Pipeline Pilot Cresset Package V2.6.0 Administrator Guide

Supported Platforms

Pipeline Pilot Server

The Cresset components are supported under Pipeline Pilot 18.1 and later releases. The tables below show the supported platforms for the Cresset Package and the underlying command line binaries. Note that the Spark™ components requires the Pipeline Server to have access to the Spark databases. The Cresset supplied databases require a minimum of 6GB of disk space up to a maximum of 40GB.

Minimum server specifications

Hardware	Specifications
RAM	4GB
Processor	Intel i5 processor or equivalent
Disk space	1GB

Recommended server specifications to install all binaries

Hardware	Specifications
RAM	8GB
Processor	Intel i7 or equivalent
Disk space	16GB

Supported Operating Systems

Windows®	Linux®
Windows Server 2019	Red Hat Enterprise Linux 7

Pipeline Pilot Clients

Installing Spark, Forge™ and Flare™ onto the client's machines will make some of the Cresset Package components easier to use. The tables below show the supported platforms for the Cresset Package and the underlying command line binaries.

Minimum client specifications

Hardware	Specifications
RAM	4GB
Processor	Intel i5 processor or equivalent
Disk space	1GB

Recommended client specifications

Hardware	Specifications
RAM	8GB
Processor	Intel i7 or equivalent
Disk space	1GB

Supported Operating Systems

Windows®	Linux®
Windows 10	Red Hat Enterprise Linux 7

Installation

The Cresset Package wraps functionality of key binaries and hence both the application binary and the Cresset Package must be installed. Operation of the binaries is subject to a license agreement and requires a valid license file (see 'Licensing' section below).

Application binaries

Installation of the Cresset application binaries is described in detail in the release notes for the individual binaries or in general at https://www.cresset-group.com/support/support-resources/installing-desktop-applications/.

To make full use of the Cresset Package, Forge, Spark, Flare and XedTools™ should be installed and licensed on the Pipeline Pilot Server. If an application is not installed, the components which call that application will not function.

Installing Spark on the client's machines will make some of the Cresset Package Spark components easier to use. Additionally, the 'Cresset Molecule Viewer (on Client)' and 'Forge Model Viewer (on Client)' components require Forge to be installed onto the client's machines. 'Flare Ligand and Protein Viewer (on Client)' requires Flare to be installed onto the client's machines.

The required versions of the applications for both the client and server are shown below. If the applications are out of date, then contact us at support@cresset-group.com to get the latest versions.

Application	Minimum Version
Forge	10.6
Flare	4.0
Spark	10.6
XedTools	3.2

Dependencies

The Cresset Package requires the following Collections to be installed:

- Chemistry Collection
- Data Modeling Collection

Cresset Package

The pkgutil tool is used to install the Cresset Package and is described in chapter 6 of the 'Application Packaging Guide' of Pipeline Pilot. Installation instructions are detailed below. You will need to use an account with the appropriate privileges.

Linux

1. Logon to the Pipeline Pilot Server

2. Setup the environment

```
> cd <Pipeline Pilot install Directory>/linux_bin
> source ./ppvars.sh
```

3. List the installed packages

```
> pkgutil -l
```

4. If cresset/chemistry is already listed then remove it

```
> pkgutil -u cresset/chemistry
> rm -rf ../apps/cresset/
```

5. Unzip the Cresset Package and place it into the apps directory on to the server

```
> unzip –d ../apps/ /path/to/Cresset_PipelinePilot_<version>.zip
```

6. Install the Cresset Package

```
> pkgutil -i cresset/chemistry
```

Windows

1. Logon to the Pipeline Pilot Server
2. Setup the environment (Note that the command prompt may require Administrator privileges depending on your Pipeline Pilot setup)

```
> cd <Pipeline Pilot install Directory>\bin
```

3. List the installed packages

```
> pkgutil.exe -l
```

4. If cresset/chemistry is already listed then remove it

```
> pkgutil.exe -u cresset/chemistry
> rmdir /S ..\apps\cresset
```

5. Unzip the Cresset Package and place it into the `<Pipeline Pilot install Directory>\apps` directory on to the server
6. Install the Cresset Package

```
> pkgutil.exe -i cresset/chemistry
```

When the clients are restarted the components will appear under **Components > Chemistry > Cresset** and examples on how to use the components will appear under **Protocols > Examples > Chemistry > Cresset**.

Global Properties

Binaries

To execute correctly, many components requires the location of the corresponding binary to be set as a Global Property.

To update the Global Properties:

1. Open the Global Properties page in the Pipeline Pilot Administration Portal.

2. In the 'Package-defined Global Protocol Properties' section set the 'Package' dropdown box to 'Cresset/Chemistry'.
3. Update each Property shown in the table below to point to where the Cresset software is installed on the pipeline server.

