Cresset Engine Broker™ V2.4.2 Release Notes

About CEBroker

The [Cresset Engine Broker](#) is a utility to connect your Cresset applications to FieldEngine resources on other computers. It allows Forge, Spark and Flare to use the full power of distributed computing resources with little or no configuration required.

Cresset's tools have always had the capability to distribute their calculations remotely using our FieldEngine technology. However, this could sometimes be difficult to configure. This tool sits in between the desktop application and existing FieldEngines and can also spawn new FieldEngine processes in response to demand. The result is a dynamically configured computing resource that is simple to set up and use and puts the power of a supercomputer on your desktop.

- Use hundreds of cores to process calculations from one Forge, Spark or Flare project

- Submit calculations to queueing systems such as Grid Engine or Platform LSF

- Connect the spare processing capacity of computers in your lab to your desktop

- Seamlessly join Windows and Linux machines into a single processing pool

- Run large virtual screening runs in a few hours.

Supported Platforms

Minimum specifications

Hardware	Specifications
RAM	1GB
Processor	Intel i3 processor or better
Disk space	100MB

Recommended specifications

Hardware	Specifications
RAM	2GB
Processor	Intel i5 processor or better
Disk space	200Mb

Supported Operating Systems

Red Hat Enterprise Linux 7® (64 bit).

Installation

1. Browse to the Linux folder of the CEBroker distribution media.
2. Install the CEBroker re-locatable rpm package using one of the command lines below (where `<vers>` is the version number, `<arch>` is the architecture and `<path>` is the install location (`/opt` by default):

```
yum install cresset-cebroker-<vers>-1.<arch>.rpm
```

or

```
rpm -i [--prefix <path>] cresset-cebroker-<vers>-1.<arch>.rpm
```

3. Alternatively, unpack the `CEBroker_<vers>.<arch>.tgz` file to a suitable location (e.g. `$HOME` or `/usr/local` or `/opt`).

In the default RPM install, CEBroker will be installed as a service called '`cresset_cebroker2`', run as the 'cebroker' user. The service will be set to start automatically (see the 'Configuration' section below).

Licensing

To run CEBroker you will require a valid license file, which will be supplied by Cresset, usually as an attachment to an email. If you cannot locate your license file, then please contact support@cresset-group.com. The license file should be placed in one of the directories detailed at https://www.cresset-group.com/support/support-resources/license-file-locations/.

Configuration

The behavior of the CEBroker service can be controlled by editing the `/etc/sysconfig/cebroker2` file. In the default installation, the broker will start up to 4 FieldEngines on the local machine on request.

The broker daemon calls a script to start FieldEngines. There are example scripts in the '`doc`' directory of the installation tree (`/opt/cresset/cebroker2` by default). The example configuration scripts cover starting FieldEngine processes on the local machine and for submitting them to a Grid Engine queue. Please contact Cresset support (support@cresset-group.com) for assistance in configuring CEBroker to your computing facilities.

Cresset desktop and command line applications can be configured to contact the broker using the machine name and port in the 'Processing' preference settings (for GUIs) or using the '-g' switch (command lines). Alternatively the environment variable '`CRESSET_BROKER`' can be used to specify the machine and port using the format `CRESSET_BROKER=hostname:port`.

Uninstalling the CEBroker

To uninstall the Cresset Engine Broker if installed from RPM, do

```
rpm -e cresset-cebroker2
```

To uninstall if installed from a tar file, just delete the CEBroker directory and remove any init scripts or system unit files that you installed to run it as a service.

Changes in version 2.4.2

*   Improved performance and behavior of the CEBroker when used to run ligand-based alignment, ligand minimization and docking experiments at a 10K scale from Flare™

*   Improved performance when working on low bandwidth internet connections

*   Fixed issue which caused the CEBroker fail to detect that a FieldEngine had shut down

*   Fixed bug which on rare occasions caused a critical error on Flare.

Changes in version 2.4

- New queueing system, handling multiple users connecting to the broker and competing for available resources
- Multiple start_XXX_engine.sh scripts are now available to support different queueing systems
- Improved handling of hostname resolution and subnet choice
- Fixed bug which caused manually connected FieldEngines to become non-contactable after a period of time

Changes in version 2.3

- New 'keepalive' messages to correctly track connected Field Engine instances
- New feature to abort any running jobs when losing the connection to the network, leaving the Field Engines connected and available
- Updated SysV and system scripts to honor the -g parameter to use GPUs
- Fixed bug which caused the CEBroker to silently fail when trying to connect to Field Engines whose name could not be resolved.

Changes in version 2.2

- Improved system integration for RHEL 7
- Fixed some possible deadlocks with network sockets
- Improved and more informative logging
- Updated to use Qt 5.9: fixes some network issues
- The username is now passed to the broker and can be passed on to the start-engines script. This allows computational resources started by the broker to be assigned to the user requesting them, facilitating cost management
- Fixed bugs that occurred if an obsolete FieldEngine tries to connect to the broker
- Fixed problems that occurred when using CEBroker without a start-engines script
- Fixed DNS issues with using FieldEngines on the Amazon cloud.

Changes in version 2.1

- Fixed several threading bugs.

Changes in version 2.0

- Version 2 represented a major change in architecture. In version 1, the CEBroker referred FieldEngine locations to the application, and subsequent communication happened directly between the application and the FieldEngine. This caused issues in cases where the FieldEngines were running in a disconnected network and could not be contacted directly by the application. In version 2 the CEBroker acts as a relay: the application communicates solely with the CEBroker, and the CEBroker communicates with the FieldEngines.

- Version 2 is not backwards compatible with Version 1. Early application versions (e.g. Spark and Forge <=10.4) cannot use version 2.

Version 1.0

- Initial release.

Known Issues and Bugs

There are no known bugs or issues.

Found a bug or problem that is not listed? Please contact us and help improve our software!

Support

Cresset	+44 (0)1223 858890
New Cambridge House	support@cresset-group.com
Bassingbourn Road	www.cresset-group.com
Litlington	Twitter: @cressetgroup
Cambridgeshire, SG8 0SS, UK	LinkedIn: Cresset group