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This is the list of scientific applications deployed on Purdue Brown cluster. More information about our center is available here (<https://www.rcac.purdue.edu/knowledge/brown>).

OPENMPI

1.1 Description

An open source Message Passing Interface implementation. The Open MPI Project is an open source Message Passing Interface implementation that is developed and maintained by a consortium of academic, research, and industry partners. Open MPI is therefore able to combine the expertise, technologies, and resources from all across the High Performance Computing community in order to build the best MPI library available. Open MPI offers advantages for system and software vendors, application developers and computer science researchers.

1.2 Versions and Dependencies

- 1.10.7
- 2.1.6
- **3.1.4**

1. zlib/1.2.11

1.3 Module

You can load the modules by:

```
module load openmpi
```


2.1 Description

Boost provides free peer-reviewed portable C++ source libraries, emphasizing libraries that work well with the C++ Standard Library.

2.2 Versions and Dependencies

- **1.64.0**
 1. zlib/1.2.11
- **1.66.0**
 1. zlib/1.2.11
- **1.70.0**
 1. zlib/1.2.11

2.3 Module

You can load the modules by:

```
module load boost
```


CMAKE

3.1 Description

A cross-platform, open-source build system. CMake is a family of tools designed to build, test and package software.

3.2 Versions and Dependencies

- 3.15.4

3.3 Module

You can load the modules by:

```
module load cmake
```


4.1 Description

FFTW is a C subroutine library for computing the discrete Fourier transform DFT in one or more dimensions, of arbitrary input size, and of both real and complex data as well as of even/odd data, i.e. the discrete cosine/sine transforms or DCT/DST. We believe that FFTW, which is free software, should become the FFT library of choice for most applications.

4.2 Versions and Dependencies

- 3.3.4
- 3.3.7

4.3 Module

You can load the modules by:

```
module load fftw
```


5.1 Description

HDF4 also known as HDF is a library and multi-object file format for storing and managing data between machines.

5.2 Versions and Dependencies

- 4.2.14

5.3 Module

You can load the modules by:

```
module load hdf
```


6.1 Description

HDF5 is a data model, library, and file format for storing and managing data. It supports an unlimited variety of datatypes, and is designed for flexible and efficient I/O and for high volume and complex data.

6.2 Versions and Dependencies

- 1.10.5
- 1.8.16

6.3 Module

You can load the modules by:

```
module load hdf5
```


7.1 Description

NetCDF is a set of software libraries and self-describing, machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data.

7.2 Versions and Dependencies

- **4.5.0**
 1. hdf/4.2.14
 2. hdf5/1.8.16
- **4.7.0**
 1. hdf/4.2.14
 2. hdf5/1.10.5

7.3 Module

You can load the modules by:

```
module load netcdf
```


NETCDF-CXX4

8.1 Description

NetCDF network Common Data Form is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data. This is the C++ distribution.

8.2 Versions and Dependencies

- **4.3.0**
 1. netcdf/4.5.0
- **4.3.1**
 1. netcdf/4.7.0

8.3 Module

You can load the modules by:

```
module load netcdf-cxx4
```


NETCDF-FORTRAN

9.1 Description

Fortran interface for NetCDF4

9.2 Versions and Dependencies

- **4.4.4**
 1. netcdf/4.5.0
- **4.5.2**
 1. netcdf/4.7.0

9.3 Module

You can load the modules by:

```
module load netcdf-fortran
```


OPENBLAS

10.1 Description

An optimized BLAS library

10.2 Versions and Dependencies

- 0.2.20
- 0.3.7

10.3 Module

You can load the modules by:

```
module load openblas
```


11.1 Description

An open source Message Passing Interface implementation.

11.2 Versions and Dependencies

- 1.10.7
- 2.1.6
- **3.1.4**

1. zlib/1.2.11

11.3 Module

You can load the modules by:

```
module load openmpi
```


ZLIB

12.1 Description

A free, general-purpose, legally unencumbered lossless data-compression library.

12.2 Versions and Dependencies

- 1.2.11

12.3 Module

You can load the modules by:

```
module load zlib
```


13.1 Description

Boost provides free peer-reviewed portable C++ source libraries, emphasizing libraries that work well with the C++ Standard Library. Boost libraries are intended to be widely useful, and usable across a broad spectrum of applications. The Boost license encourages both commercial and non-commercial use.

13.2 Versions and Dependencies

- **1.64.0**
 1. zlib/1.2.11
- **1.66.0**
 1. zlib/1.2.11
- **1.70.0**
 1. zlib/1.2.11

13.3 Module

You can load the modules by:

```
module load boost
```


CMAKE

14.1 Description

A cross-platform, open-source build system. CMake is a family of tools designed to build, test and package software.

14.2 Versions and Dependencies

- 3.15.4

14.3 Module

You can load the modules by:

```
module load cmake
```


15.1 Description

FFTW is a C subroutine library for computing the discrete Fourier transform DFT in one or more dimensions, of arbitrary input size, and of both real and complex data as well as of even/odd data, i.e. the discrete cosine/sine transforms or DCT/DST. We believe that FFTW, which is free software, should become the FFT library of choice for most applications.

15.2 Versions and Dependencies

- 3.3.4
- 3.3.7

15.3 Module

You can load the modules by:

```
module load fftw
```


16.1 Description

HDF4 also known as HDF is a library and multi-object file format for storing and managing data between machines.

16.2 Versions and Dependencies

- 4.2.14

16.3 Module

You can load the modules by:

```
module load hdf
```


17.1 Description

HDF5 is a data model, library, and file format for storing and managing data. It supports an unlimited variety of datatypes, and is designed for flexible and efficient I/O and for high volume and complex data.

17.2 Versions and Dependencies

- 1.10.5
- 1.8.16

17.3 Module

You can load the modules by:

```
module load hdf5
```


18.1 Description

LibTIFF - Tag Image File Format TIFF Library and Utilities.

18.2 Versions and Dependencies

- **4.0.10**
 1. zlib/1.2.11

18.3 Module

You can load the modules by:

```
module load libtiff
```


19.1 Description

Put a proper description of your package here.

19.2 Versions and Dependencies

- 3.14

19.3 Module

You can load the modules by:

```
module load libv8
```


20.1 Description

NetCDF network Common Data Form is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data. This is the C distribution.

20.2 Versions and Dependencies

- **4.5.0**
 1. hdf/4.2.14
 2. hdf5/1.8.16
- **4.7.0**
 1. hdf/4.2.14
 2. hdf5/1.10.5

20.3 Module

You can load the modules by:

```
module load netcdf
```


NETCDF-CXX4

21.1 Description

NetCDF network Common Data Form is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data. This is the C++ distribution.

21.2 Versions and Dependencies

- **4.3.0**
 1. netcdf/4.5.0
- **4.3.1**
 1. netcdf/4.7.0

21.3 Module

You can load the modules by:

```
module load netcdf-cxx4
```


NETCDF-FORTRAN

22.1 Description

NetCDF network Common Data Form is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data. This is the Fortran distribution.

22.2 Versions and Dependencies

- **4.4.4**
 1. netcdf/4.5.0
- **4.5.2**
 1. netcdf/4.7.0

22.3 Module

You can load the modules by:

```
module load netcdf-fortran
```


OPENBLAS

23.1 Description

An optimized BLAS (Basic Linear Algebra Subprograms) library.

23.2 Versions and Dependencies

- 0.3.7

23.3 Module

You can load the modules by:

```
module load openblas
```


24.1 Description

An open source Message Passing Interface implementation. The Open MPI Project is an open source Message Passing Interface implementation that is developed and maintained by a consortium of academic, research, and industry partners. Open MPI is therefore able to combine the expertise, technologies, and resources from all across the High Performance Computing community in order to build the best MPI library available. Open MPI offers advantages for system and software vendors, application developers and computer science researchers.

