



# FOQUS (Framework for Optimization, Quantification of Uncertainty and Sensitivity)

## INSTALL MANUAL

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## 1. READ THIS FIRST

**Most users should not need this manual. The best way to install FOQUS is to use the FOQUS Bundle installer, which in addition to installing FOQUS, installs TurbineLite, SimSinter, and PSUADE.** This installation manual provides additional information about the FOQUS installer and installation on non-windows operating systems like Linux and OS X. This manual also contains information useful to developers of FOQUS, and users wishing to build a custom installer with different versions of third-party libraries.

## 2. INTRODUCTION

There are two methods of installation. The first method is to use the Windows installer. The installer provides FOQUS and all third-

### 3.1. Python

Package: Python  
 Version: 2.7.3 or higher (not Python 3) (32-bit recommended on Windows)  
 Copyright: Copyright (c) 2001-2013 Python Software Foundation  
 Purpose: Needed for FOQUS and the graphical interface  
 Homepage: <http://python.org>  
 Download: <http://python.org/download/>  
 Description: Python interpreter  
 License: <http://docs.python.org/2/license.html>

### 3.2. PySide

Package: PySide  
 Version: 1.2.1 or higher (32-bit recommended on Windows)  
 Copyright: Copyright (C) 2013 Digia Plc and/or its subsidiaryies  
 Purpose: Provides a graphical user interface (GUI) toolkit  
 Homepage: <http://qt-project.org/wiki/Category:LanguageBindings::PySide>  
 Download: [http://qt-project.org/wiki/PySide\\_Binaries\\_Windows](http://qt-project.org/wiki/PySide_Binaries_Windows)  
 Description: A python interface for the Qt graphical interface library. On Windows PySide provides the Qt libraries. On other platforms such as Linux PySide and Qt may be packaged separately.  
 License: LGPL version 2.1, see <http://qt-project.org/wiki/About-PySide>

### 3.3. Numpy

Package: Numpy  
 Version: 1.7 or higher (32-bit recommended on Windows)  
 Copyright: Copyright (c) 2005-2013, NumPy Developers  
 Purpose: Needed for the optimization framework  
 Homepage: <http://www.numpy.org/>  
 Download: <http://sourceforge.net/projects/numpy/files/>  
 Description: Array processing/mathematics module for Python  
 License: <http://www.numpy.org/license.html>

### 3.4. SciPy

Package: SciPy  
 Version: 0.12.0 or higher (32-bit recommended on Windows)  
 Copyright: Copyright (c) 2003-2013, SciPy Developers  
 Purpose: Needed for some optimization solvers and some UQ GUI components  
 Homepage: <http://www.scipy.org/>  
 Download: <http://sourceforge.net/projects/scipy/files/>  
 Description: Common numerical methods for Python  
 License: <http://www.scipy.org/scipylib/license.html>

### 3.5. Matplotlib

Package: Matplotlib  
 Version: 1.3.0 or higher (32-bit recommended on Windows)  
 Copyright: Copyright (c) 2013, Matplotlib Development Team  
 Purpose: Needed to visualize optimization and UQ results  
 Homepage: <http://matplotlib.org/>  
 Download: <http://matplotlib.org/downloads.html> (Windows 32 bit)  
 Description: A Python plotting library  
 License: <http://matplotlib.org/users/license.html>

### 3.6. pyparsing

Package: pyparsing  
 Version: 2.0.1  
 Copyright: Copyright (c) 2003-2013, Paul T. McGuire  
 Purpose: Needed by Matplotlib  
 Homepage: <http://pyparsing.wikispaces.com/>  
 Download: <http://sourceforge.net/projects/pyparsing/>  
 Description: For parsing expressions  
 License: <http://pyparsing.wikispaces.com/share/view/5698048?replyId=5724804>

### 3.7. pywin32 (Windows only)

Package: pywin32  
 Version: Build 218  
 Copyright: Copyright (c) 1994-2008, Mark Hammond  
 Purpose: Needed to determine short names for Window files in UQ module  
 Homepage: <http://sourceforge.net/projects/pywin32/>  
 Download: <http://sourceforge.net/projects/pywin32/files/pywin32/>  
 Description: Python for Windows extensions  
 License: Python Software Foundation License

### 3.8. Python-Dateutils

Package: Python-Dateutils  
 Version: 1.5  
 Copyright: Copyright (c) 2003-2011, Gustavo Niemeyer  
 Purpose: Used by the Turbine client software and Matplotlib  
 Homepage: <http://labix.org/python-dateutil>  
 Download: <http://labix.org/python-dateutil>  
 Description: Dateutils is used by Matplotlib and the Turbine Client libraries  
 License: Python Software Foundation License

