also provided. This consists of localName (the original name of the file), byteSize, format, archiveDate, createDate (when the original file was created/modified) and userID. See gd_query for further information on these
standard metadata fields (dictionary keys). You can specify your own overriding values for localName and format if you prefer. You can also include the optional user defined standard metadata fields comment, version and tree. To help data organisation the tree field can be assigned a hierarchy string, similar to a directory path, e.g. 'myuserID/designs/testmodel'.

**Querying file metadata**

To query file metadata pass a query string to the gd_query function. A query takes the form 'field.subfield = value', where = can be replaced by other comparison operators. A field is equivalent to a key in a dictionary, and a subfield is equivalent to a key in a subdictionary. More than one query condition can be included in the string using & to join them together. A call to gd_query returns a list of dictionaries, one for each matching result.

```python
>>> result = gd_query('standard.version=1.2.0 & product>25.4')
>>> print result[0]

{'standard': {'byteSize': 24, 'localName': 'file.dat', 'comment': 'Test design model file', 'version': '1.2.0', 'archiveDate': '2005-04-13 18:19:39', 'ID': 'file_dat_df89e3cd-675e-454c-a43f-c1e71de446f0', 'format': 'dat', 'createDate': '2004-09-15 15:25:33', 'datagroups': '', 'userID': 'jlw'},
'model': {'name': 'test_design', 'params': [1, 4.7, 5.3]},
'product': 25.5431}
```

gd_display is a convenient way to view your query results.

```python
>>> gd_display(result)
```
It is possible to select which metadata fields are returned in the query results. This is done by passing a string containing a comma separated list of these fields as the third argument to `gd_query`. The second argument specifies that we want to query files, but is normally omitted because it is the default.

```python
>>> r = gd_query('product>25','file','standard.ID, model.*')
>>> gd_display(r)
```

To search for some text within a metadata value use the 'like' operator together with `%` to specify any characters, or `_` to specify one character.

```python
>>> gd_query('standard.comment like %design m_del%')
```

The * wildcard can be used to represent an anonymous subfield, or any number of subfields if it appears at the beginning.

```python
>>> gd_query('*.name = test_design')
```
Use `gd_query()` without any input arguments to start the Query Graphical User Interface (GUI), see Figure 2. You can set query conditions for standard metadata by selecting an operator (=, > etc) from the drop down list next to the relevant metadata item and typing in a value. Further query conditions for user defined metadata can be entered in the ‘Query custom metadata or variables’ text field. In the following text field you can enter a comma separated list to specify which metadata items are returned for each matching query result.

Click the ‘Submit Query’ button to run your query. The corresponding `gd_query` script command is displayed, followed by the results of the query.

Figure 2 The Query GUI can be used to submit queries and view results.

Hyperlinks are provided in the query results for downloading and browsing data.
Figure 3 demonstrates that a file can be downloaded by clicking on its standard.ID hyperlink. In the Save dialog box you can use the default file name value (original name of file) or specify a new file name. Browsing data is further discussed in the Grouping data section.

Retrieving files
A file can be retrieved to the local filesystem by specifying its unique ID. This string is returned by `gd_archive` when the file is archived, and also appears in the metadata query results as `['standard'][ 'ID']`.

```python
>>> ID = result[0][ 'standard'][ 'ID']
>>> print ID
file_dat_c6afa4b4-03cb-49a4-8c4e-008c38aae413
```
The file can be retrieved to a specific file location.

```python
>>> gd_retrieve(ID,'C:/filesdir/myfile.dat')
'C:/filesdir/myfile.dat'
```

Alternatively the file can be retrieved to a specified directory (the original file name is used).

```python
>>> gd_retrieve(ID,'C:/filesdir')
'C:\filesdir\file.dat'
```

**Archiving, querying and retrieving Jython variables**

To archive a variable (v) simply pass it to `gd_archive` with an optional metadata structure (m).

```python
>>> v = {'width': 12, 'height': 6}
>>> m = {'standard': {'comment': 'measurements variable'}}
>>> varID = gd_archive(v,m)
```

It is possible to query the contents of an archived dictionary. Including ‘var’ as the second argument indicates that you want to query the contents of a variable (as opposed to the metadata of the variable).

```python
>>> result = gd_query('height=6','var')
>>> gd_display(result[0])
```

```plaintext
*** Content of the dictionary ***
standard.datagroups:
standard.varID: var_7c73ac04-cb90-4b28-988c-1e0562e4659d
height: 6
width: 12
```

The contents of the variable are returned along with a small subset of its metadata (standard.varID and standard.datagroups) which may be required for further queries. You can also query a variable's full metadata by including ‘varmeta’ as the second argument.
A variable can be retrieved into the local Jython workspace by specifying its unique ID. This string is returned when the variable is archived (e.g. `varID`) and also appears in the variable query results as `['standard']['varID']` and in the metadata query results as `['standard']['ID']`.

```plaintext
>>> v2 = gd_retrieve(varID)
>>> print v2
{'height': 6, 'width': 12}
```

### Grouping data
Related data can be logically grouped together using a datagroup as follows:

Specify metadata that applies to the whole group.

```plaintext
>>> dgmetadata = {'standard': {'comment': 'Group for experiment 123'}}
```

Call `gd_datagroup` to create a datagroup, giving it a name.

```plaintext
>>> datagroupID = gd_datagroup('Experiment 123',dgmetadata)
```

Add archived files or variables to the datagroup.

```plaintext
>>> gd_datagroupadd(datagroupID,fileID)
>>> gd_datagroupadd(datagroupID,varID)
```
Archive a new file (with no metadata this time) and add it to the datagroup.

```python
>>> gd_archive('C:/anotherfile.txt', None, datagroupID)
```

The datagroup metadata now contains references to the files and variables it contains. Datagroup metadata can be queried by including 'datagroup' as the second argument.

```python
>>> r = gd_query('standard.datagroupname=Experiment 123', 'datagroup')
```

```python
>>> gd_display(r)
```

```
*** Content of the dictionary 1 (Total dictionaries : 1) ***
standard.ID: dg_111385dd-44b8-4ac4-9ec3-f7f19af85e6e
standard.datagroupname: Experiment 123
standard.archiveDate: 2004-10-07 11:42:03
standard.userID: jlw
standard.comment: Group for experiment 123
standard.datagroups:
standard.subdatagroups:
standard.files.fileID: file_dat_c6afa4b4-03cb-49a4-8c4e...
standard.files.fileID: anotherfile_txt_8886aa7a-5464-48...
standard.vars.varID: var_7c73ac04-cb90-4b28-988c-1e0562...
*** No more results. ***
```

Metadata for the files and variables also contain references to the datagroup(s) that they belong to, with a standard.datagroups.datagroupID field for each datagroup.

Datagroups can be added to other datagroups to create a hierarchy as follows:

```python
>>> parentDatagroupID = datagroupID
>>> childDatagroupID = gd_datagroup('child datagroup')
```

Add the child datagroup (also called a subdatagroup) to the parent datagroup.

```python
>>> gd_datagroupadd(parentDatagroupID, childDatagroupID)
```

Find all the datagroups that are in the parent datagroup.
Find all the datagroups that contain the child datagroup.

```python
>>> parents = gd_query('standard.subdatagroups.datagroupID=' +
                     childDatagroupID,'datagroup')
```

Using the Query GUI you can browse between related datagroups, files and variables by clicking on hyperlinks. In Figure 4 a query on datagroup metadata has been made by selecting datagroup from the drop down list at the top of the window, then...
specifying the query conditions. The matching datagroup shown in the figure has related subdatagroups, files and variables which are displayed as hyperlinks. Clicking on the standard.vars.varID link brings up a new window containing the metadata for that variable. Clicking on standard.ID in this window will display the contents of the variable itself.