24.2 Versions and Dependencies

- 1.10.7
 - 2.1.6
 - **3.1.4**
1. zlib/1.2.11

24.3 Module

You can load the modules by:

```
module load openmpi
```


25.1 Description

Qt is a comprehensive cross-platform C++ application framework.

25.2 Versions and Dependencies

- 5.12.5

25.3 Module

You can load the modules by:

```
module load qt
```


26.1 Description

Tcl Tool Command Language is a very powerful but easy to learn dynamic programming language, suitable for a very wide range of uses, including web and desktop applications, networking, administration, testing and many more. Open source and business-friendly, Tcl is a mature yet evolving language that is truly cross platform, easily deployed and highly extensible.

26.2 Versions and Dependencies

- 8.6.8
 1. zlib/1.2.11

26.3 Module

You can load the modules by:

```
module load tcl
```


27.1 Description

TeX Live is a free software distribution for the TeX typesetting system. Heads up, its is not a reproducible installation. At any point only the most recent version can be installed. Older versions are included for backward compatibility, i.e., if you have that version already installed.

27.2 Versions and Dependencies

- 20200406

27.3 Module

You can load the modules by:

```
module load texlive
```


28.1 Description

Tk is a graphical user interface toolkit that takes developing desktop applications to a higher level than conventional approaches. Tk is the standard GUI not only for Tcl, but for many other dynamic languages, and can produce rich, native applications that run unchanged across Windows, Mac OS X, Linux and more.

28.2 Versions and Dependencies

- 8.6.8
 1. tcl/8.6.8

28.3 Module

You can load the modules by:

```
module load tk
```


29.1 Description

Automated units conversion

29.2 Versions and Dependencies

- 2.2.24

29.3 Module

You can load the modules by:

```
module load udunits2
```


ZLIB

30.1 Description

A free, general-purpose, legally unencumbered lossless data-compression library.

30.2 Versions and Dependencies

- 1.2.11

30.3 Module

You can load the modules by:

```
module load zlib
```


31.1 Description

Boost provides free peer-reviewed portable C++ source libraries, emphasizing libraries that work well with the C++ Standard Library.

31.2 Versions and Dependencies

- **1.64.0**
 1. zlib/1.2.11
- **1.66.0**
 1. zlib/1.2.11
- **1.70.0**
 1. zlib/1.2.11

31.3 Module

You can load the modules by:

```
module load boost
```


CMAKE

32.1 Description

A cross-platform, open-source build system. CMake is a family of tools designed to build, test and package software.

32.2 Versions and Dependencies

- 3.15.4

32.3 Module

You can load the modules by:

```
module load cmake
```


33.1 Description

FFTW is a C subroutine library for computing the discrete Fourier transform DFT in one or more dimensions, of arbitrary input size, and of both real and complex data as well as of even/odd data, i.e. the discrete cosine/sine transforms or DCT/DST. We believe that FFTW, which is free software, should become the FFT library of choice for most applications.

33.2 Versions and Dependencies

- 3.3.4
- 3.3.7

33.3 Module

You can load the modules by:

```
module load fftw
```


34.1 Description

HDF4 also known as HDF is a library and multi-object file format for storing and managing data between machines.

34.2 Versions and Dependencies

- 4.2.14

34.3 Module

You can load the modules by:

```
module load hdf
```


35.1 Description

HDF5 is a data model, library, and file format for storing and managing data. It supports an unlimited variety of datatypes, and is designed for flexible and efficient I/O and for high volume and complex data.

35.2 Versions and Dependencies

- 1.10.5
- 1.8.16

35.3 Module

You can load the modules by:

```
module load hdf5
```


36.1 Description

NetCDF is a set of software libraries and self-describing, machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data.

36.2 Versions and Dependencies

- **4.5.0**
 1. hdf/4.2.14
 2. hdf5/1.8.16
- **4.7.0**
 1. hdf/4.2.14
 2. hdf5/1.10.5

36.3 Module

You can load the modules by:

```
module load netcdf
```


37.1 Description

NetCDF network Common Data Form is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data. This is the C++ distribution.

37.2 Versions and Dependencies

- **4.3.0**
 1. netcdf/4.5.0
- **4.3.1**
 1. netcdf/4.7.0

37.3 Module

You can load the modules by:

```
module load netcdf-cxx4
```


NETCDF-FORTRAN

38.1 Description

Fortran interface for NetCDF4

38.2 Versions and Dependencies

- **4.4.4**
 1. netcdf/4.5.0
- **4.5.2**
 1. netcdf/4.7.0

38.3 Module

You can load the modules by:

```
module load netcdf-fortran
```


OPENBLAS

39.1 Description

An optimized BLAS library

39.2 Versions and Dependencies

- 0.2.20
- 0.3.7

39.3 Module

You can load the modules by:

```
module load openblas
```


40.1 Description

An open source Message Passing Interface implementation.

40.2 Versions and Dependencies

- 1.10.7
- 2.1.6
- **3.1.4**

1. zlib/1.2.11

40.3 Module

You can load the modules by:

```
module load openmpi
```


ZLIB

41.1 Description

A free, general-purpose, legally unencumbered lossless data-compression library.

41.2 Versions and Dependencies

- 1.2.11

41.3 Module

You can load the modules by:

```
module load zlib
```


42.1 Description

Boost provides free peer-reviewed portable C++ source libraries, emphasizing libraries that work well with the C++ Standard Library.

42.2 Versions and Dependencies

- **1.64.0**
 1. zlib/1.2.11
- **1.66.0**
 1. zlib/1.2.11
- **1.70.0**
 1. zlib/1.2.11

42.3 Module

You can load the modules by:

```
module load boost
```


CMAKE

43.1 Description

A cross-platform, open-source build system. CMake is a family of tools designed to build, test and package software.

43.2 Versions and Dependencies

- 3.15.4

43.3 Module

You can load the modules by:

```
module load cmake
```


44.1 Description

FFTW is a C subroutine library for computing the discrete Fourier transform DFT in one or more dimensions, of arbitrary input size, and of both real and complex data as well as of even/odd data, i.e. the discrete cosine/sine transforms or DCT/DST. We believe that FFTW, which is free software, should become the FFT library of choice for most applications.

44.2 Versions and Dependencies

- 3.3.4

44.3 Module

You can load the modules by:

```
module load fftw
```


45.1 Description

HDF4 also known as HDF is a library and multi-object file format for storing and managing data between machines.

45.2 Versions and Dependencies

- 4.2.14

45.3 Module

You can load the modules by:

```
module load hdf
```


46.1 Description

HDF5 is a data model, library, and file format for storing and managing data. It supports an unlimited variety of datatypes, and is designed for flexible and efficient I/O and for high volume and complex data.

46.2 Versions and Dependencies

- 1.10.5
- 1.8.16

46.3 Module

You can load the modules by:

```
module load hdf5
```


47.1 Description

NetCDF is a set of software libraries and self-describing, machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data.

47.2 Versions and Dependencies

- **4.5.0**
 1. hdf/4.2.14
 2. hdf5/1.8.16
- **4.7.0**
 1. hdf/4.2.14
 2. hdf5/1.10.5

47.3 Module

You can load the modules by:

```
module load netcdf
```


NETCDF-CXX4

48.1 Description

NetCDF network Common Data Form is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data. This is the C++ distribution.

48.2 Versions and Dependencies

- **4.3.0**
 1. netcdf/4.5.0
- **4.3.1**
 1. netcdf/4.7.0

48.3 Module

You can load the modules by:

```
module load netcdf-cxx4
```


NETCDF-FORTRAN

49.1 Description

Fortran interface for NetCDF4

49.2 Versions and Dependencies

- **4.4.4**
 1. netcdf/4.5.0
- **4.5.2**
 1. netcdf/4.7.0

49.3 Module

You can load the modules by:

```
module load netcdf-fortran
```


OPENBLAS

50.1 Description

An optimized BLAS library

50.2 Versions and Dependencies

- 0.2.20
- 0.3.7

50.3 Module

You can load the modules by:

```
module load openblas
```


51.1 Description

An open source Message Passing Interface implementation.