### 3.9. Python-ntlm

Package: Python-ntlm  
 Version: 1.0.1  
 Copyright: Copyright (c) 2001 Dmitry A. Rozmanov  
 Purpose: Used by the Turbine client software  
 Homepage: <https://code.google.com/p/python-ntlm/>  
 Download: <https://code.google.com/p/python-ntlm/source/checkout>  
 Description: Python-ntlm is used for authentication features in the Turbine Client library  
 License: LGPL v3

### 3.10. Py4J

Package: Py4J  
 Version: 0.8.1  
 Copyright: Copyright (C) 2009, Barthelemy Dagenais  
 Purpose: Used by the data management framework  
 Homepage: <http://py4j.sourceforge.net/>  
 Download: <http://py4j.sourceforge.net/download.html>  
 Description: Allows Java objects to be used in Python  
 License: BSD

### 3.11. networkx

Package: networkx  
 Version: 1.91  
 Copyright: Copyright (C) 2004-2012, NetworkX Developers  
 Purpose: Used by the data management framework for display dependencies  
 Homepage: <https://networkx.github.io/>  
 Download: <https://networkx.github.io/download.html>  
 Description: Graph and Graph visualization software  
 License: BSD type, <https://networkx.github.io/documentation/latest/reference/legal.html>

### 3.12. pycrypto

Package: pycrypto  
 Version: 2.6.1  
 Copyright: Mostly Public Domain, HMAC.py is Copyright Python Foundation  
 Purpose: Used by data management framework  
 Homepage: <https://www.dlitz.net/software/pycrypto/>  
 Download: <https://www.dlitz.net/software/pycrypto/>  
 Description: Python cryptography module.  
 License: Mostly Public Domain, HMAC.py has Python License and was derived from Python 2.2



### 3.13. adodbapi

Package: adodbapi  
 Version: 2.6.0.6  
 Copyright: Copyright (C) 2002 Henrik Ekelund, versions 2.1 and later by Vernon Cole  
 Purpose: Direct access to TurbineLite database  
 Homepage: <http://adodbapi.sourceforge.net/>  
 Download: <http://sourceforge.net/projects/adodbapi/>  
 Description: Module for ADO database interface  
 License: LGPL 2.1 or optionally a later version

### 3.14. GitPython

Package: GitPython  
 Version: 1.0.1  
 Copyright: Copyright (C) 2008, 2009 Michael Trier and contributors, 2010-2015 Sebastian Thiel  
 Purpose: For performing Git operations in DMF  
 Homepage: <https://pypi.python.org/pypi/GitPython/1.0.1>  
 Download: <https://pypi.python.org/pypi/GitPython/1.0.1>  
 Description: Module for interfacing with Git  
 License: BSD (<https://github.com/gitpython-developers/GitPython/blob/master/LICENSE>)

### 3.15. GitDB

Package: gitdb  
 Version: 0.6.4  
 Copyright: Copyright (C) 2011, Sebastian Thiel  
 Purpose: For performing Git operations in DMF  
 Homepage: <https://pypi.python.org/pypi/gitdb>  
 Download: <https://pypi.python.org/pypi/gitdb>  
 Description: GitPython dependency  
 License: BSD (<https://github.com/gitpython-developers/gitdb/blob/master/LICENSE>)

### 3.16. D3

Package: D3  
 Version: 3.5.6  
 Copyright: Copyright (C) 2015 Mike Bostock  
 Purpose: Used by DMF to display data dependencies  
 Homepage: <http://d3js.org/>  
 Download: <http://d3js.org/>  
 Description: Visualization library  
 License: BSD (<https://github.com/mbostock/d3/blob/master/LICENSE>)

### 3.17. SLF4J

Package: slf4j  
 Version: 1.7.10  
 Purpose: Logging in DMF Java code  
 Homepage: <http://www.slf4j.org>  
 Download: <http://www.slf4j.org/download.html>  
 Description: Java logging library jar  
 License: MIT (<http://www.slf4j.org/license.html>)

### 3.18. JSON.org

Package: json.org  
 Version: 20150729  
 Purpose: Creation and processing of JSON data objects in Java for DMF  
 Homepage: <http://www.json.org/java/index.html>  
 Download: <http://www.json.org/java/index.html>  
 Description: Java JSON data object library  
 License: Custom (<http://www.json.org/license.html>)

## 4. OPTIONAL PACKAGES

The following packages are optional and may be installed before or after installing FOQUS. These generally operate as separate programs. FOQUS will function without these packages, however some feature may not work. The need for these packages depends on how you want to use FOQUS.