**Granting access to data.**
The gd_addusers function allows you to grant other users permission to query particular files, variables and datagroups that you own. These users may also retrieve the variables to their local Jython workspace and the files to their local filesystem (providing they have read permission for the appropriate directory on the Globus file server).

In the following example the user with username ‘bob’ is given access to an archived variable.

```python
>>> users = ['bob']
>>> gd_addusers(varID, users)
```

Access may also be granted as part of the metadata when a file or variable is archived, or when a datagroup is created.

```python
>>> m = {'access': {'users': ['bob']}}
>>> gd_archive('C:/file.dat', m)
```

**Further information.**
All of these functions have help information which can be viewed by using the gd_help command in the Jython environment.

```python
>>> gd_help(gd_datagroupadd)
```
NAME

    gd_datagroupadd( datagroupID, dataID )

DESCRIPTION

    Add an archived file, variable or subdatagroup to a datagroup.

    datagroupID  -- Unique identifier of the datagroup.
    dataID       -- Unique identifier of the file, variable or subdatagroup to add to the datagroup.

    Returns 1 if the operation was successful and 0 if it failed (for example if the datagroup does not exist).

Further descriptions and examples for each function are available in the next section of this document.
Function Reference

**gd_addusers**

Grants an array of users or user groups permission to access some data (file, variable or datagroup).

**Syntax**

```python
success = gd_addusers(ID, users, accesstype='users')
success = gd_addusers(datagroupID, users, accesstype='users')
```

**Description**

- `success = gd_addusers(ID, users)` grants other users permission to query or retrieve a file or variable, specified by its ID. A userID for each user should be provided in the `users` list. Alternatively a single user can be specified as a string.

- `success = gd_addusers(datagroupID, users)` is similar but grants other users permission to query a datagroup, specified by its ID.

- `success = gd_addusers(ID, groups, 'groups')` grants a group of users permission to query or retrieve a file or variable, specified by its ID. A groupID for each user group should be provided in the `groups` list. Alternatively a single group can be specified as a string. Every registered user is a member of the built in group 'allusers' and other user groups can be set up by the database administrator.

- `success = gd_addusers(datagroupID, groups, 'groups')` is similar but grants a group of users permission to query a datagroup, specified by its ID.

The function returns 1 if successful, or 0 if failed (for example if one of the users already has access permission or does not exist). All valid userIDs or groupsIDs in the list will be granted permission, and a warning message will be displayed for any that fail.

**Example**

Grant users with user IDs `user1` and `user2` access to an archived file.

```python
from gddatabase import *
fileID = gd_archive('C:/file.dat')
```
users = ['user1', 'user2']
gd_addusers(fileID, users)

Grant all registered users access to an archived file.

gd_addusers(fileID, 'allusers', 'groups')

**Notes**
You must be the owner of the data to give others permission to access it.

A valid proxy certificate is required (see `gd_createproxy` from the Geodise Compute Toolbox).

Your certificate subject must have been added to the authorisation database.

**See also**
`gd_archive, gd_datagroup, gd_query, gd_createproxy`
gd_archive

Stores a file or variable with some metadata into the archive.

Syntax

\[
\begin{align*}
\text{ID} &= \text{gd_archive}(	ext{filename}, \text{metadata=\text{None}}, \text{datagroupID=''} ) \\
\text{ID} &= \text{gd_archive}(\text{v}, \text{metadata=\text{None}}, \\
&\quad \quad \quad \text{datagroupID=''}, \text{datatype=''} ) \\
\end{align*}
\]

Description

\[ \text{ID} = \text{gd_archive} (\text{filename}) \]

takes a string representing a filename and archives that file in a file store (specified in the ClientConfig.xml file). Some standard information about the file (metadata) is automatically generated and can be later queried with \textit{gd_query}. A unique identifier (ID) for the archived file is returned which can be used to retrieve the file with \textit{gd_retrieve}.

\[ \text{ID} = \text{gd_archive} (\text{filename}, \text{metadata}) \]

archives a file with some user defined metadata which can later be queried with \textit{gd_query}. Standard metadata about the file is also generated.

\[ \text{ID} = \text{gd_archive} (\text{filename}, \text{metadata, datagroupID}) \]

archives a file and adds it to a datagroup specified by datagroupID. A datagroup is used to group together a collection of related files, variables and other datagroups, see \textit{gd_datagroup} and \textit{gd_datagroupadd}. To specify a datagroupID without including user defined file metadata, use a keyword argument for datagroupID, e.g. \textit{gd_archive} (myfilename, datagroupID=mydatagroupID).

\[ \text{ID} = \text{gd_archive} (\text{v}) \]

takes a variable and archives it in a database (accessible via the webservises specified in the ClientConfig.xml file). \textit{v} can be of type string, integer, float, complex, dictionary, list, or tuple. Some standard metadata about the variable is generated automatically and can be later queried with \textit{gd_query}. A unique identifier (ID) for the archived variable is returned which can be used to retrieve the variable to the workspace with \textit{gd_retrieve}. A variable can also be assigned user defined metadata and added to a datagroup by supplying a datagroupID in the same way as a file.

\[ \text{ID} = \text{gd_archive} (\text{v}, \text{metadata, datagroupID, 'var'}) \]

should be used when archiving a variable that is a string. If \textit{v} has any other type it will be
automatically detected, but when it is a string ‘var’ must be specified to indicate it is a variable and not a filename. If there is no user defined metadata or data group ID, use a keyword argument for datatype, e.g. `gd_archive(v, datatype='var')`.

**Input Arguments**

**metadata**

The keys (referred to as fields) in the `metadata` dictionary must be strings but the values can contain any combination of variables (string, integer, float, complex, dictionary, list, or tuple) necessary to describe the data. There are two special subdictionaries, `standard` and `access`, which may only contain certain values.

Some metadata is automatically generated (even when no metadata is passed to the function) and stored in the `standard` subdictionary of the `metadata` dictionary. For files and variables this consists of ID, userID and archiveDate, and for files only: byteSize, format, localName (the original name of the file) and createDate (when the original file was created/modified). Optional comment, version and tree fields can be added to `standard` and overriding values for localName and format can also be specified. The tree value is a string which can be used to represent a user defined hierarchy for the data, similar to a directory path, e.g. 'myuserID/designs/testmodel'. See `gd_query` for further information on these standard fields. Any other fields set in the `standard` subdictionary will be overwritten or removed.

The `access` subdictionary of `metadata` controls who may query and retrieve the data. The person who archived the data automatically has access to it and does not need to be added. `access` can contain two fields, each of which can be a single string or a list of strings:

- **users**
  
  User ID strings specifying which users may access the data.

- **groups**
  
  Group ID strings specifying which groups of users may access the data (currently a group must be created in the database by an administrator).