51.2 Versions and Dependencies

- 1.10.7
- 2.1.6
- **3.1.4**

1. zlib/1.2.11

51.3 Module

You can load the modules by:

```
module load openmpi
```


ZLIB

52.1 Description

A free, general-purpose, legally unencumbered lossless data-compression library.

52.2 Versions and Dependencies

- 1.2.11

52.3 Module

You can load the modules by:

```
module load zlib
```


53.1 Versions and Dependencies

- 2017
- 2018
- 2019
- 2020
- 2021
- 6.14-6

53.2 Module

You can load the modules by:

```
module load abaqus
```


54.1 Description

Boost provides free peer-reviewed portable C++ source libraries, emphasizing libraries that work well with the C++ Standard Library.

54.2 Versions and Dependencies

- **1.64.0**
 1. zlib/1.2.11
- **1.66.0**
 1. zlib/1.2.11

54.3 Module

You can load the modules by:

```
module load boost
```


CMAKE

55.1 Description

A cross-platform, open-source build system. CMake is a family of tools designed to build, test and package software.

55.2 Versions and Dependencies

- 3.15.4

55.3 Module

You can load the modules by:

```
module load cmake
```


56.1 Description

FFTW is a C subroutine library for computing the discrete Fourier transform DFT in one or more dimensions, of arbitrary input size, and of both real and complex data as well as of even/odd data, i.e. the discrete cosine/sine transforms or DCT/DST. We believe that FFTW, which is free software, should become the FFT library of choice for most applications.

56.2 Versions and Dependencies

- 3.3.4
- 3.3.7

56.3 Module

You can load the modules by:

```
module load fftw
```


57.1 Description

HDF4 also known as HDF is a library and multi-object file format for storing and managing data between machines.

57.2 Versions and Dependencies

- 4.2.14

57.3 Module

You can load the modules by:

```
module load hdf
```


58.1 Description

HDF5 is a data model, library, and file format for storing and managing data. It supports an unlimited variety of datatypes, and is designed for flexible and efficient I/O and for high volume and complex data.

58.2 Versions and Dependencies

- 1.10.5
- 1.8.16

58.3 Module

You can load the modules by:

```
module load hdf5
```


59.1 Description

Intel MPI

59.2 Versions and Dependencies

- 5.1.3.223

59.3 Module

You can load the modules by:

```
module load impi
```


60.1 Description

NetCDF is a set of software libraries and self-describing, machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data.

60.2 Versions and Dependencies

- **4.5.0**
 1. hdf/4.2.14
 2. hdf5/1.8.16
- **4.7.0**
 1. hdf/4.2.14
 2. hdf5/1.10.5

60.3 Module

You can load the modules by:

```
module load netcdf
```


NETCDF-CXX4

61.1 Description

NetCDF network Common Data Form is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data. This is the C++ distribution.

61.2 Versions and Dependencies

- **4.3.0**
 1. netcdf/4.5.0
- **4.3.1**
 1. netcdf/4.7.0

61.3 Module

You can load the modules by:

```
module load netcdf-cxx4
```


NETCDF-FORTRAN

62.1 Description

Fortran interface for NetCDF4

62.2 Versions and Dependencies

- **4.4.4**
 1. netcdf/4.5.0
- **4.5.2**
 1. netcdf/4.7.0

62.3 Module

You can load the modules by:

```
module load netcdf-fortran
```


OPENBLAS

63.1 Description

An optimized BLAS library

63.2 Versions and Dependencies

- 0.2.20
- 0.3.7

63.3 Module

You can load the modules by:

```
module load openblas
```


64.1 Description

An open source Message Passing Interface implementation.

64.2 Versions and Dependencies

- 1.10.7
- 2.1.6
- **3.1.4**

1. zlib/1.2.11

64.3 Module

You can load the modules by:

```
module load openmpi
```


ZLIB

65.1 Description

A free, general-purpose, legally unencumbered lossless data-compression library.

65.2 Versions and Dependencies

- 1.2.11

65.3 Module

You can load the modules by:

```
module load zlib
```


66.1 Description

Used to invoke Simulia Abaqus.

66.2 Versions and Dependencies

- 2017
- 2018
- 2019
- 2020
- 2021
- 6.14-6

66.3 Module

You can load the modules by:

```
module load abaqus
```


67.1 Description

Boost provides free peer-reviewed portable C++ source libraries, emphasizing libraries that work well with the C++ Standard Library. Boost libraries are intended to be widely useful, and usable across a broad spectrum of applications. The Boost license encourages both commercial and non-commercial use.

67.2 Versions and Dependencies

- **1.64.0**
 1. zlib/1.2.11
- **1.66.0**
 1. zlib/1.2.11
- **1.70.0**
 1. zlib/1.2.11

67.3 Module

You can load the modules by:

```
module load boost
```


CMAKE

68.1 Description

A cross-platform, open-source build system. CMake is a family of tools designed to build, test and package software.

68.2 Versions and Dependencies

- 3.15.4

68.3 Module

You can load the modules by:

```
module load cmake
```


69.1 Description

FFTW is a C subroutine library for computing the discrete Fourier transform DFT in one or more dimensions, of arbitrary input size, and of both real and complex data as well as of even/odd data, i.e. the discrete cosine/sine transforms or DCT/DST. We believe that FFTW, which is free software, should become the FFT library of choice for most applications.

69.2 Versions and Dependencies

- 3.3.4
- 3.3.7

69.3 Module

You can load the modules by:

```
module load fftw
```


70.1 Description

HDF4 also known as HDF is a library and multi-object file format for storing and managing data between machines.

70.2 Versions and Dependencies

- 4.2.14

70.3 Module

You can load the modules by:

```
module load hdf
```


71.1 Description

HDF5 is a data model, library, and file format for storing and managing data. It supports an unlimited variety of datatypes, and is designed for flexible and efficient I/O and for high volume and complex data.

71.2 Versions and Dependencies

- 1.10.5
- 1.8.16

71.3 Module

You can load the modules by:

```
module load hdf5
```


72.1 Description

Intel MPI

72.2 Versions and Dependencies

- 2017.1.132

72.3 Module

You can load the modules by:

```
module load impi
```


73.1 Description

NetCDF network Common Data Form is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data. This is the C distribution.

73.2 Versions and Dependencies

- **4.5.0**
 1. hdf/4.2.14
 2. hdf5/1.8.16
- **4.7.0**
 1. hdf/4.2.14
 2. hdf5/1.10.5

73.3 Module

You can load the modules by:

```
module load netcdf
```


NETCDF-CXX4

74.1 Description

NetCDF network Common Data Form is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data. This is the C++ distribution.

74.2 Versions and Dependencies

- **4.3.0**
 1. netcdf/4.5.0
- **4.3.1**
 1. netcdf/4.7.0

74.3 Module

You can load the modules by:

```
module load netcdf-cxx4
```


NETCDF-FORTRAN

75.1 Description

NetCDF network Common Data Form is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data. This is the Fortran distribution.

75.2 Versions and Dependencies

- **4.4.4**
 1. netcdf/4.5.0
- **4.5.2**
 1. netcdf/4.7.0

75.3 Module

You can load the modules by:

```
module load netcdf-fortran
```


OPENBLAS

76.1 Description

An optimized BLAS (Basic Linear Algebra Subprograms) library.

76.2 Versions and Dependencies

- 0.2.20
- 0.3.7

76.3 Module

You can load the modules by:

```
module load openblas
```


77.1 Description

An open source Message Passing Interface implementation. The Open MPI Project is an open source Message Passing Interface implementation that is developed and maintained by a consortium of academic, research, and industry partners. Open MPI is therefore able to combine the expertise, technologies, and resources from all across the High Performance Computing community in order to build the best MPI library available. Open MPI offers advantages for system and software vendors, application developers and computer science researchers.