**These packages are not provided with the Windows FOQUS or FOQUS Bundle installers and must be downloaded and installed separately.**

### 4.1.GAMS

Package: GAMS  
 Version: 24.1.3 (32-bit)  
 Purpose: Needed to run the heat integration  
 Homepage: <http://www.gams.com/>  
 Download: <http://www.gams.com/download/> (Windows 32 bit)  
 Description: The General Algebraic Modeling System (GAMS) is a high-level modeling system for mathematical programming and optimization, which consists of a language compiler and a stable of integrated high-performance solvers. The heat integration tool is modeled and implemented in GAMS.  
 License: The purchase information for user licenses can be found in <http://www.gams.com/sales/sales.htm>.

## 4.2. Java

Package: Java  
 Version: Oracle Java 8 or higher  
 Purpose: Needed to run the data management framework and iREVEAL plug-in  
 Homepage: <https://www.java.com/en/>  
 Download: <https://www.java.com/en/>  
<http://www.oracle.com/technetwork/java/javase/downloads/jdk8-downloads-2133151.html> (JDK 8)  
 Description: Java runtime environment to execute Java code. Java JDK for compilation of additional dependencies in for server based DMF.  
 License: <http://www.oracle.com/technetwork/java/javase/downloads/jre-6u21-license-159054.txt>

## 4.3. Apache Ant

Package: Apache Ant  
 Version: 1.9.6  
 Purpose: To compile additional dependencies in the server based DMF.  
 Homepage: <http://ant.apache.org/index.html>  
 Download: <http://ant.apache.org/srcdownload.cgi>  
 Description: Java library and command line tool for building Java applications.  
 License: <http://www.apache.org/licenses/LICENSE-2.0.html> (Apache Version 2.0)

## 4.4. Git

Package: Git  
 Version: 2.6.0 or higher  
 Purpose: Needed to run the data management framework lite  
 Homepage: <https://git-scm.com/>  
 Download: <https://git-scm.com/>  
 Description: Git used as a repository to store data for the DMF lite  
 License: <https://github.com/git/git> (GPLv2)

## 4.5. CMA

Package: CMA  
 Version: 1.1.02  
 Copyright: Copyright (c) 2014 Inria  
 Author: Nikolaus Hansen  
 Purpose: Derivative free optimization algorithm (included in FOQUS, no need to install)  
 Homepage: <https://www.lri.fr/~hansen/cmaesintro.html>  
 Download: [https://www.lri.fr/~hansen/cmaes\\_inmatlab.html#python](https://www.lri.fr/~hansen/cmaes_inmatlab.html#python)  
 Description: Python module for CMA-ES. This is the only fully functional derivative-free optimization (DFO) algorithm currently implemented. This module can be used with parallel objective function evaluation and can be restarted if optimization is interrupted or more iteration is desired.

License: BSD 3-Clause (included in cma.py comments)

## 4.6.NLopt

Package: NLopt  
 Version: 2.4.2  
 Purpose: Optional DFO solvers, contains gradient methods, but not supported by FOQUS  
 Homepage: <http://ab-initio.mit.edu/wiki/index.php/NLopt>  
 Download: <http://ab-initio.mit.edu/wiki/index.php/NLopt>  
 Description: A selection of optimization solvers currently does not support parallel objective or check pointing.  
 License: LGPL, some solvers have less restrictive licensing

## 4.7.Alfresco OpenCMIS Extension

Package: alfresco-opencmis-extensions  
 Version: 0.7  
 Purpose: Used by the DMF to communicate with Alfresco  
 Homepage: <https://code.google.com/a/apache-extras.org/p/alfresco-opencmis-extension/>  
 Download: <https://code.google.com/a/apache-extras.org/p/alfresco-opencmis-extension/downloads/list>  
 Description: Java library dependency for communicating with Alfresco CMIS interface  
 License: Apache License 2.0 (<http://www.apache.org/licenses/LICENSE-2.0>)

## 4.8.Apache Chemistry

Package: Apache Chemistry  
 Version: 0.10.0  
 Purpose: Used by the DMF to communicate with Alfresco  
 Homepage: <https://chemistry.apache.org/>  
 Download: <https://chemistry.apache.org/java/download.html>  
 Description: Java library dependency for communicating with CMIS repositories  
 License: Apache License 2.0 (<http://www.apache.org/licenses/LICENSE-2.0>)

## 5. CCSI SOFTWARE DEPENDENCIES

There are several other CCSI software packages that FOQUS depends upon for full functionality. The easiest way to install these is to use the FOQUS Bundle installer, which installs everything needed to run FOQUS. These packages may also be downloaded and install individually from the CCSI web site.

