

Table of Contents

Software Environment	1
<u>Software: Overview</u>	1
<u>Operating Systems</u>	2
<u>Modules</u>	3
<u>Table of All Modules</u>	5
Licensed Application Software	8
<u>Licensed Application Software: Overview</u>	8
<u>Tecplot</u>	9
<u>IDL</u>	10
<u>Matlab</u>	11
<u>Gaussian</u>	12
<u>FieldView</u>	13
<u>Gridgen</u>	14

Software Environment

Software: Overview

Software on the NAS HECC systems include the operating systems, programming environments, licensed or open source software, etc. The following lists the few directories where you can find most of the software you need.

- **/bin** : essential user commands binaries, such as **cp**, **ls**, **mv**, **vi**, etc.
- **/lib** : essential shared libraries and kernel modules, such as **libc**, **libm**, etc.
- **/usr/bin** : most user commands, such as **cat**, **diff**, **ldd**, etc.
- **/usr/lib** : libraries for programming and packages, such as **libstdc++**, **libGL**, etc.
- **/usr/include** : system's general-use include files for the C programming language
- **/usr/local/bin** : binaries added for local use, such as **acct_ytd**, **bbftp**, etc.
- **/usr/local/lib** : shell start up files, such as **glocal.cshrc** for NAS systems
- **/PBS** : software for submitting, monitoring and managing PBS jobs
- **/nasa** : licensed or open source software modules

Except for those under **/nasa**, the binaries, libraries and include files above should have been included in your default search path.

Read the articles on [Modules](#) to learn how to use licensed or open source software managed by modules.

In addition, on Pleiades there are some useful tools provided by members of the Application Performance and Productivity Group. They are stored under the directory **/u/scicon/tools**.

Operating Systems

All NAS HECC systems (including Pleiades and Columbia) are running SGI ProPack for Linux which is designed to enhance the Linux experience for SGI systems.

To find the Linux kernel version number on a host, use:

```
%uname -r
```

To find the SGI release number on a host, use:

```
%cat /etc/sgi-release
```

All Pleiades front-ends and compute nodes are running with ProPack 7SP1.

All Columbia systems, including both front-ends and compute systems, are running with ProPack 6SP5.

Modules

A system called "modules" to centralize the location of licensed products from vendors or software from public domain is installed on all NAS HECC systems.

To use the modules commands, you have to do either one of the following first:

1. Source the following files in your **.cshrc** or **.profile**

In **.cshrc** (for csh users):

```
source /usr/local/lib/global.cshrc
```

In **.profile** (for bash users):

```
source /usr/local/lib/global.profile
```

2. In the shell that you want to use the module commands, do one of the following:

For csh users:

```
%source /usr/share/modules/init/csh
```

For bash users:

```
%. /usr/share/modules/init/bash
```

The following are useful module commands to remember:

module avail

- Used to find out what modules are available.

module list

- Used to list which modules are loaded in your environment.

module purge

- Used to unload all loaded modulefiles.

module load *module_name1 module_name2 ... module_nameN*

- Used to load the desired modules.

module switch *old_module_name new_module_name*

- Used to switch between two modules.

module show *module_name*

- Used to show changes to the environment that will happen if you load *module_name*.

Table of All Modules

The table below shows the available software managed through modules on Pleiades and/or Columbia. To request installation of a software as a module, please send an email to support@nas.nasa.gov

Note that the name of a software module may contain:

- software name
- vendor name
- version number
- varieties such as what compiler and/or what library is used to build the software

For example:

- `comp-intel/11.1.072` represents the Intel Compiler version 11.1.072.
- `mpi-sgi/mpt.2.04.10789` represents the SGI MPI library version mpt.2.04.10789.
- `mpi-mvapich2/1.4.1/intel` represents the MVAPICH2 MPI library version 1.4.1 built with an Intel compiler.

Use the `module avail` command to see all the available versions and provide the full name of a module when you decide to load a module.