77.2 Versions and Dependencies

- 1.10.7
 - 2.1.6
 - **3.1.4**
1. zlib/1.2.11

77.3 Module

You can load the modules by:

```
module load openmpi
```


78.1 Description

Tcl Tool Command Language is a very powerful but easy to learn dynamic programming language, suitable for a very wide range of uses, including web and desktop applications, networking, administration, testing and many more. Open source and business-friendly, Tcl is a mature yet evolving language that is truly cross platform, easily deployed and highly extensible.

78.2 Versions and Dependencies

- 8.6.8
 1. zlib/1.2.11

78.3 Module

You can load the modules by:

```
module load tcl
```


79.1 Description

Tk is a graphical user interface toolkit that takes developing desktop applications to a higher level than conventional approaches. Tk is the standard GUI not only for Tcl, but for many other dynamic languages, and can produce rich, native applications that run unchanged across Windows, Mac OS X, Linux and more.

79.2 Versions and Dependencies

- **8.6.8**

1. tcl/8.6.8

79.3 Module

You can load the modules by:

```
module load tk
```


ZLIB

80.1 Description

A free, general-purpose, legally unencumbered lossless data-compression library.

80.2 Versions and Dependencies

- 1.2.11

80.3 Module

You can load the modules by:

```
module load zlib
```


81.1 Versions and Dependencies

- 2017
- 2018
- 2019
- 2020
- 2021
- 6.14-6

81.2 Module

You can load the modules by:

```
module load abaqus
```


82.1 Description

Boost provides free peer-reviewed portable C++ source libraries, emphasizing libraries that work well with the C++ Standard Library.

82.2 Versions and Dependencies

- **1.64.0**
 1. zlib/1.2.11
- **1.66.0**
 1. zlib/1.2.11
- **1.70.0**
 1. zlib/1.2.11

82.3 Module

You can load the modules by:

```
module load boost
```


CMAKE

83.1 Description

A cross-platform, open-source build system. CMake is a family of tools designed to build, test and package software.

83.2 Versions and Dependencies

- 3.15.4

83.3 Module

You can load the modules by:

```
module load cmake
```


84.1 Description

FFTW is a C subroutine library for computing the discrete Fourier transform DFT in one or more dimensions, of arbitrary input size, and of both real and complex data as well as of even/odd data, i.e. the discrete cosine/sine transforms or DCT/DST. We believe that FFTW, which is free software, should become the FFT library of choice for most applications.

84.2 Versions and Dependencies

- 3.3.4
- 3.3.7

84.3 Module

You can load the modules by:

```
module load fftw
```


85.1 Description

HDF4 also known as HDF is a library and multi-object file format for storing and managing data between machines.

85.2 Versions and Dependencies

- 4.2.14

85.3 Module

You can load the modules by:

```
module load hdf
```


86.1 Description

HDF5 is a data model, library, and file format for storing and managing data. It supports an unlimited variety of datatypes, and is designed for flexible and efficient I/O and for high volume and complex data.

86.2 Versions and Dependencies

- 1.10.5
- 1.8.16

86.3 Module

You can load the modules by:

```
module load hdf5
```


87.1 Description

Intel MPI

87.2 Versions and Dependencies

- 2018.1.163

87.3 Module

You can load the modules by:

```
module load impi
```


88.1 Description

NetCDF is a set of software libraries and self-describing, machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data.

88.2 Versions and Dependencies

- **4.5.0**
 1. hdf/4.2.14
 2. hdf5/1.8.16
- **4.7.0**
 1. hdf/4.2.14
 2. hdf5/1.10.5

88.3 Module

You can load the modules by:

```
module load netcdf
```


NETCDF-CXX4

89.1 Description

NetCDF network Common Data Form is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data. This is the C++ distribution.

89.2 Versions and Dependencies

- **4.3.0**
 1. netcdf/4.5.0
- **4.3.1**
 1. netcdf/4.7.0

89.3 Module

You can load the modules by:

```
module load netcdf-cxx4
```


NETCDF-FORTRAN

90.1 Description

Fortran interface for NetCDF4

90.2 Versions and Dependencies

- **4.4.4**
 1. netcdf/4.5.0
- **4.5.2**
 1. netcdf/4.7.0

90.3 Module

You can load the modules by:

```
module load netcdf-fortran
```


OPENBLAS

91.1 Description

An optimized BLAS library

91.2 Versions and Dependencies

- 0.2.20
- 0.3.7

91.3 Module

You can load the modules by:

```
module load openblas
```


92.1 Description

An open source Message Passing Interface implementation.

92.2 Versions and Dependencies

- 1.10.7
- 2.1.6
- **3.1.4**

1. zlib/1.2.11

92.3 Module

You can load the modules by:

```
module load openmpi
```


93.1 Description

A free, general-purpose, legally unencumbered lossless data-compression library.

93.2 Versions and Dependencies

- 1.2.11

93.3 Module

You can load the modules by:

```
module load zlib
```


94.1 Versions and Dependencies

- 2017
- 2018
- 2019
- 2020
- 2021
- 6.14-6

94.2 Module

You can load the modules by:

```
module load abaqus
```


95.1 Description

Boost provides free peer-reviewed portable C++ source libraries, emphasizing libraries that work well with the C++ Standard Library.

95.2 Versions and Dependencies

- **1.64.0**
 1. zlib/1.2.11
- **1.66.0**
 1. zlib/1.2.11
- **1.70.0**
 1. zlib/1.2.11

95.3 Module

You can load the modules by:

```
module load boost
```


CMAKE

96.1 Description

A cross-platform, open-source build system. CMake is a family of tools designed to build, test and package software.

96.2 Versions and Dependencies

- 3.15.4

96.3 Module

You can load the modules by:

```
module load cmake
```


97.1 Description

FFTW is a C subroutine library for computing the discrete Fourier transform DFT in one or more dimensions, of arbitrary input size, and of both real and complex data as well as of even/odd data, i.e. the discrete cosine/sine transforms or DCT/DST. We believe that FFTW, which is free software, should become the FFT library of choice for most applications.

97.2 Versions and Dependencies

- 3.3.4
- 3.3.7

97.3 Module

You can load the modules by:

```
module load fftw
```


98.1 Description

HDF4 also known as HDF is a library and multi-object file format for storing and managing data between machines.

98.2 Versions and Dependencies

- 4.2.14

98.3 Module

You can load the modules by:

```
module load hdf
```


99.1 Description

HDF5 is a data model, library, and file format for storing and managing data. It supports an unlimited variety of datatypes, and is designed for flexible and efficient I/O and for high volume and complex data.

99.2 Versions and Dependencies

- 1.10.5
- 1.8.16

99.3 Module

You can load the modules by:

```
module load hdf5
```


100.1 Description

Intel MPI

100.2 Versions and Dependencies

- 2019.3.199

100.3 Module

You can load the modules by:

```
module load impi
```


101.1 Description

NetCDF is a set of software libraries and self-describing, machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data.

101.2 Versions and Dependencies

- **4.5.0**
 1. hdf/4.2.14
 2. hdf5/1.8.16
- **4.7.0**
 1. hdf/4.2.14
 2. hdf5/1.10.5

101.3 Module

You can load the modules by:

```
module load netcdf
```


NETCDF-CXX4

102.1 Description

NetCDF network Common Data Form is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data. This is the C++ distribution.

102.2 Versions and Dependencies

- **4.3.0**
 1. netcdf/4.5.0
- **4.3.1**
 1. netcdf/4.7.0

102.3 Module

You can load the modules by:

```
module load netcdf-cxx4
```


NETCDF-FORTRAN

103.1 Description

Fortran interface for NetCDF4

103.2 Versions and Dependencies

- **4.4.4**
 1. netcdf/4.5.0
- **4.5.2**
 1. netcdf/4.7.0

103.3 Module

You can load the modules by:

```
module load netcdf-fortran
```


OPENBLAS

104.1 Description

An optimized BLAS library

104.2 Versions and Dependencies

- 0.2.20
- 0.3.7

104.3 Module

You can load the modules by:

```
module load openblas
```


OPENMPI

105.1 Description

An open source Message Passing Interface implementation.