**Examples**

Archive a file with no user defined metadata.
from gddatabase import *
ID = gd_archive ('C:/file.dat')
print ID

```
file_dat_ce868f40-8de0-445e-8ae5-36c05eec25a9
```

Archive a file with some metadata, \( m \) (user defined metadata and a standard comment), and give access permission to user1 and user2.

\[
m = \{ \text{'model': \{ 'name': 'test\_design'\}} \}
m[\text{'params']} = [1, 4.7, 5.3]
m[\text{'iterations'}] = 9000
m[\text{'standard']} = { \text{'comment': 'Comment about file'}}
m[\text{'access'}] = { \text{'users': ['user1','user2']}}
gd_archive('C:/file.dat',m)
\]

Archive a file and add it to a datagroup, with no user defined metadata.

\[
dID = gd_datagroup('design opt 2004-09-03')
gd_archive('C:/file.dat',datagroupID=dID)
\]

Archive a structure with some user defined metadata.

\[
v.width = 12
v.height = 6
m.\text{standard}.\text{comment} = \text{'measurement variables'}
gd_archive(v,m)
\]

Notes
A valid proxy certificate is required to archive a file or variable (see \texttt{gd\_createproxy} from the Geodise Compute Toolbox).

You must have access to the host machine the files will be archived on. Your certificate subject must be added to the gridmap file on the host and to the authorisation database.
See also

gd_addusers, gd_retrieve, gd_query, gd_datagroup, gd_datagroupadd,
gd_createproxy
gd_datagroup

Creates a new datagroup, used to group together archived files, variables and subdatagroups.

Syntax

datagroupID = gd_datagroup(datagroupname,metadata=None,
                                   datagrouptype='')

Description

datagroupID = gd_datagroup(datagroupname) creates a new, empty datagroup with a datagroup name. The datagroupname argument can act as a user defined identifier for the datagroup, although it does not have to be unique. Some standard information about the datagroup (metadata) is also generated which can be later queried with gd_query. A unique identifier (datagroupID) is returned which can then be used to add files and variables to the datagroup while they are being archived with gd_archive. Files, variables and other datagroups already in the archive can be added to a datagroup with gd_datagroupadd.

         datagroupID = gd_datagroup(datagroupname,metadata) creates a new, empty datagroup with a datagroup name and some user defined metadata which can later be queried with gd_query. Standard metadata about the datagroup is also generated.

         datagroupID = gd_datagroup(datagroupname,metadata,
[a => monitor']) is useful for monitoring a group of data produced by a computational job. It is similar to an ordinary datagroup but stores extra index information that allows a user of gd_query to easily find the datagroup associated with their most recent job, or the most recent job meeting certain metadata criteria. This functionality is provided for convenience so that the user does not have to remember any particular metadata field names or values, or what time the datagroup was created.

Input Arguments

metadata The keys (referred to as fields) in the metadata dictionary must be strings but the values can contain any combination of variables (string, integer, float, complex, dictionary, list, or tuple) necessary to describe the datagroup. There are two special subdictionaries, standard and access, which may only contain certain values.
Some metadata is automatically generated (even when no metadata is passed to the function) and stored in the standard subdictionary of the metadata dictionary. For datagroups this consists of ID, userID and archiveDate. Optional comment, version and tree fields can also be added to standard. The tree field is a string which can be used to represent a user defined hierarchy for the data, similar to a directory path, e.g. 'myuserID/designs/testmodel'. See gd_query for further information on these standard fields. Any other fields set in the standard subdictionary will be overwritten or removed.

The access subdictionary of metadata controls who may query the datagroup. The person who created the datagroup automatically has access to it and does not need to be added. access can contain two fields, each of which can be a single string or a list of strings:

- **users**: User ID strings specifying which users may access the datagroup.
- **groups**: Group ID strings specifying which groups of users may access the datagroup (currently a user group must be created in the database by an administrator).

**Examples**

Create a datagroup with some metadata, m (user defined metadata and a standard comment), and give access permission to user1 and user2.

```python
from gddatabase import *

m = {'expnum': 123}
m['standard'] = {'comment': 'Data for experiment 123'}
m['access'] = {'users': ['user1','user2']}
datagroupID = gd_datagroup('design opt 2004-09-03',m)
print datagroupID

dg_ce868f40-8ds0-455e-9ae5-36c05epc25a9
```
Add a file to the datagroup when it is archived.

```python
gd_archive('C:/file.dat', datagroupID=datagroupID)
```

Add a variable to the datagroup after it has been archived.

```python
v = {'width': 12}
varID = gd_archive(v)
gd_datagroupadd(datagroupID,varID)
```

Create a monitored datagroup and find it with a query.

```python
monID = gd_datagroup('design job 2004-09-03', datagrouptype='monitor')
gd_datagroupadd(monID,varID)
gd_query('standard.jobIndex = max','monitor')
```

Further examples are given in `gd_datagroupadd` and `gd_query`.

**Notes**

A valid proxy certificate is required (see `gd_createproxy` from the Geodise Compute Toolbox).

Your certificate subject must have been added to the authorisation database.

**See also**

`gd_datagroupadd, gd_archive, gd_retrieve, gd_query, gd_createproxy`
**gd_datagroupadd**

Adds an archived file, variable or subdatagroup to a datagroup.

**Syntax**

```
success = gd_datagroupadd(datagroupID,ID)
success = gd_datagroupadd(datagroupID,subdatagroupID)
```

**Description**

```
success = gd_datagroupadd(datagroupID,ID) adds a file or variable to a datagroup. The datagroup is specified by its unique identifier datagroupID and the identifier of the file or variable to add is specified with ID. The datagroup must have been created with gd_datagroup and the file or variable must have been archived using gd_archive. The function returns 1 if successful, or 0 if failed (for example if the datagroup does not exist).
```

```
success = gd_datagroupadd(datagroupID,subdatagroupID) adds a datagroup (subdatagroupID) to another datagroup (datagroupID). The datagroup to be added is known as a subdatagroup. Both datagroups must have been created with gd_datagroup.
```

**Examples**

Add a file and a variable to a datagroup after they have been archived.

```
from gddatabase import *
datagroupID = gd_datagroup('design opt 2004-09-03')

fileID = gd_archive('C:/file.dat')
gd_datagroupadd(datagroupID,fileID)

v = {'width': 12}
varID = gd_archive(v)
gd_datagroupadd(datagroupID,varID)
```

Add a datagroup to another datagroup

```
datagroupID = gd_datagroup('parent datagroup')
subdatagroupID = gd_datagroup('child datagroup')
```
Notes
Only the owner of a datagroup can add data to it.

Attempting to add a file, variable or subdatagroup twice to the same datagroup will cause an error.

Attempting to add a datagroup to another datagroup that it is already the parent or ancestor of will cause an error. E.g. If datagroup \( b \) is added to datagroup \( a \), and datagroup \( c \) is added to \( b \), then \( a \) cannot be added to \( b \) or \( c \).

A valid proxy certificate is required (see `gd_createproxy` from the Geodise Compute Toolbox).

Your certificate subject must have been added to the authorisation database.

See also
`gd_datagroup, gd_archive, gd_retrieve, gd_query, gd_createproxy`
gd_dbsetup

Creates and populates the .geodise directory with configuration files.

Syntax

gd_dbsetup(hostprompt=1)

Description

gd_dbsetup() creates a .geodise directory in the user’s home directory if one does not exist then copies the necessary configuration files into it. The user is prompted to configure the name of the Globus server and directory where gd_archive will store data files and this information is saved in .geodise/ClientConfig.xml.

Example locations for the .geodise directory are:

Windows C:\Documents and Settings\your_username\.geodise
Linux $HOME/.geodise

gd_dbsetup(0) creates a .geodise directory as above but does not prompt for the name of the Globus server and directory where gd_archive will store data files, using default values instead. The default settings are either taken from a previous copy of ClientConfig.xml in .geodise or from ClientConfig.xml in the distribution.