Available Modules (as of 30 August 2010)

Software	Platforms	Function
Intel compiler	Pleiades/Columbia	Compiler
Intel mkl	Pleiades/Columbia	Math/Scientific Library
Intel mpi	Pleiades/Columbia	MPI Library
SGI mpt	Pleiades/Columbia	MPI Library
SGI scsl	Columbia	Math/Scientific Library
automake	Columbia	Makefile Tool
boost	Columbia	C++ Library
cpan	Pleiades	Comprehensive Perl Archive Network
cscope	Columbia	Source Code Browsing Tool
drm	Pleiades	X Window Library Tool
eclipse	Pleiades	Software Development Environment
emacs	Pleiades	Text Editor
fieldview	Pleiades/Columbia	Data Visualization and Analysis Tool
flex	Pleiades	Text Scanner Generation Tool
fluent	Pleiades	CFD Modeling Application
gaussian	Pleiades/Columbia	Quantum Chemistry Application

gcc	Pleiades/Columbia	GNU C/C++ Compiler
gd	Pleiades/Columbia	Images Creation Library
git	Pleiades/Columbia	Version Control System
glib	Pleiades/Columbia	Low-level Core Library
gmp	Pleiades/Columbia	Math Library
gnuplot	Pleiades/Columbia	Data Visualization Tool
grace	Pleiades/Columbia	Data Visualization Tool
grads	Pleiades/Columbia	Data Visualization and Analysis Tool
gridgen	Pleiades/Columbia	CFD Grid Generation Tool
gsl	Pleiades/Columbia	GNU Scientific Library
hcss	Pleiades/Columbia	Herschel Common Science System
hdf4	Pleiades/Columbia	I/O Library and Tools
hdf5	Pleiades/Columbia	I/O Library and Tools
idl	Pleiades/Columbia	Data Visualization and Analysis Tool
idn	Pleiades	GNU Libidn
imagemagick	Pleiades/Columbia	Image Tool
java-sdk	Columbia	Programming Language
jpeg	Columbia	Image Tool
jvm	Pleiades	Java Virtual Machine
libxml	Columbia	C Parser and Toolkit
lsdyna3d	Pleiades/Columbia	Finite Element Application
matlab	Pleiades/Columbia	Numerical Computing Environment and Programming Language
mlp	Columbia	Multi-Level Parallelism Library
mpfr	Pleiades	Multiple-Precision Floating-point Computations Library
mpich2	Columbia	MPI Library
mvapich2	Pleiades	MPI Library
ncarg	Pleiades/Columbia	Graphics Library for Scientific Data
ncl	Pleiades/Columbia	NCAR Command Language
nco	Pleiades/Columbia	netCDF Operators
netcdf	Pleiades/Columbia	I/O Library
octave	Pleiades/Columbia	Numerical Computations Language
paraview	Pleiades	Data Visualization and Analysis Tool
parmetis	Pleiades/Columbia	Math/Numerical Library
pdf	Columbia	PDF File Generation Library
perl	Columbia	Programming Language
petsc	Columbia	Math/Numerical Library
parallel netcdf	Pleiades/Columbia	Parallel I/O Library
png	Columbia	Portable Network Graphics Format

pyMPI	Columbia	MPI Program Development with Python
python	Pleiades/Columbia	Programming Language
ruby	Pleiades	Programming Language
svn	Pleiades/Columbia	Revision Control Application
swig	Pleiades/Columbia	Software Development Tool
tcl-tk	Pleiades/Columbia	Scripting Language
tecplot	Pleiades/Columbia	Data Visualization and Analysis Tool
texlive	Pleiades	TeX System Application
totalview	Pleiades/Columbia	Debugger
udunits	Pleiades/Columbia	Data Format Library
visit	Pleiades/Columbia	Data Visualization and Analysis Tool
xv	Pleiades	Images Display Application
xxdiff	Pleiades	Graphical File And Directories Comparator And Merge Tool
yaml	Pleiades/Columbia	Human-Readable Data Serialization Format
zlib	Columbia	Data Compression Library

Licensed Application Software

Licensed Application Software: Overview

A few licensed applications from different vendors are installed on NAS HECC systems under the `/nasa` directory. They are either purchased by NAS (with justification that many users need it) or by users themselves. If you would like to use a licensed application which is not yet available on NAS HECC systems, you may have to purchase the license yourself.

Tecplot

Two Tecplot products are available on the HECC systems: Tecplot 360 and Tecplot Chorus.