105.2 Versions and Dependencies

- 1.10.7
- 2.1.6
- **3.1.4**

1. zlib/1.2.11

105.3 Module

You can load the modules by:

```
module load openmpi
```


106.1 Description

A free, general-purpose, legally unencumbered lossless data-compression library.

106.2 Versions and Dependencies

- 1.2.11

106.3 Module

You can load the modules by:

```
module load zlib
```


107.1 Description

Boost provides free peer-reviewed portable C++ source libraries, emphasizing libraries that work well with the C++ Standard Library.

107.2 Versions and Dependencies

- **1.66.0**
 1. impi/5.1.3.223
 2. zlib/1.2.11

107.3 Module

You can load the modules by:

```
module load boost
```


108.1 Description

FFTW is a C subroutine library for computing the discrete Fourier transform DFT in one or more dimensions, of arbitrary input size, and of both real and complex data as well as of even/odd data, i.e. the discrete cosine/sine transforms or DCT/DST. We believe that FFTW, which is free software, should become the FFT library of choice for most applications.

108.2 Versions and Dependencies

- **3.3.7**

1. impi/5.1.3.223

108.3 Module

You can load the modules by:

```
module load fftw
```


PARALLEL-NETCDF

109.1 Description

PnetCDF Parallel netCDF is a high-performance parallel I/O library for accessing files in format compatibility with Unidatas NetCDF, specifically the formats of CDF-1, 2, and 5.

109.2 Versions and Dependencies

- **1.10.0**

1. impi/5.1.3.223

109.3 Module

You can load the modules by:

```
module load parallel-netcdf
```


110.1 Description

[//spack.readthedocs.io/en/latest/mirrors.html](https://spack.readthedocs.io/en/latest/mirrors.html)

110.2 Versions and Dependencies

- 16

1. impi/2017.1.132
2. netcdf-fortran/4.4.4

110.3 Module

You can load the modules by:

```
module load amber
```


111.1 Description

Boost provides free peer-reviewed portable C++ source libraries, emphasizing libraries that work well with the C++ Standard Library.

111.2 Versions and Dependencies

- **1.66.0**
 1. impi/2017.1.132
 2. zlib/1.2.11
- **1.70.0**
 1. impi/2017.1.132
 2. zlib/1.2.11

111.3 Module

You can load the modules by:

```
module load boost
```


112.1 Description

FFTW is a C subroutine library for computing the discrete Fourier transform DFT in one or more dimensions, of arbitrary input size, and of both real and complex data as well as of even/odd data, i.e. the discrete cosine/sine transforms or DCT/DST. We believe that FFTW, which is free software, should become the FFT library of choice for most applications.

112.2 Versions and Dependencies

- 3.3.7

1. impi/2017.1.132

112.3 Module

You can load the modules by:

```
module load fftw
```


GROMACS

113.1 Description

GROMACS GROningen MAchine for Chemical Simulations is a molecular dynamics package primarily designed for simulations of proteins, lipids and nucleic acids. It was originally developed in the Biophysical Chemistry department of University of Groningen, and is now maintained by contributors in universities and research centers across the world.

113.2 Versions and Dependencies

- **2018.4**
 1. fftw/3.3.7
 2. impi/2017.1.132
- **2019.2**
 1. fftw/3.3.7
 2. impi/2017.1.132

113.3 Module

You can load the modules by:

```
module load gromacs
```


LAMMPS

114.1 Versions and Dependencies

- 31Mar17
- 7Aug19

114.2 Module

You can load the modules by:

```
module load lammeps
```


PARALLEL-NETCDF

115.1 Description

PnetCDF Parallel netCDF is a high-performance parallel I/O library for accessing files in format compatibility with Unidatas NetCDF, specifically the formats of CDF-1, 2, and 5.

115.2 Versions and Dependencies

- **1.10.0**

1. impi/2017.1.132

115.3 Module

You can load the modules by:

```
module load parallel-netcdf
```


QUANTUM-ESPRESSO

116.1 Description

Quantum-ESPRESSO is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials.

116.2 Versions and Dependencies

- **6.2.1**

1. fftw/3.3.7
2. impi/2017.1.132
3. intel/17.0.1.132

- **6.3**

1. fftw/3.3.7
2. impi/2017.1.132
3. intel/17.0.1.132

116.3 Module

You can load the modules by:

```
module load quantum-espresso
```


117.1 Description

Boost provides free peer-reviewed portable C++ source libraries, emphasizing libraries that work well with the C++ Standard Library.

117.2 Versions and Dependencies

- **1.66.0**
 1. impi/2018.1.163
 2. zlib/1.2.11
- **1.70.0**
 1. impi/2018.1.163
 2. zlib/1.2.11

117.3 Module

You can load the modules by:

```
module load boost
```


118.1 Description

FFTW is a C subroutine library for computing the discrete Fourier transform DFT in one or more dimensions, of arbitrary input size, and of both real and complex data as well as of even/odd data, i.e. the discrete cosine/sine transforms or DCT/DST. We believe that FFTW, which is free software, should become the FFT library of choice for most applications.

118.2 Versions and Dependencies

- **3.3.7**

1. [impi/2018.1.163](#)

118.3 Module

You can load the modules by:

```
module load fftw
```


PARALLEL-NETCDF

119.1 Description

PnetCDF Parallel netCDF is a high-performance parallel I/O library for accessing files in format compatibility with Unidatas NetCDF, specifically the formats of CDF-1, 2, and 5.

119.2 Versions and Dependencies

- **1.10.0**

1. impi/2018.1.163

119.3 Module

You can load the modules by:

```
module load parallel-netcdf
```


120.1 Description

Boost provides free peer-reviewed portable C++ source libraries, emphasizing libraries that work well with the C++ Standard Library.

120.2 Versions and Dependencies

- **1.66.0**
 1. impi/2019.3.199
 2. zlib/1.2.11
- **1.70.0**
 1. impi/2019.3.199
 2. zlib/1.2.11

120.3 Module

You can load the modules by:

```
module load boost
```


121.1 Description

FFTW is a C subroutine library for computing the discrete Fourier transform DFT in one or more dimensions, of arbitrary input size, and of both real and complex data as well as of even/odd data, i.e. the discrete cosine/sine transforms or DCT/DST. We believe that FFTW, which is free software, should become the FFT library of choice for most applications.

121.2 Versions and Dependencies

- **3.3.7**

1. [impi/2019.3.199](#)

121.3 Module

You can load the modules by:

```
module load fftw
```


PARALLEL-NETCDF

122.1 Description

PnetCDF Parallel netCDF is a high-performance parallel I/O library for accessing files in format compatibility with Unidatas NetCDF, specifically the formats of CDF-1, 2, and 5.

122.2 Versions and Dependencies

- **1.10.0**

1. impi/2019.3.199

122.3 Module

You can load the modules by:

```
module load parallel-netcdf
```


123.1 Description

Boost provides free peer-reviewed portable C++ source libraries, emphasizing libraries that work well with the C++ Standard Library.

123.2 Versions and Dependencies

- **1.66.0**
 1. openmpi/1.10.7-old
 2. zlib/1.2.11

123.3 Module

You can load the modules by:

```
module load boost
```


124.1 Description

FFTW is a C subroutine library for computing the discrete Fourier transform DFT in one or more dimensions, of arbitrary input size, and of both real and complex data as well as of even/odd data, i.e. the discrete cosine/sine transforms or DCT/DST. We believe that FFTW, which is free software, should become the FFT library of choice for most applications.