Notes

The file .geodise/ClientConfig.xml can be edited to manually configure settings such as which Globus file store to archive files on, see installation document for more information.
**gd_db_version**

Gets the Geodise Database Toolbox version number.

**Syntax**

```python
version = gd_db_version()
```

**Description**

`version = gd_db_version()` returns the version of the current Geodise Database Toolbox for Jython release as a string of the form MAJOR.MINOR.POINT.
**gd_display**

Displays the results of a query (a list of dictionaries), or a single dictionary.

**Syntax**

```
    gd_display(qresults)
    gd_display(qresults{i})
```

**Description**

`gd_display(qresults)` can be used to display a list of dictionaries, e.g. the results of a call to the `gd_query` or `gd_querydeleted` function. This is a convenient way of viewing dictionaries to get an overview of their contents.

`gd_display(qresults{i})` displays the contents of a dictionary, e.g. a single result from a query where `i` is the index of a dictionary in the list.

**Example**

Display all the results from a query.

```python
from gddatabase import *
r = gd_query('iterations = 9000')
gd_display(r)
```

```
*** Content of dictionary 1 (Total dictionaries: 2) ***
standard.ID: file_dat_66830074-e749-4de0-b976-61f4d32
standard.localName: file.dat
standard.byteSize: 245
standard.format: dat
standard.createDate: 2004-08-23 10:40:33
standard.archiveDate: 2004-09-03 15:25:45
standard.userID: jlw
standard.comment: Comment about file
standard.datagroups:
    model.name: test_design
    params: [1, 4.7, 5.3]
    iterations: 9000
Press ENTER to continue ..., q to quit:
```
To display just one result from a query use that result’s index.

\[ \text{gd_display(r[0])} \]

**See also**

[gd_query](#), [gd_querydeleted](#)
**gd_markfordeletion**

Marks data for deletion from the archive.

**Syntax**

\[
\text{marktotal} = \text{gd\_markfordeletion}(\text{ID})
\]

\[
\text{marktotal} = \text{gd\_markfordeletion}(\text{IDs})
\]

**Description**

\[
\text{marktotal} = \text{gd\_markfordeletion}(\text{ID})
\]
takes an ID string and marks the corresponding file, variable or datagroup for deletion from the archive. The function returns 1 if successful or 0 if failed, in which case the reason is displayed in a warning message (for example the ID does not exist). Once data is marked for deletion it is no longer visible using \text{gd\_query}, \text{gd\_retrieve} or any other Database Toolbox functions (apart from \text{gd\_unmarkfordeletion} or \text{gd\_querydeleted}). The data is then eligible for permanent deletion by an administrator.

\[
\text{marktotal} = \text{gd\_markfordeletion}(\text{IDs})
\]
is similar but takes a list of ID strings and marks the corresponding files, variables and datagroups for deletion from the archive. The function returns \text{marktotal}, the total number of IDs successfully marked for deletion, and displays warning messages for those that were unsuccessful.

**Examples**

Mark a single file for deletion from the archive.

```python
from gddatabase import *
ID = gd_archive('C:/file.dat')
marktotal = gd_markfordeletion(ID)
print marktotal
```

```
1
```

Query variable metadata, and then mark the corresponding variables for deletion from the archive.

```python
q = 'standard.archiveDate > 2004-12-01 & a.b < -500'
qresults = gd_query(q, 'varmeta')
IDs = []
```
for i in range(len(qresults)):
    IDs.append(qresults[i]['standard']['ID'])

marktotal = gd_markfordeletion(IDs)
print marktotal

5

Notes
Only the owner of the data (the person who archived it) can mark it for deletion.

A valid proxy certificate is required (see \texttt{gd_createproxy} from the Geodise Compute Toolbox).

See also
\texttt{gd_unmarkfordeletion, gd_querydeleted, gd_createproxy}
**gd_query**

Performs queries over metadata or Python dictionaries stored in the archive.

**Syntax**

```python
qresults = gd_query(query=None, datasource='file',
                    resultfields='*')
```

**Description**

`gd_query()` with no input arguments starts the query GUI, a Graphical User Interface for querying metadata and structures which also allows hyperlink browsing between related data. See the Geodise Database Toolbox Tutorial for more details.

`qresults = gd_query(query)` sends a query string to the database requesting all file metadata that meets the criteria specified in the string. A query takes the form `'field.subfield = value'`, where `=` can be replaced by other comparison operators. A field is equivalent to a key in a dictionary, and a subfield is equivalent to a key in a subdictionary. More than one query condition can be included in the string using `&` to join them together. The function returns a list of metadata dictionaries, one for each matching result.

`qresults = gd_query(query, datasource)` sends a query string to the database requesting matching archived variables or metadata of a certain type, depending on the value of the `datasource` string. To query metadata set `datasource` to 'file' (default), 'varmeta' (metadata about variables), 'datagroup' or 'monitor'. A list of matching dictionaries is returned, one for each result. To query variables stored in the database set `datasource` to 'var'. In this case the function will return a list of matching variables. The only variables that can be queried in this way are dictionaries, because they contain named fields that can be searched for.

`qresults = gd_query(query, datasource, resultfields)` sends a query string to the database as above but only returns selected fields for each matching result. The `resultfields` string is a comma separated list indicating which fields should be returned for each result, for example just the `standard.ID` fields (i.e. `{'standard': {'ID': id_value}}`). The default, `*`, returns all fields. To view the query results, use function `gd_display`. 

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Input Arguments

query  A query takes the form 'field.subfield = value' where field is a key in the archived metadata/variable dictionary and subfield is a key in a subdictionary, for example iterations or standard.ID. The value is an alphanumeric value the field should contain, and can also be thought of as the value part of a dictionary entry. The operator & (meaning ‘and’) can be used to specify more than one search condition.

The following operators can be used to compare fields with values:

=    Equal to
!=   Not equal to
>    Greater than
<    Less than
>=   Greater than or equal to
<=   Less than or equal to
like  Similar to
not like  Not similar to

Similarity matches with like and not like use the following wildcards:

_    Matches any single character.
%    Matches any string of any length (including 0).

For example, 'standard.localName like %dat%' will match strings containing the phrase ‘dat’, and 'model.name like _est%' will match strings starting with any character followed by ‘est’ and then any string. To search for the characters _ and %, precede them with the \ escape character.

The operators do case sensitive comparison when used with string values. To make an operator case insensitive surround it with two # characters. For example, #=#, #!=#, #like#, #not like#.
Another wildcard, *, provides flexibility in describing the field path. For example, `model.name` can be replaced by `*.name` for a less specific search.