- TurbineLite – Job queuing system from simulation jobs
- SimSinter – Standard .NET interface to simulation software, and graphical interface for configuration files that define simulation inputs and outputs
- PSUADE – Needed for UQ portions of FOQUS.

The following CCSI packages are not currently provided by the FOQUS Bundle, but provide additional surrogate model functionality to FOQUS. They can be downloaded from the CCSI website:

- ALAMO – build simple algebraic surrogate models
- iREVEAL – Surrogate models for CFDs

## 6. WINDOWS INSTALLATION PROCEEDURE

This is officially supported and tested for Windows 7, 32 and 64 bit. It may also work on other versions of Windows; however it has not been fully tested. This section provides information about the FOQUS windows installer. The best way to install FOQUS is to use the FOQUS Bundle installer, which provides additional required CCSI software.

### 6.1. Install

1. Uninstall any previously installed version of FOQUS (see Section 4.2)
2. Download the MSI file from  
<https://www.acceleratecarboncapture.org/drupal/product/foqus>
3. In the Windows file explorer double click the installer
4. The installation will proceed without asking any questions
5. The working directory for a user is set the first time you run FOQUS. This setting is stored in \$HOME/.foqus.cfg on Linux or Mac, and %APPDATA%.foqus.cfg on Windows. The working directory can be changed in the FOQUS settings, or be editing the confutation file.
6. Install optional software.
7. See Section 10 for testing the installation.

The install location is generally C:\Program Files\FOQUS\foqus\_version\ or C:\Program Files (x86)\FOQUS\foqus\_version\

Start menu items are created for documentation and starting FOQUS. The Turbine\_console menu item sets up an environment with the Turbine client scripts in the PATH for easy use.

### 6.2. Uninstall

1. Open the Windows Control Panel
2. Select programs
3. Select uninstall a program
4. Right click on FOQUS and select uninstall

## 7. MANUAL INSTALLATION PROCEEDURE

This procedure should work on platforms that support Python and PySide. This should work on Linux and Mac, however these platforms are not as well tested as Windows 7. The Windows MSI installer is generally the preferred install method. On Linux most of the third party Python modules are packaged by the distribution maintainers, and can be installed through the

distribution's package manager. TurbineLite and SimSinter only run on Windows, so FOQUS running on non-windows platforms will either not run windows based simulators or run them on remote machines.

## 7.1. Installation

1. Install Python 2.7.3 (or higher in the 2.7 series) (<http://python.org/download/>). There are also several Python distributions that will provide most or all of the required packages (See <http://www.scipy.org/install.html> for a list of additional Python distributions). In Linux Python is generally available through the standard package manager.
2. Install the required packages. Download information is provided, but you will need to select the appropriate package and version for your system. For a Linux install, these packages should be available in the distributions package management system.
  - Install PySide version 1.2 or higher ([http://qt-project.org/wiki/PySide\\_Binaries\\_Windows](http://qt-project.org/wiki/PySide_Binaries_Windows))
  - Install Numpy version 1.7 or higher (<http://sourceforge.net/projects/numpy/files/>)
  - Install SciPy version 0.12 or higher (<http://sourceforge.net/projects/scipy/files/>)
  - Install Matplotlib version 1.3 or higher (<http://matplotlib.org/downloads.html>)
  - Install pywin32 (windows only) <http://sourceforge.net/projects/pywin32/files/pywin32/>
  - Install Python-requests
  - Install networkx
  - Install py4j
  - Other required third-party packages are automatically installed
3. Install FOQUS. The install may require admin or root privileges.
  - Download the FOQUS source zip from [https://www.acceleratecarboncapture.org/drupal/product/sim-based\\_optimize](https://www.acceleratecarboncapture.org/drupal/product/sim-based_optimize)
  - Extract the files to a convenient directory.
  - Open a terminal or command prompt Window.
  - At the command prompt change to the directory of the install files.
  - Change to the foqus subdirectory
  - Type “setup.py install” in Windows or “python setup.py install” in Linux. You may need to install as root in Linux or have admin privileges in Windows. The install argument is important, without it nothing will be installed. If you do not have root privileges, you may use the “setup.py install --user” command.
4. The working directory is set the first time you run FOQUS. This setting is stored in \$HOME/.foqus.cfg in Linux or Mac, and %APPDATA%.foqus.cfg in windows. The working directory can be changed in the FOQUS settings.
5. Install optional software.