124.2 Versions and Dependencies

- **3.3.7**

1. openmpi/1.10.7-old

124.3 Module

You can load the modules by:

```
module load fftw
```


PARALLEL-NETCDF

125.1 Description

PnetCDF Parallel netCDF is a high-performance parallel I/O library for accessing files in format compatibility with Unidatas NetCDF, specifically the formats of CDF-1, 2, and 5.

125.2 Versions and Dependencies

- **1.10.0**

1. openmpi/1.10.7-old

125.3 Module

You can load the modules by:

```
module load parallel-netcdf
```


126.1 Description

Boost provides free peer-reviewed portable C++ source libraries, emphasizing libraries that work well with the C++ Standard Library.

126.2 Versions and Dependencies

- **1.66.0**
 1. openmpi/2.1.6-old
 2. zlib/1.2.11
- **1.70.0**
 1. openmpi/2.1.6-old
 2. zlib/1.2.11

126.3 Module

You can load the modules by:

```
module load boost
```


127.1 Description

FFTW is a C subroutine library for computing the discrete Fourier transform DFT in one or more dimensions, of arbitrary input size, and of both real and complex data as well as of even/odd data, i.e. the discrete cosine/sine transforms or DCT/DST. We believe that FFTW, which is free software, should become the FFT library of choice for most applications.

127.2 Versions and Dependencies

- **3.3.7**

1. openmpi/2.1.6-old

127.3 Module

You can load the modules by:

```
module load fftw
```


OPENFOAM

128.1 Versions and Dependencies

- 5.0_slurm
- 6.0
- 7.0

128.2 Module

You can load the modules by:

```
module load openfoam
```


PARALLEL-NETCDF

129.1 Description

PnetCDF Parallel netCDF is a high-performance parallel I/O library for accessing files in format compatibility with Unidatas NetCDF, specifically the formats of CDF-1, 2, and 5.

129.2 Versions and Dependencies

- **1.10.0**

1. openmpi/2.1.6-old

129.3 Module

You can load the modules by:

```
module load parallel-netcdf
```


PARAVIEW

130.1 Description

ParaView is an open-source, multi-platform data analysis and visualization application.

130.2 Versions and Dependencies

- 5.4.0
- 5.6.2

130.3 Module

You can load the modules by:

```
module load paraview
```


131.1 Description

Boost provides free peer-reviewed portable C++ source libraries, emphasizing libraries that work well with the C++ Standard Library.

131.2 Versions and Dependencies

- **1.66.0**
 1. openmpi/3.1.4-old
 2. zlib/1.2.11
- **1.70.0**
 1. openmpi/3.1.4-old
 2. zlib/1.2.11

131.3 Module

You can load the modules by:

```
module load boost
```


132.1 Description

FFTW is a C subroutine library for computing the discrete Fourier transform DFT in one or more dimensions, of arbitrary input size, and of both real and complex data as well as of even/odd data, i.e. the discrete cosine/sine transforms or DCT/DST. We believe that FFTW, which is free software, should become the FFT library of choice for most applications.

132.2 Versions and Dependencies

- 3.3.7
 1. openmpi/3.1.4-old

132.3 Module

You can load the modules by:

```
module load fftw
```


133.1 Description

Meep or MEEP is a free finite-difference time-domain FDTD simulation software package developed at MIT to model electromagnetic systems.

133.2 Versions and Dependencies

- **1.20.0**
 1. fftw/3.3.7
 2. hdf5/1.8.16
 3. openmpi/3.1.4-old

133.3 Module

You can load the modules by:

```
module load meep
```


PARALLEL-NETCDF

134.1 Description

PnetCDF Parallel netCDF is a high-performance parallel I/O library for accessing files in format compatibility with Unidatas NetCDF, specifically the formats of CDF-1, 2, and 5.

134.2 Versions and Dependencies

- **1.10.0**
 1. openmpi/3.1.4-old

134.3 Module

You can load the modules by:

```
module load parallel-netcdf
```


PARAVIEW

135.1 Description

ParaView is an open-source, multi-platform data analysis and visualization application.

135.2 Versions and Dependencies

- **5.9.1**

1. libtiff/4.0.10
2. openmpi/3.1.4-old
3. zlib/1.2.11

135.3 Module

You can load the modules by:

```
module load paraview
```


ANACONDA

136.1 Description

Python distribution, virtual environments, and package manager.

136.2 Versions and Dependencies

- 2019.10-py27
- 2020.02-py37
- 2020.11-py38
- 5.1.0-py27
- 5.1.0-py36
- 5.3.1-py27
- 5.3.1-py37

136.3 Module

You can load the modules by:

```
module load anaconda
```


137.1 Description

This module loads the ANSYS software suite. Note: Users may experience reduced functionality, including model size restrictions, unless a research license is used.

137.2 Versions and Dependencies

- 17.1
- 18.2
- 19.2
- 2019R3
- 2020R1
- 2021R2
- 2022R1

137.3 Module

You can load the modules by:

```
module load ansys
```


ANSYSEM

138.1 Description

Ansys Mechanical enables you to solve complex structural engineering problems and make better, faster design decisions. With the finite element analysis (FEA) solvers available in the suite, you can customize and automate solutions for your structural mechanics problems and parameterize them to analyze multiple design scenarios. Ansys Mechanical is a dynamic tool that has a complete range of analysis tools.

138.2 Versions and Dependencies

- 19.2
- 2020r1
- 2021r2

138.3 Module

You can load the modules by:

```
module load ansysem
```


139.1 Description

The AWS Command Line Interface CLI is a unified tool to manage your AWS services from command line. For more information: <https://aws.amazon.com/cli/>

139.2 Versions and Dependencies

- 2.4.15

139.3 Module

You can load the modules by:

```
module load aws-cli
```


BIOCONTAINERS

140.1 Description

This module enables a collection of BioContainers application containers.

140.2 Versions and Dependencies

- default

140.3 Module

You can load the modules by:

```
module load biocontainers
```


141.1 Description

Once this module is loaded, modules maintained by Bioinformatics become available for use. Note that some bioinformatics modules depend on deprecated RCAC softwares, therefore, you may need to load the 'modtree/deprecated' module.

141.2 Module

You can load the modules by:

```
module load bioinfo
```


142.1 Description

Boost provides free peer-reviewed portable C++ source libraries, emphasizing libraries that work well with the C++ Standard Library. Boost libraries are intended to be widely useful, and usable across a broad spectrum of applications. The Boost license encourages both commercial and non-commercial use.

142.2 Versions and Dependencies

- **1.64.0**
 - 1. zlib/1.2.11
- **1.66.0**
 - 1. zlib/1.2.11
- **1.70.0**
 - 1. zlib/1.2.11

142.3 Module

You can load the modules by:

```
module load boost
```


143.1 Description

CDO is a collection of command line Operators to manipulate and analyse Climate and NWP model Data.

143.2 Versions and Dependencies

- **1.9.5**
 1. fftw/3.3.7
 2. hdf5/1.8.16
 3. netcdf/4.5.0
 4. udunits2/2.2.24

143.3 Module

You can load the modules by:

```
module load cdo
```


CMAKE

144.1 Description

A cross-platform, open-source build system. CMake is a family of tools designed to build, test and package software.

144.2 Versions and Dependencies

- 3.15.4
- 3.20.6

144.3 Module

You can load the modules by:

```
module load cmake
```


145.1 Description

COMSOL Multiphysics® is a general-purpose simulation software used in all fields of engineering, manufacturing, and scientific research. The software brings fully coupled multiphysics and single-physics modeling capabilities, simulation data management, and user-friendly tools for building simulation applications.