In addition to user defined metadata fields, the following standard metadata fields can be queried:

<table>
<thead>
<tr>
<th>Field</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>standard.ID</code></td>
<td>ID that uniquely identifies a file, variable or datagroup.</td>
</tr>
<tr>
<td><code>standard.datagroupname</code></td>
<td>Name of datagroup. Only used when querying datagroups.</td>
</tr>
<tr>
<td><code>standard.localName</code></td>
<td>Name of a local file before it was archived.</td>
</tr>
<tr>
<td><code>standard.byteSize</code></td>
<td>Size in bytes of a file.</td>
</tr>
<tr>
<td><code>standard.format</code></td>
<td>Format of file (default is its extension).</td>
</tr>
<tr>
<td><code>standard.createDate</code></td>
<td>Date the file was created/modified.</td>
</tr>
<tr>
<td><code>standard.archiveDate</code></td>
<td>Date the file or variable was archived, or the datagroup was created.</td>
</tr>
<tr>
<td><code>standard.userID</code></td>
<td>ID of the user who archived the data or created the datagroup.</td>
</tr>
<tr>
<td><code>standard.comment</code></td>
<td>Comment about the file, variable or datagroup.</td>
</tr>
<tr>
<td><code>standard.version</code></td>
<td>User defined version number for the file, variable or datagroup.</td>
</tr>
<tr>
<td><code>standard.tree</code></td>
<td>String representing a user defined data hierarchy, similar to a directory path.</td>
</tr>
<tr>
<td><code>standard.files.fileID</code></td>
<td>Each file in a datagroup.</td>
</tr>
<tr>
<td><code>standard.vars.varID</code></td>
<td>Each variable in a datagroup.</td>
</tr>
<tr>
<td><code>standard.subdatagroups.datagroupID</code></td>
<td>Each subdatagroup in a datagroup.</td>
</tr>
<tr>
<td><code>standard.datagroups.datagroupID</code></td>
<td>Each datagroup a file, variable or</td>
</tr>
</tbody>
</table>
Datagroups are collections that can contain files, variables or other datagroups, see [gd_datagroup](gd_datagroup) and [gd_datagroupadd](gd_datagroupadd).

The fields in an archived dictionary variable can also be queried in conjunction with the standard metadata fields for that variable.

**datasource** The data source indicates which type of data to query, and can be specified by one of the following strings (the default datasource value is 'file'):

- `'file'` Metadata about files.
- `'datagroup'` Metadata about datagroups.
- `'monitor'` Metadata about monitorable datagroups.
- `'varmeta'` Metadata about Jython variables.
- `'var'` Jython variables.

A datagroup that was created with the ‘monitor’ flag can be queried as an ordinary datagroup, or as a collection of data about a computational job, by setting datasource to ‘monitor’. This provides a quick and easy query mechanism for finding a user’s most recent job, or the latest job meeting certain other metadata criteria. It is provided for convenience so that the user does not have to remember any particular field names, values, or what time the datagroup was created. In addition to standard.ID, standard.userID and user defined metadata, the following standard metadata can be used together with ‘monitor’ to query a job monitoring datagroup.

- **standard.jobIndex** Job index. Special query syntax
  `jobIndex = max` gets the highest index (most recent job).
- **standard.jobName** Name of job (same as datagroupname).
- **standard.startDate** Start date of job (when the datagroup was created).
Examples
Query file metadata to find files archived on or after 1st September 2004 where iterations = 9000. A datasource argument is not required because ‘file’ is the default.

```python
from gddatabase import *
q = 'standard.archiveDate>=2004-09-01 & iterations=9000'
qresults = gd_query(q)
print len(qresults)

2

print qresults[0].keys()

['standard', 'model', 'iterations', 'params']

print qresults[0]

{'standard':
  {'byteSize': 24,
   'localName': 'file.dat',
   'comment': 'Comment about file',
   'archiveDate': '2004-09-03 15:25:45',
   'ID': 'file_dat_66830074-e749-4de0-b976-61f4d32',
   'format': 'dat',
   'createDate': '2004-08-23 10:40:33',
   'datagroups': '',
   'userID': 'jlw'},
  'model': {'name': 'test_design'},
  'iterations': 9000,
  'params': [1, 4.7, 5.3]}
```

The above output has been formatted for this document. See `gd_display` for an example of displaying the full contents of query results in an easy to read format.

```python
print qresults[0]['standard']['archiveDate']
```
Query to find files which have a name field equal to ‘test_design’ in their metadata and only return the fields standard.ID and params.

```python
q = '*.name = test_design'
qresults = gd_query(q,'file','standard.ID, params')
print qresults[0]
```

```python
{'standard':
 {'ID': 'file_dat_66830074-e749-4de0-b976-61f4d32'},
 'params':[1, 4.7, 5.3])
```

Query to find datagroups with comments containing the text ‘experiment’.

```python
q = 'standard.comment like %experiment%'
r = gd_query(q,'datagroup')
```

Query variable metadata to find the metadata for all variables that are in a particular datagroup.

```python
q = 'standard.datagroups.datagroupID = dg_ce868f40-8ds0-455...' 
r = gd_query(q,'varmeta')
```

Query variables to find dictionaries where the value of field width is between 9 and 14 inclusive.

```python
r = gd_query('width >= 9 & width <= 14', 'var')
```

Find files that have a comment in their metadata, using "" (two double quotes) to indicate an empty value.

```python
r = gd_query('standard.comment != ""')
```

Find the latest job monitoring datagroup then find the latest job monitoring datagroup which matches some other criteria.
m = {'modelver': 0.6}; m2 = {'modelver': 0.71}
gd_datagroup('design model job xyz', m, 'monitor')
gd_datagroup('design model job abc', m, 'monitor')
gd_datagroup('design model job 999', m2, 'monitor')

r1 = gd_query('standard.jobIndex = max', 'monitor')
print r1[0]['standard']['jobName']

design model job 999

r2 = gd_query('standard.jobIndex = max & modelver <= 0.6', 'monitor')
print r2[0]['standard']['jobName']

design model job abc

Notes
When querying standard date information (archiveDate or createDate), specify the date/time using the International Standard Date and Time Notation (ISO 8601) which is: "YYYY-MM-DD hh:mm:ss" (hh:mm:ss is optional).

Only results for data you are authorised to access will be returned. Function gd_addusers can be used to grant access to others.

A valid proxy certificate is required to query the database (see gd_createproxy from the Geodise Compute Toolbox).

Your certificate subject must have been added to the authorisation database.

See also
gd_display, gd_createproxy, gd_archive, gd_retrieve, gd_datagroup, gd_datagroupadd, gd_addusers
**gd_querydeleted**

Performs queries over metadata or Python dictionaries marked for deletion in the archive.

**Syntax**

```
qresults = gd_querydeleted(query, datasource='file',
                         resultfields='*')
```

**Description**

`qresults = gd_query(query, datasource, resultfields)` has exactly the same functionality as `gd_query` but performs the queries over data that has been marked for deletion using the `gd_markfordeletion` function.

`gd_querydeleted` returns a list of metadata dictionaries, one for each matching result. The `['standard']['ID']` value from each result can be passed to the `gd_unmarkfordeletion` function, which can recover data that was mistakenly marked for deletion. This function will only return results for data that has not already been permanently deleted from the archive by an administrator.

A brief description of the input arguments is given here, see `gd_query` for further information. To view the query results, use function `gd_display`.

**Input Arguments**

- **query**: A query takes the form `'field.subfield = value'` where `field` is a key in the archived metadata/variable dictionary and `subfield` is a key in a subdictionary, for example `iterations` or `standard.ID`. The value is an alphanumeric value the field should contain, and can also be thought of as the value part of a dictionary entry. The operator `&` (meaning ‘and’) can be used to specify more than one search condition.

- **datasource**: The data source indicates which type of data to query, and can be specified by one of the following strings (the default `datasource` value is 'file'):

  - `'file'`  
  - `'datagroup'`
'monitor'  Metadata about monitorable datagroups.
'varmeta'  Metadata about Jython variables.
'var'  Jython variables.

resultfields  The resultfields string is a comma separated list indicating which fields should be returned for each result, for example just the standard.ID fields (i.e. {'standard':{'ID':id_value}}).
The default, *, returns all fields.