6. See Section 10 for information about testing the install.

## 7.2.Uninstall

The following steps can be used to uninstall FOQUS, if it was installed manually by the above procedure. You may wish to leave the Turbine Client files, if you want to uninstall FOQUS but not the Turbine Client.

- Determine the directory where the python packages are installed. On a standard Windows install this would be C:\Python27\Lib\site-packages.
- Go to the site packages directory.
- Delete the FOQUS files and directories.
  - Delete foqus\_\*
- Delete the Turbine client egg file (TurbineClient-\*.egg).
- Open the easy-install.pth file in WordPad (NotePad will not properly recognize the line breaks).
- Delete lines for FOQUS and the Turbine Client
  - ./turbineclient\*
  - ./foqus\_\*
- In the Windows file explorer go to the Python scripts directory (Usually c:\Python27\Scripts).
- Delete the file foqus.py
- Delete the turbine client scripts turbine\_\*

## 8. RUNNING FOQUS FROM AN SVN CHECKOUT

1. Install Python and Modules from Section 3. Python 2.7.x is required, but newer versions of the listed modules are most likely fine.
2. Install TurbineClient
  - a. Check the TurbineClient out from svn.
  - b. Install using setup.py script and follow instructions provide with TurbineClient
3. Check out the FOQUS project from svn/
4. You should now be able to run the foqus.py script without installing FOQUS.
5. (Optional) Install any optional modules from Section 4 that you need

## 9. BUILDING A WINDOWS INSTALLER

The following section provides instructions for building Windows installer MSI file. Py2exe and WiX are used to create a windows MSI installer that does not require separate installation of third-party software. Py2exe bundles everything into a self-contained directory including the python interpreter, modules, the Turbine Client, and FOQUS. This is packaged for installation by WiX.

1. Two additional pieces of software are required to build the MSI file. Both are freely available.

- a. Py2exe creates the exe files and bundles the required Python modules. It can be downloaded from <http://www.py2exe.org/>
  - b. WiX creates Windows installer MSI files and can be downloaded from <http://wixtoolset.org/>
2. Install Python and the required modules. See the procedure in section 5.1 steps 1 and 2.
3. Run the “python setup.py wix” from the command line, in the same directory as the batch file.
4. The above step should have created an MSI called foqus\_installer.msi.

## 10.OPTIMZIATION PLUG-INS

The FOQUS working directory contains a subdirectory called user\_plugins. This directory contains Python code for user provided optimization plug-ins. FOQUS will check this directory when it starts to see what optimization methods are available. If you have not set the FOQUS working directory, you should run FOQUS once and exit before installing plugins to create the directory structure, or you can create the user\_plugins subdirectory yourself to add plugins before starting FOQUS the first time.

At this early development stage, only the CMA-ES plug-in is fully functional. This plug-in requires a third party Python module that is made available by Nikolaus Hansen (<https://www.lri.fr/~hansen/>) under a BSD style license. This module is included with the FOQUS installer. If you are using an older version of FOQUS and have installed cma.py in your user\_plugins directory, you should delete it.

## 11. TESTING

This section provides a simple test procedure to see if FOQUS was installed properly. This method assumes you used the Windows MSI installer, but a similar procedure can be used to test other install methods.

The Turbine Gateway installation is required to run simulations, but the FOQUS installation can be tested on some provided example problems without it. This test does not require turbine.

1. From the Windows start menu select the CCSI Tools -> FOQUS folder, and then select FOQUS.
2. The first time FOQUS start you will be asked to select a working directory. This is the directory where FOQUS will store its files. This directory should be dedicated to FOQUS, and used for nothing else. The directory selection dialog will allow you to create new directories.
3. From the FOQUS home screen select Open.
4. A file selection dialog will open.
  - a. The example files will be in the examples folder in the location where FOQUS was installed.
  - b. Browse to {FOQUS install location}\examples\optimization\Rosenbrock.json
  - c. Open the Rosenbrock.json example file
5. Click the optimization icon at the top of the window.



6. Click the Run tab, and push the start button
7. The optimization should complete in 10 to 40 seconds.
8. If errors occur, refer to the debugging section of the user's manual and contact [ccsi-support@acceleratecarboncapture.org](mailto:ccsi-support@acceleratecarboncapture.org).