145.2 Versions and Dependencies

- 5.3a
- 5.4
- 5.5_b359
- 5.6

145.3 Module

You can load the modules by:

```
module load comsol
```


146.1 Description

CPLEX is a high-performance mathematical programming solver for linear programming, mixed integer programming, and quadratic programming

146.2 Versions and Dependencies

- 12.8.0

146.3 Module

You can load the modules by:

```
module load cplex
```


CURL

147.1 Description

cURL is an open source command line tool and library for transferring data with URL syntax

147.2 Versions and Dependencies

- 7.63.0
 - 1. zlib/1.2.11

147.3 Module

You can load the modules by:

```
module load curl
```


148.1 Description

ENVI is the industry standard for image processing and analysis software. It is used by image analysts, GIS professionals and scientists to extract timely, reliable and accurate information from geospatial imagery. This geospatial software is scientifically proven, easy to use and tightly integrated with Esri's ArcGIS platform.

148.2 Versions and Dependencies

- 5.5.2

148.3 Module

You can load the modules by:

```
module load envi
```


FFMPEG

149.1 Description

FFmpeg is a complete, cross-platform solution to record, convert and stream audio and video.

149.2 Versions and Dependencies

- 4.2.1

149.3 Module

You can load the modules by:

```
module load ffmpeg
```


150.1 Description

FFTW is a C subroutine library for computing the discrete Fourier transform DFT in one or more dimensions, of arbitrary input size, and of both real and complex data as well as of even/odd data, i.e. the discrete cosine/sine transforms or DCT/DST. We believe that FFTW, which is free software, should become the FFT library of choice for most applications.

150.2 Versions and Dependencies

- 3.3.4
- 3.3.7

150.3 Module

You can load the modules by:

```
module load fftw
```


GAMESS

151.1 Description

GAMESS is a program for ab initio molecular quantum chemistry.

151.2 Versions and Dependencies

- 18.Aug.2016.R1
- 30.Jun.2019.R1

151.3 Module

You can load the modules by:

```
module load gamess
```


GAUSSIAN09

152.1 Description

Gaussian is a computer program used by chemists, chemical engineers, biochemists, physicists and other scientists. It utilizes fundamental laws of quantum mechanics to predict energies, molecular structures, spectroscopic data (NMR, IR, UV, etc) and much more advanced calculations.

152.2 Versions and Dependencies

- E.01

152.3 Module

You can load the modules by:

```
module load gaussian09
```


GAUSSIAN16

153.1 Description

Gaussian is a computer program used by chemists, chemical engineers, biochemists, physicists and other scientists. It utilizes fundamental laws of quantum mechanics to predict energies, molecular structures, spectroscopic data (NMR, IR, UV, etc) and much more advanced calculations.

153.2 Versions and Dependencies

- A.03
- B.01

153.3 Module

You can load the modules by:

```
module load gaussian16
```


GAUSSVIEW

154.1 Description

Gaussview is a graphical interface used with Gaussian. It aids in the creation of Gaussian input files, enables the user to run Gaussian calculations from a graphical interface without the need for using a command line instruction, and helps in the interpretation of Gaussian output (e.g., you can use it to plot properties, animate vibrations, visualize computed spectra, etc.).

154.2 Versions and Dependencies

- 5.0.8
- 6.0.16

154.3 Module

You can load the modules by:

```
module load gaussview
```


155.1 Description

The GNU Compiler Collection includes front ends for C, C++, Objective-C, Fortran, Ada, and Go, as well as libraries for these languages.

155.2 Versions and Dependencies

- 4.8.5
- **5.2.0**
 1. gmp/6.1.2
 2. mpc/1.1.0
 3. mpfr/3.1.6
- **6.3.0**
 1. gmp/6.1.2
 2. mpc/1.1.0
 3. mpfr/3.1.6
- **7.3.0**
 1. gmp/6.1.2
 2. mpc/1.1.0
 3. mpfr/3.1.6
- **8.3.0**
 1. gmp/6.1.2
 2. mpc/1.1.0
 3. mpfr/3.1.6

155.3 Module

You can load the modules by:

```
module load gcc
```

156.1 Description

GDAL Geospatial Data Abstraction Library is a translator library for raster and vector geospatial data formats that is released under an X/MIT style Open Source license by the Open Source Geospatial Foundation. As a library, it presents a single raster abstract data model and vector abstract data model to the calling application for all supported formats. It also comes with a variety of useful command line utilities for data translation and processing.

156.2 Versions and Dependencies

- **2.4.2**

1. hdf/4.2.14
2. hdf5/1.8.16
3. libtiff/4.0.10
4. netcdf/4.5.0
5. proj/5.2.0
6. zlib/1.2.11

- **3.4.2**

1. curl/7.63.0
2. geos/3.7.2
3. hdf/4.2.14
4. hdf5/1.10.5
5. libtiff/4.0.10
6. netcdf/4.7.0
7. proj/8.1.0
8. zlib/1.2.11

156.3 Module

You can load the modules by:

```
module load gdal
```


157.1 Description

GEOS Geometry Engine - Open Source is a C++ port of the Java Topology Suite JTS. As such, it aims to contain the complete functionality of JTS in C++. This includes all the OpenGIS Simple Features for SQL spatial predicate functions and spatial operators, as well as specific JTS enhanced topology functions.

157.2 Versions and Dependencies

- 3.7.2

157.3 Module

You can load the modules by:

```
module load geos
```


158.1 Description

GMP is a free library for arbitrary precision arithmetic, operating on signed integers, rational numbers, and floating-point numbers.

158.2 Versions and Dependencies

- 6.1.2

158.3 Module

You can load the modules by:

```
module load gmp
```


159.1 Description

GMT Generic Mapping Tools is an open source collection of about 80 command-line tools for manipulating geographic and Cartesian data sets including filtering, trend fitting, gridding, projecting, etc. and producing PostScript illustrations ranging from simple x-y plots via contour maps to artificially illuminated surfaces and 3D perspective views.

159.2 Versions and Dependencies

- **5.4.4**
 1. fftw/3.3.7
 2. gdal/2.4.2
 3. netcdf/4.5.0
 4. openblas/0.2.20

159.3 Module

You can load the modules by:

```
module load gmt
```


GNUPLOT

160.1 Description

Gnuplot is a portable command-line driven graphing utility for Linux, OS/2, MS Windows, OSX, VMS, and many other platforms. The source code is copyrighted but freely distributed i.e., you don't have to pay for it. It was originally created to allow scientists and students to visualize mathematical functions and data interactively, but has grown to support many non-interactive uses such as web scripting. It is also used as a plotting engine by third-party applications like Octave. Gnuplot has been supported and under active development since 1986

160.2 Versions and Dependencies

- 5.2.7

160.3 Module

You can load the modules by:

```
module load gnuplot
```


GRADS

161.1 Description

The Grid Analysis and Display System (GrADS) is an interactive desktop tool that is used for easy access, manipulation, and visualization of earth science data. GrADS has two data models for handling gridded and station data.

161.2 Versions and Dependencies

- 2.2.1

161.3 Module

You can load the modules by:

```
module load grads
```


162.1 Description

The GNU Scientific Library GSL is a numerical library for C and C++ programmers. It is free software under the GNU General Public License. The library provides a wide range of mathematical routines such as random number generators, special functions and least-squares fitting. There are over 1000 functions in total with an extensive test suite.

162.2 Versions and Dependencies

- 2.4

162.3 Module

You can load the modules by:

```
module load gsl
```


163.1 Description

The Gurobi Optimizer was designed from the ground up to be the fastest, most powerful solver available for your LP, QP, QCP, and MIP (MILP, MIQP, and MIQCP) problems. Note: Gurobi is licensed software. You will need to create an account on the Gurobi homepage and download Gurobi Optimizer yourself.

163.2 Versions and Dependencies

- 9.0.1
- 9.5.1

163.3 Module

You can load the modules by:

```
module load gurobi
```


HADOOP

164.1 Description

The Apache Hadoop software library is a framework that allows for the distributed processing of large data sets across clusters of computers using simple programming models.