Examples
Query variable metadata that has been marked for deletion, and then unmark the corresponding variables so that they are no longer eligible for deletion from the archive.

```
from gddatabase import *
q = 'standard.archiveDate > 2004-12-01 & a.b < -500'
qresults = gd_querydeleted(q,'varmeta')
IDs = []
for i in range(len(qresults)):
    IDs.append(qresults[i]['standard']['ID'])
unmarktotal = gd_unmarkfordeletion(IDs)
print unmarktotal
```

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Notes
When querying standard date information (archiveDate or createDate), specify the date/time using the International Standard Date and Time Notation (ISO 8601) which is: "YYYY-MM-DD hh:mm:ss" (hh:mm:ss is optional).

Only results for data marked for deletion and owned by the user (i.e. data the user archived/created) will be returned.

If the marked data has been permanently deleted from the archive by an administrator it cannot be queried.
A valid proxy certificate is required (see `gd_createproxy` from the Geodise Compute Toolbox).

Your certificate subject must have been added to the authorisation database.

**See also**

`gd_unmarkfordeletion`, `gd_markfordeletion`, `gd_display`, `gd_query`, `gd_createproxy`
**gd_retrieve**

Retrieves a file, variable or metadata from the archive to the local machine.

**Syntax**

```python
filename = gd_retrieve(ID, localpath=None, datatype=None, prompt='')
metadata = gd_retrieve(ID, localpath=None, datatype='')
v = gd_retrieve(ID)
```

**Description**

The ID needed to retrieve some data can be found in its metadata as ['standard'][ID], and is also returned by `gd_archive`.

`filename = gd_retrieve(ID, filename)` retrieves a file from the archive based on its unique identifier (ID) and saves it to a local file specified by the `filename` string. The function returns the retrieved file's new location as a string, which is equal to the `filename` argument in this case. If a file exists with the same name a prompt will appear asking whether to overwrite it.

`filename = gd_retrieve(ID, directory)` retrieves a file from the archive based on its unique identifier (ID) and saves it to a local directory specified by the `directory` string. The original name of the file will be used, which is determined by the ['standard']['localName'] property in the file's metadata, see `gd_archive` and `gd_query`. The function returns the retrieved file's new location as a string.

`filename = gd_retrieve(ID, filename, prompt='overwrite')` will retrieve a file and save it to the local file system. If a file exists with the same name it will be overwritten without prompting. This is also the case when a `directory` is given as the second argument.

`metadata = gd_retrieve(ID, datatype='metadata')` will return a metadata structure which corresponds to the file, variable or datagroup identified by ID. This is a shortcut, as the same result can be achieved using `gd_query`.

`v = gd_retrieve(ID)` returns a variable from the archive to the Jython workspace based on its unique identifier (ID).
Examples

Retrieve a file and save it with a specific file name.

```python
from gddatabase import *
fileID = gd_archive('C:/file.dat')
gd_retrieve(fileID, 'C:/filesdir/myfile.dat')

'C:/filesdir/myfile.dat'
```

Retrieve a file to a directory and use its original name.

```python
gd_retrieve(fileID, 'C:/filesdir')

'C:\filesdir\file.dat'
```

Retrieve a variable to the Jython workspace.

```python
v = {'width': 12, 'height': 6}
varID = gd_archive(v)
x = gd_retrieve(varID)
print x

{'height': 6, 'width': 12}
```

Retrieve some metadata about a file.

```python
m = gd_retrieve(fileID, datatype='metadata')
```

Notes
You can only retrieve data that you archived or that someone else has given you permission to access.

A valid proxy certificate is required to retrieve a file, variable or metadata (see `gd_createproxy` from the Geodise Compute Toolbox).
You must have access to the host machine the files will be retrieved from. Your certificate subject must be added to the gridmap file on the host and to the authorisation database.

See also

`gd_archive`, `gd_datagroup`, `gd_datagroupadd`, `gd_query`, `gd_createproxy`
gd_unmarkfordeletion

Recovers data marked for deletion, if it has not been permanently deleted by an administrator.

Syntax

unmarktotal = gd_unmarkfordeletion(ID)
unmarktotal = gd_unmarkfordeletion(IDs)

Description

unmarktotal = gd_unmarkfordeletion(ID) takes an ID string and unmarks the corresponding file, variable or datagroup so it is no longer marked for deletion from the archive. This is a safety measure to recover data that was mistakenly marked for deletion. This function is only applicable for data that has not already been permanently deleted from the archive by an administrator. The function returns 1 if successful or 0 if failed, in which case the reason is displayed in a warning message (for example the ID does not exist). If data is successfully unmarked it is visible again to gd_query, gd_retrieve and other Database Toolbox functions.

unmarktotal = gd_unmarkfordeletion(IDs) is similar but takes a list of ID strings and unmarks the corresponding files, variables and datagroups so they are no longer marked for deletion from the archive. The function returns unmarktotal, the total number of IDs successfully unmarked for deletion, and displays warning messages for those that were unsuccessful.

Examples

Unmark a single file so that it is no longer eligible for deletion from the archive.

```
from gddatabase import *
ID = gd_archive('C:/file.dat')
gd_markfordeletion(ID)
unmarktotal = gd_unmarkfordeletion(ID)
print unmarktotal
```

1

Query variable metadata that has been marked for deletion, and then unmark the corresponding variables so that they are no longer eligible for deletion from the
archive.

```
q = 'standard.archiveDate > 2004-12-01 & a.b < -500'
qresults = gd_querydeleted(q, 'varmeta')
IDs = []
for i in range(len(qresults)):
    IDs.append(qresults[i]['standard']['ID'])

unmarktotal = gd_unmarkfordeletion(IDs)
print unmarktotal
```

5

**Notes**
Only the owner of the data (the person who archived it) can unmark it for deletion.

If the marked data has been permanently deleted from the archive by an administrator it cannot be recovered.

A valid proxy certificate is required (see *gd_createproxy* from the Geodise Compute Toolbox).

**See also**
gd_markfordeletion, gd_querydeleted, gd_createproxy
XML Toolbox

Introduction

The XML Toolbox for Jython allows users to convert and store variables and structures from the Jython workspace into the plain text XML format, and from this XML format to Jython. This XML format can be used to store parameter structures, variables and results from engineering applications in non-proprietary files, or XML-capable databases, and can be used for the transfer of data across the Grid. The toolbox contains bi-directional conversion routines implemented as four small intuitive and easy-to-use Python functions. As an additional feature, this toolbox allows the transparent transfer of data from the Jython scripting environment to the Matlab Problem Solving Environment and vice versa.

- Jython structures and variables can be stored in an XML format and used by other tools.
- XML representations can be stored and queried using the functions provided by the Geodise Database Toolbox.
- The ability to leverage XML and database technologies makes the data available beyond the Jython environment, and facilitates data sharing and reuse between users, e.g. with those of the XML Toolbox for Matlab.
- Access to XML data-driven tools such as Web Services becomes more transparent to engineering users.

The size of data structures the XML Toolbox can deal with is only limited by the available memory; as an indication, 60MB large data structures can be easily converted on a 256MB PC running Jython.

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Table 5 XML Toolbox functions
**Tutorial**

The XML Toolbox for Jython can be used independently of the Compute and Database Toolboxes. No proxy certificate is required to make use of its functionality. Two jar archives (which are included in the *lib* subdirectory) are required for it to work: jdom.jar and jnumeric-0.1a3.jar (or a similar version).