Property	Default Value (Linux, Windows)	Components
ForgeAlign_exe	/opt/cresset/Forge/bin/falign C:\Program Files\Cresset-BMD\Forge\falign.exe	Forge Align
ForgeBuild_exe	/opt/cresset/Forge/bin/fbuild C:\Program Files\Cresset-BMD\Forge\fbuild.exe	Forge Build
ForgeScore_exe	/opt/cresset/Forge/bin/fscore C:\Program Files\Cresset-BMD\Forge\fscore.exe	Forge Score
ActivityMiner_exe	/opt/cresset/Forge/bin/aminer C:\Program Files\Cresset-BMD\Forge\aminer.exe	Activity Miner
FieldTemplater_exe	/opt/cresset/Forge/bin/ftemplater C:\Program Files\Cresset-BMD\Forge\ftemplater.exe	FieldTemplater
ForgeSurface_exe	/opt/cresset/Forge/bin/fsurface C:\Program Files\Cresset-BMD\Forge\fsurface.exe	Forge Surface Writer
Sparkcl_exe	/opt/cresset/Spark/bin/sparkcl C:\Program Files\Cresset-BMD\Spark\sparkcl.exe	Spark Database Search Spark Database Search (on Client) Spark Database List Viewer Visual Spark Database Selector
Sparkdb_exe	/opt/cresset/Spark/bin/sparkdb C:\Program Files\Cresset-BMD\Spark\sparkdb.exe	Generate Spark Database
xedex_exe	/opt/cresset/xed/bin/xedex C:\Program Files (x86)\Cresset-BMD\XED\xedex.exe	XedeX
xedmin_exe	/opt/cresset/xed/bin/xedmin C:\Program Files (x86)\Cresset-BMD\XED\xedmin.exe	XedMin
xedconvert_exe	/opt/cresset/xed/bin/xedconvert C:\Program Files (x86)\Cresset-BMD\XED\xedconvert.exe	Cresset Molecule Writer
pyflare_exe	/opt/cresset/Flare/bin/pyflare C:\Program Files\Cresset-BMD\Flare\pyflare.exe	pyflare

Blaze

The Blaze components require the URL to the Blaze REST service. Each user of the Blaze component will also require a username and password for the Blaze Server. See the Blaze manual for instructions. Note the Blaze REST interface was added in Blaze 10.2.

Property	Example Value	Components
BlazeUrl	http://example.com/blaze/ui/rest.cgi	Blaze

N.B. Pipeline Pilot does not permit the blinding of passwords in all situations. In particular, the Blaze search node requires use of a plain text password to enable selection of the collections to search. If this is unacceptable to you then please [contact us](#) to discuss alternatives.
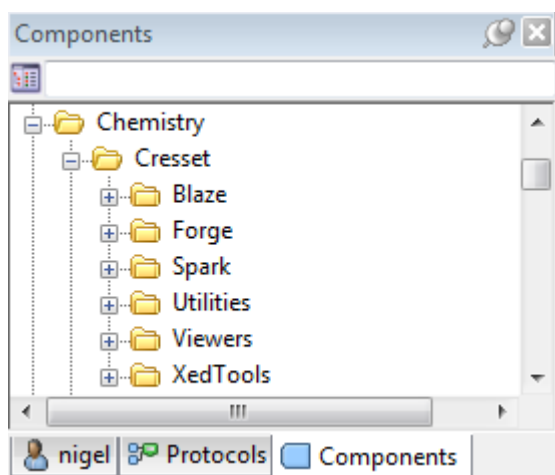
Cresset Engine Broker™

The [Cresset Engine Broker](#) can enable several components to use the power of your computing cluster to reduce the time it takes for the node to run. To use the Cresset Engine Broker set the CressetEngineBroker property to 'hostname:port' where 'hostname' is the name or IP address of the server running the Cresset Engine Broker and 'port' is the port the Cresset Engine Broker is running on.

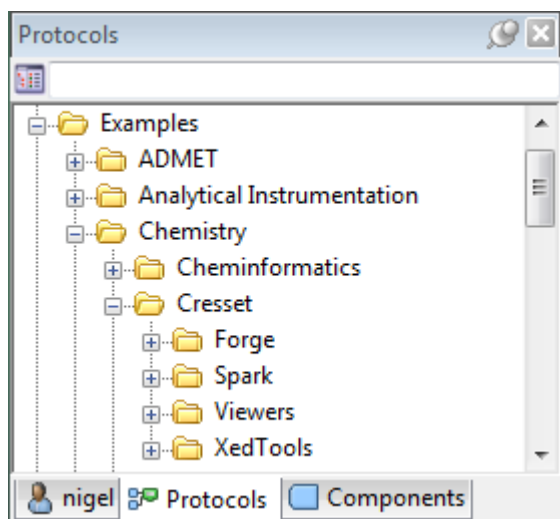| Property	Example Value	Components
CressetEngineBroker	example:9000	Forge Align Forge Build Forge Score Activity Miner FieldTemplater Spark Database Search Spark Database Search (on Client) Generate Spark Database pyflare

Alternatively, the environment variable 'CRESSET_BROKER' can be set on each PipelinePilot server instead of using the global property.

Verify Installation

1. Start the 'Pipeline Pilot Client'
2. Select the Components tab
3. Verify that the **Chemistry > Cresset** directory is present.

4. Select the Protocols tab
5. Verify that the Examples > Chemistry > Cresset directory is present.

Licensing

The software used by the Cresset Package requires a valid license file. If you are a customer and cannot locate your license file, then please contact Cresset support (support@cresset-group.com). Alternatively, contact us at enquiries@cresset-group.com for more information. License files should be placed in one of the locations detailed at https://www.cresset-group.com/support/support-resources/license-file-locations/.

Known Issues and Bugs

There are no known bugs or issues with the supported Pipeline Pilot versions (>18.1).

Support

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