Tecplot 360

Tecplot 360 is a CFD and Numerical Simulation Visualization Software used in post-processing simulation results. Common tasks associated with post-processing analysis of flow solver (for example, Fluent, STAR-CD, OpenFOAM) can include such tasks as:

- Calculating grid quantities (for example, aspect ratios, skewness, orthogonality, and stretch factors)
- Normalizing data; Deriving flow field functions like pressure coefficient or vorticity magnitude
- Verifying solution convergence
- Estimating the order of accuracy of solutions
- Interactively exploring data through cut planes (a slice through a region), iso-surfaces (3-D maps of concentrations), particle paths (dropping an object in the "fluid" and watching where it goes).

As of Dec. 2008, the Tecplot 360 license at NAS no longer has restrictions on the number of copies of Tecplot 360 that can be run concurrently.

Note: If you have set the stacksize with a command like `limit stacksize unlimited`, you will have to reduce the stacksize for Tecplot to run. For example:

```
%limit stacksize 2000000
```

Tecplot Chorus

Tecplot Chorus is a new simulation analytics framework that unites physics visualization with data management and analytics in a single environment.

Currently, one Tecplot Chorus license is available to use on Pleiades or NAS supported desktop systems.

For more information on these versions of Tecplot, please visit [Tecplot's documentation page](#).

See also: <http://en.wikipedia.org/wiki/Tecplot>

IDL

IDL is a software for data analysis, visualization, and cross-platform application development. IDL combines tools for any type of project, from "quick-look," interactive analysis and display to large-scale commercial programming projects.

For more information, please visit the [IDL home page](#).

Current licenses of IDL at NAS allow 10 users to use it at the same time. If you are not able to use IDL because the licenses are being used, try using it at a later time, or load an IDL module and issue the command `lmstat -a` to find out how many licenses are in use.

See also: [http://en.wikipedia.org/wiki/IDL_\(programming_language\)](http://en.wikipedia.org/wiki/IDL_(programming_language))

Matlab

Matlab is a numerical computing environment and programming language. Created by The MathWorks, Matlab allows easy matrix manipulation, plotting of functions and data, implementation of algorithms, creation of user interfaces, and interfacing with programs in other languages. Although it specializes in numerical computing, an optional toolbox interfaces with the Maple symbolic engine, allowing it to be part of a full computer algebra system.

A total of 8 licenses are available to use on either Pleiades or Columbia or NAS supported desktop systems. To find out how many licenses are currently in use, use:

```
%module load matlab/2010b  
%matstat
```

For more information, please visit the [Matlab web site](#) at MathWorks.

Note: Our version of **glibc** has not been tested with Matlab 2010. Please proceed with this in mind.

See also: <http://en.wikipedia.org/wiki/Matlab>

Gaussian

Gaussian 03 is a suite of electronic structure programs. It is used by chemists, chemical engineers, biochemists, physicists and others for research in established and emerging areas of chemical interest.

Starting from the basic laws of quantum mechanics, Gaussian predicts the energies, molecular structures, and vibrational frequencies of molecular systems, along with numerous molecular properties derived from these basic computation types. It can be used to study molecules and reactions under a wide range of conditions, including both stable species and compounds which are difficult or impossible to observe experimentally such as short-lived intermediates and transition structures.

For more information, please see the [Gaussian manual](#) or the [Gaussian web site](#).

Two versions (c.02 and e.01) of Gaussian 03 have been installed on Columbia systems. To use the older c.02 version, do the following in your PBS script:

```
module load gaussian.03.c02
source $g03root/g03/bsd/g03.login
```

```
g03 input output
```

To use the newer e.01 version (built with **intel-comp.10.0.023** and **intel-mkl.9.1.023**), do:

```
module load gaussian.03.e.01
source $g03root/g03/bsd/g03.login
```

```
g03 input output
```

If you are a bash user, then do:

```
. /usr/share/modules/init/bash
module load gaussian.03.e.01
. $g03root/g03/bsd/g03.profile
```

```
g03 input output
```

See also: <http://en.wikipedia.org/wiki/GAUSSIAN>

FieldView

FieldView is Intelligent Light's CFD post-processing software to quickly identify important flow features and characteristics in simulations. It allows interactive exploration for thorough understanding of results. You can use it to examine and compare cases, extract critical values, and make presentations.

Current license allows up to 4 concurrent uses.

For more information, see Intelligent Light's [FieldView home page](#).

Gridgen

Gridgen is Pointwise's meshing software used by engineers and scientists to generate high quality grids for engineering analysis.

For more information, please visit the [Gridgen home page](#) at the Pointwise web site.