**Getting started**

Before using the Geodise XML Toolbox in the Jython environment, you need to import the *gdxml* module. There is an example in the *demo_xml.py* script.

Use either

1. >>> import gdxml
   and then, for example, to call xml_format() use:
   >>> gdxml.xml_format(…)

   or

2. >>> from gdxml import xml_format
   and then, for example, to call xml_format() use:
   >>> xml_format(…)

   or

3. >>> from gdxml import *
   and then, for example, to call xml_format() use:
   >>> xml_format(…)

**Converting Python data types to XML**

All common Python built-in data types can be converted into XML (with or without data type attributes) with the simple-to-use command *xml_format*. We highlight the differences in XML output structure in the following three examples.

```python
>>> v = {}
>>> v['a'] = 1.2345
>>> v['b'] = 'This is a string.'
>>> v['c'] = ('alpha','beta')
>>> v['d'] = 12345
>>> v['e'] = {'sub' : {'subsub' : 'subsubsub'}}
```

This first example shows the formatting of the variable *v* with no additional input parameters specified. The XML is formatted in such a way that any subsequent parsing of the created XML string with *xml_parse* reconstructs an exact copy of the original Jython data structure.

```python
>>> xmlstr = xml_format(v)
>>> print xmlstr
```
The XML attributes idx, type and size, which allow the exact reconstruction of the data types in Jython, can be turned off by specifying the second parameter in the xml_format function call as 'off'. This results in a more generic formatting of the structure, however, the XML contents are now interpreted purely as strings when parsed back into Jython as type and size information are lost:

```python
>>> xmlstr = xml_format(v, 'off')
>>> print xmlstr

<root>
  <b>This is a string.</b>
  <a>1.2345</a>
  <e>
    <sub>
      <subsub>subsubsub</subsub>
    </sub>
  </e>
  <d>12345</d>
  <c>
    <item>alpha</item>
    <item>beta</item>
  </c>
</root>
```

The user can write the XML representation of a Jython variable immediately into an XML file using the command xml_save. This command uses the same XML format as the function xml_format.

**Converting XML to Python data types**

As XML can contain any arbitrary contents as long as they follow the W3C XML Recommendation (www.w3.org), parsing and translating of these constructs into a Jython-specific environment can be complex. The function xml_parse allows the conversion of XML strings in two ways into Jython data structures. These correspond to the techniques shown above for xml_format with and without the XML attributes.
If the XML contains specific type attributes, such as created by `xml_format` with attributes switched on (i.e. the `idx`, `type`, `size` attributes), the XML Toolbox will be able to re-create the Python data type and content described by the XML string.

For example,

```xml
xmlstr = '<root idx="1" type="integer" size="1 1">42</root>'
```

can be parsed using the command

```python
>>> v = xml_parse(xmlstr)
```

and returns the variable

```python
>>> print v
42
```

As a more complex example,

```python
# Paste this assignment into a Python script and run it:
xmlstr = ""
<root xml_tb_version="3.1" idx="1" type="struct" size="1 1">
  <a idx="1" type="double" size="1 1">1.2345</a>
  <b idx="1" type="double" size="2 4">1 5 2 6 3 7 4 8</b>
  <c idx="1" type="char" size="1 17">This is a string.</c>
  <d idx="1" type="cell" size="1 2">
    <item idx="1" type="char" size="1 5">alpha</item>
    <item idx="2" type="char" size="1 4">beta</item>
  </d>
  <e idx="1" type="boolean" size="1 1">0</e>
  <f idx="1" type="struct" size="1 1">
    <sub1 idx="1" type="struct" size="1 1">
      <subsub1 idx="1" type="double" size="1 1">1</subsub1>
      <subsub2 idx="1" type="double" size="1 1">2</subsub2>
    </sub1>
  </f>
  <g idx="1" type="struct" size="1 2">
    <aa idx="1" type="cell" size="1 2">
      <item idx="1" type="char" size="1 5">g1aa1</item>
      <item idx="2" type="char" size="1 5">g1aa2</item>
    </aa>
    <aa idx="2" type="cell" size="1 1">
      <item idx="1" type="char" size="1 5">g2aa1</item>
    </aa>
  </g>
</root>
"
```
can be parsed using the command

```python
>>> v = xml_parse(xmlstr)
```

and returns the (immutable, non-sorted) data structure

```python
>>> print v
{'b': [[1.0, 2.0, 3.0, 4.0], [5.0, 6.0, 7.0, 8.0]],
'a': 1.2345,
'g': [{'aa': ['g1aa1', 'g1aa2']}, {'aa': ['g2aa1']}],
'f': {'sub1': {'subsub1': 1.0, 'subsub2': 2.0}},
'e': 0,
'd': ['alpha', 'beta'],
'c': 'This is a string.'}
```

which corresponds exactly to the Jython variable used in `xml_format` to create the XML string.

If we use the same command, `xml_parse`, but tell the parser to ignore the attributes with the command

```python
>>> v_wo_att = xml_parse(xmlstr,'off')
>>> print v_wo_att
```

we obtain a dictionary where types and sizes of the data will not be adapted to match standard Python data types, that means that all alphanumeric content will be returned as strings.

```python
{'b': '1 5 2 6 3 7 4 8',
'a': '1.2345',
'g': [{'aa': 'g1aa2'}, {'aa': 'g2aa1'}],
'f': {'sub1': {'subsub1': '1', 'subsub2': '2'}},
'e': '0',
'd': 'beta',
'c': 'This is a string.'}
```

The structural information (in fields f and g) is still preserved, although nested list contents, such as in field b, and numeric values, such as in fields a and e, are returned as pure strings.
Function Reference

xml_format

Converts a Jython variable into an XML string.

Syntax

```python
xmlstr = xml_format(v, attswitch='on', name='root')
```

Description

xml_format converts Jython variables and data structures (including deeply nested data structures) into XML and returns the XML as string.

Input Arguments

- `v`: Jython variable of type int, float, long, string, dictionary, list, tuple, complex

  - `attswitch`: optional, default='on':
    - 'on' writes header attributes `idx`, `size`, `type` for identification by Jython when parsing the XML later;
    - 'off' writes "plain" XML without header attributes.

  - `name`: optional, give root element a specific name, e.g. 'project'.

Output Arguments

- `xmlstr`: string, containing XML description of the variable `v`.

The root element of the created XML string is called 'root' by default but this can be overwritten with the `name` input parameter. A default `xml_tb_version` attribute of "X.Y-py" is added to the root element unless `attswitch` is set to 'off'. X and Y are Version numbers which identify the toolbox used.

If `attswitch` is set to 'on' (by default), the attributes `idx`, `type`, and `size` will be added to the XML element headers. This allows `xml_parse` to parse and convert the XML string correctly back into the original Jython variable or data structure. If `attswitch` is set to 'off', some of the information is lost and subsequently the contents of XML elements will be read in as strings when converting back using
xml_parse (see tutorial section).

Examples

This example shows how to convert a simple number into an XML string. Note that we could have used xml_format(5.0) instead.

```python
from gdxml import *

v = 5.0
xmlstr = xml_format(v)
print xmlstr
```

```xml
<root xml_tb_version="0.1-py" idx="1" type="double"
    size="1 1">5</root>
```

We can tell the command to ignore all the attributes and obtain the following XML:

```python
xmlstr = xml_format(v,'off')
print xmlstr
```

```xml
<root>5</root>
```

The root elements can be assigned a different name by adding this as third parameter to the xml_format function:

```python
xmlstr = xml_format(v,'off','myXmlNumber')
print xmlstr
```

```xml
<myXmlNumber>5</myXmlNumber>
```

Strings can also be converted into XML:

```python
v = 'The Hitchhikers Guide to the Galaxy'
xmlstr = xml_format(v)
print xmlstr
```

```xml
<root xml_tb_version="0.1-py" idx="1" type="char" size="1 35">
The Hitchhikers Guide to the Galaxy</root>
```
One of the most powerful ways to use the XML Toolbox is to convert whole deeply nested data structures into XML:

```python
v = {'project' : {'name' : 'my Project no. 001'}}
v['project']['date'] = '2005-01-01'
v['project']['uid'] = '208d0174-a752-f391-faf2-45bc397'
v['comment'] = 'This is a new project'

xmlstr = xml_format(v,'off')
print xmlstr

<root>
  <project>
    <name>my Project no. 001</name>
    <date>2004-09-09 16:18:29</date>
    <uid>208d0174-a752-f391-faf2-45bc397</uid>
  </project>
  <comment>This is a new project</comment>
</root>
```

See also

- `xml_parse`
- `xml_load`
- `xml_save`
**xml_load**

Loads an XML file and converts its content into a Jython variable.

**Syntax**

```python
v = xml_load(filename, attswitch='on')
```

**Description**

`xml_load` reads the file given in parameter `filename` and uses `xml_parse` to convert it into a Jython data structure or variable. If the file cannot be found, an error will be displayed.

**Input Arguments**

- `filename` : filename of xml file to load (if extension .xml is omitted, `xml_load` tries to append it if the file cannot be found).
- `attswitch` : optional, default='on':
  - 'on' takes into account XML attributes `idx`, `size`, `type`
  - 'off' ignores attributes in XML element headers.

**Output Arguments**

- `v` : Jython data structure or variable.

**Examples**

This example simply loads the sample file from the given location and converts its contents to a Jython data structure. (The file has previously been created using `xml_save`).

```python
from gdxml import *

v = xml_load('c:/data/myfavourite.xml')
print v
```

```python
{'name' : 'Google',
'url' : 'http://www.google.com',
'rating' : 5,
'description' : 'Great search functionality for the web'}
```

In the following example, we perform the same action, however, as we are specifying
the additional parameter 'off' for attributes, the \texttt{idx}, \texttt{size}, and \texttt{type} attributes are ignored and the result is slightly different: \texttt{v['rating']} in this case is returned as a string variable, '5'.

\begin{verbatim}
v = xml_load('c:/data/myfavourite.xml','off')
print v

({'name': 'Google',
  'url': 'http://www.google.com',
  'rating': '5',
  'description': 'Great search functionality for the web'})
\end{verbatim}

\textbf{See also}
\begin{itemize}
  \item \texttt{xml_format}, \texttt{xml_parse}, \texttt{xml_save}
\end{itemize}
xml_parse

Parses an XML string, xmlstr, and returns the corresponding Jython variable v.

Syntax

\[
v = \text{xml_parse}(\text{xmlstr}, \text{attswitch}=\text{'on'})\]

Description

This is a non-validating parser. XML processing entries or comments starting with '<?' or '<!', are ignored by the parser.

Input Arguments

xmlstr       XML string, for example read from a file.

attswitch    optional, default='on':
'on' reads XML header attributes idx, size, type if present and interprets these to create the correct Jython data types.
'off' ignores XML element header attributes and interprets contents as strings.

Output Arguments

v             Jython variable or structure.

Examples

This example shows how to define a simple XML string and parse it into a Jython variable. As the idx, type, and size attributes are defined, the resulting Jython data structure conforms to these specifications (list of size [1x2]).

\[
\text{xmlstr} = \text{'}<\text{root}\text{ idx}=\text{''1'' type=\text{''double'' size=\text{''1 2''}}}>3.1416
1.4142</\text{root}>\text{'}
\]

from gdxml import *
V1 = xml_parse(xmlstr)
print V1

\[
[3.1416, 1.4142] \% (type jclass org.python.core.PyList)
\]

Again, setting the attswitch parameter to 'off' lets the parser ignore the attributes
and the returned variable is interpreted as a string.

```python
V2 = xml_parse(xmlstr,'off')
print V2

'3.1416 1.4142'   % (type jclass org.python.core.PyString)
```

Let's define a more complex data set in XML and convert it into a Jython data structure:

```python
# Paste this assignment into a Python script and run it:
xmlstr = ""
<root>
  <project>
    <name>myProjectName</name>
    <date>2004-09-13</date>
    <bytes>10472</bytes>
  </project>
  <project>
    <name>myProject Two</name>
    <date>2004-09-13</date>
    <bytes>9851</bytes>
  </project>
</root>
"

v = xml_parse(xmlstr)
print v
```

```python
[['project':
  {'bytes': '10472',
   'date': '2004-09-13',
   'name': 'myProjectName'},
  {'project':
   {'bytes': '9851',
    'date': '2004-09-13',
    'name': 'myProject Two'}}]
```

See also

xml_format, xml_load, xml_save
**xml_save**

Stores XML representation of a Jython variable or data structure in XML format in a file.

**Syntax**

```python
xml_save(filename, v, attswitch='on')
```

**Description**

xml_save stores a Jython variable in plain text XML format into the file specified by the user.

**Input Arguments**

The Jython variable `v` can be any of the types supported by `xml_format`.

- `filename`: full filename (including path and extension).
- `v`: Jython variable or data structure to store in file.
- `attswitch`: optional, 'on' stores XML type attributes `idx`, `size`, `type` (default), 'off' doesn't store XML type attributes.

**Examples**

This example saves a Jython dictionary as XML in a file at a given location.

```python
from gdxml import *

v = {}
v['name'] = 'Google'
v['url'] = 'http://www.google.com'
v['rating'] = 5
v['description'] = 'Great search functionality for the web'
xml_save('c:/data/myfavourite.xml', v)
```

**Notes**

xml_save uses xml_format and then stores the resulting XML string in the file with the given filename.

**See also**

`xml_format`, `xml_parse`, `xml_load`
Utilities

The following utility functions are available with the Geodise Toolboxes for Jython.

Function Reference

**gd_help**

Print help information about a GeodiseLab module or function.

Syntax

```
gd_help(target,hidden=1)
```

Description

This command prints information about any module, function or class in the Jython workspace. The inline documentation of the object is printed, and the contents of the object are formatted and displayed.

```
gd_help(target)  where target is the module, function or class to be displayed. When target is a function the input arguments will be inspected and printed. When target is a module or class the contents of the object will be recursively inspected ("private" functions will not be displayed).
```

```
gd_help(target,hidden) when hidden is false all of the functions contained in module and classes will be displayed, otherwise private functions (those whose name begin with an underscore) will not be printed.
```

Note

The function gd_help is available in the modules gdcompute, gddatabase and gdxml.

Example

```
>>> from gdxml import gd_help, xml_format
>>> gd_help(xml_format)
```
Help on function xml_format:

NAME
xml_format( V, attswitch='on', name='root' )

DESCRIPTION
Formats the variable V into a name-based tag XML string.

V          -- a string, number, complex, list, tuple, dictionary,
              or instance
attswitch  -- 'on'-- writes attributes, 'off'-- writes "plain" XML
name       -- give root element a specific name, eg. 'project'