164.2 Versions and Dependencies

- 2.7.7

164.3 Module

You can load the modules by:

```
module load hadoop
```


165.1 Description

HDF4 also known as HDF is a library and multi-object file format for storing and managing data between machines.

165.2 Versions and Dependencies

- 4.2.14

165.3 Module

You can load the modules by:

```
module load hdf
```


166.1 Description

HDF5 is a data model, library, and file format for storing and managing data. It supports an unlimited variety of datatypes, and is designed for flexible and efficient I/O and for high volume and complex data.

166.2 Versions and Dependencies

- 1.10.5
- 1.8.16

166.3 Module

You can load the modules by:

```
module load hdf5
```


167.1 Description

HSPICE is an analog circuit simulator capable of performing transient, steady state, and frequency domain analyses.

167.2 Versions and Dependencies

- 2017.12
- 2019.06
- 2020.12

167.3 Module

You can load the modules by:

```
module load hspice
```


HYPER-SHELL

168.1 Description

Process shell commands over a distributed, asynchronous queue.

168.2 Versions and Dependencies

- 1.8.3
- 2.0.0

168.3 Module

You can load the modules by:

```
module load hyper-shell
```


169.1 Description

envi @5.5.2

169.2 Versions and Dependencies

- 8.7

169.3 Module

You can load the modules by:

```
module load idl
```


170.1 Description

Intel Parallel Studio.

170.2 Versions and Dependencies

- 16.0.1.150
- 17.0.1.132
- 18.0.1.163
- 19.0.3.199

170.3 Module

You can load the modules by:

```
module load intel
```


171.1 Description

The Julia Language: A fresh approach to technical computing. Julia is a high-level, high-performance, dynamic programming language. While it is a general-purpose language and can be used to write any application, many of its features are well suited for numerical analysis and computational science.

171.2 Versions and Dependencies

- 1.7.1

171.3 Module

You can load the modules by:

```
module load julia
```


JUPYTERHUB

172.1 Description

Complete Jupyter Hub/Lab/Notebook environment.

172.2 Versions and Dependencies

- 2.0.0

1. texlive

172.3 Module

You can load the modules by:

```
module load jupyterhub
```


LEARNING

173.1 Versions and Dependencies

- **conda-5.1.0-py27-cpu**
 1. anaconda/5.1.0-py27
- **conda-5.1.0-py36-cpu**
 1. anaconda/5.1.0-py36

173.2 Module

You can load the modules by:

```
module load learning
```


174.1 Description

LibTIFF - Tag Image File Format TIFF Library and Utilities.

174.2 Versions and Dependencies

- **4.0.10**
 1. zlib/1.2.11

174.3 Module

You can load the modules by:

```
module load libtiff
```


MATHEMATICA

175.1 Description

Mathematica (Wolfram Language and other tools) provide a language, software system for technical computing in R&D and education, and computer algebra system.

175.2 Versions and Dependencies

- 11.3
- 12.1
- 12.3
- 9.0

175.3 Module

You can load the modules by:

```
module load mathematica
```


176.1 Description

MATLAB MATrix LABoratory is a multi-paradigm numerical computing environment and fourth-generation programming language. A proprietary programming language developed by MathWorks, MATLAB allows matrix manipulations, plotting of functions and data, implementation of algorithms, creation of user interfaces, and interfacing with programs written in other languages, including C, C++, C#, Java, Fortran and Python.

176.2 Versions and Dependencies

- R2017a
- R2018a
- R2019a
- R2020a
- R2020b
- R2021b

176.3 Module

You can load the modules by:

```
module load matlab
```


MODTREE

177.1 Description

This module helps users to switch to the new software stack provided by RCAC. You do not need to explicitly load this module unless you are switching from the deprecated module tree.

177.2 Versions and Dependencies

- deprecated
- new

177.3 Module

You can load the modules by:

```
module load modtree
```


178.1 Description

Gnu Mpc is a C library for the arithmetic of complex numbers with arbitrarily high precision and correct rounding of the result.

178.2 Versions and Dependencies

- **1.1.0**
 1. gmp/6.1.2
 2. mpfr/3.1.6

178.3 Module

You can load the modules by:

```
module load mpc
```


179.1 Description

The MPFR library is a C library for multiple-precision floating-point computations with correct rounding.

179.2 Versions and Dependencies

- **3.1.6**
 1. gmp/6.1.2

179.3 Module

You can load the modules by:

```
module load mpfr
```


180.1 Description

NCL is an interpreted language designed specifically for scientific data analysis and visualization. Supports NetCDF 3/4, GRIB 1/2, HDF 4/5, HDF-EOD 2/5, shapefile, ASCII, binary. Numerous analysis functions are built-in.

180.2 Versions and Dependencies

- **6.4.0**

1. gdal/2.4.2
2. hdf/4.2.14
3. hdf5/1.8.16
4. netcdf/4.5.0
5. udunits2/2.2.24

180.3 Module

You can load the modules by:

```
module load ncl
```


181.1 Description

The NCO toolkit manipulates and analyzes data stored in netCDF-accessible formats

181.2 Versions and Dependencies

- **4.6.7**
 1. netcdf/4.5.0
 2. udunits2/2.2.24

181.3 Module

You can load the modules by:

```
module load nco
```


182.1 Description

Simple viewer for NetCDF files.

182.2 Versions and Dependencies

- **2.1.7**
 1. netcdf/4.5.0
 2. udunits2/2.2.24

182.3 Module

You can load the modules by:

```
module load ncview
```


183.1 Description

NetCDF network Common Data Form is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data. This is the C distribution.

183.2 Versions and Dependencies

- **4.5.0**
 1. hdf/4.2.14
 2. hdf5/1.8.16
- **4.7.0**
 1. hdf/4.2.14
 2. hdf5/1.10.5

183.3 Module

You can load the modules by:

```
module load netcdf
```


NETCDF-CXX4

184.1 Description

NetCDF network Common Data Form is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data. This is the C++ distribution.

184.2 Versions and Dependencies

- **4.3.0**
 1. netcdf/4.5.0
- **4.3.1**
 1. netcdf/4.7.0

184.3 Module

You can load the modules by:

```
module load netcdf-cxx4
```


NETCDF-FORTRAN

185.1 Description

NetCDF network Common Data Form is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data. This is the Fortran distribution.

185.2 Versions and Dependencies

- **4.4.4**
 1. netcdf/4.5.0
- **4.5.2**
 1. netcdf/4.7.0

185.3 Module

You can load the modules by:

```
module load netcdf-fortran
```


NETLIB-LAPACK

186.1 Description

LAPACK version 3.X is a comprehensive FORTRAN library that does linear algebra operations including matrix inversions, least squared solutions to linear sets of equations, eigenvector analysis, singular value decomposition, etc. It is a very comprehensive and reputable package that has found extensive use in the scientific community.

186.2 Versions and Dependencies

- 3.6.0

186.3 Module

You can load the modules by:

```
module load netlib-lapack
```


187.1 Description

GNU Octave is a high-level language, primarily intended for numerical computations. It provides a convenient command line interface for solving linear and nonlinear problems numerically, and for performing other numerical experiments using a language that is mostly compatible with Matlab. It may also be used as a batch-oriented language.

187.2 Versions and Dependencies

- **4.4.0**

1. openblas/0.2.20

187.3 Module

You can load the modules by:

```
module load octave
```


OPENBLAS

188.1 Description

An optimized BLAS (Basic Linear Algebra Subprograms) library.

188.2 Versions and Dependencies

- 0.2.20
- 0.3.7

188.3 Module

You can load the modules by:

```
module load openblas
```


PANOPLY

189.1 Description

Panoply is a Java-based cross-platform NetCDF, HDF and GRIB Data Viewer.

189.2 Versions and Dependencies

- **4.11.0**

1. – AAAA, BBBB, CCCC

189.3 Module

You can load the modules by:

```
module load panoply
```


190.1 Description

PROJ is a generic coordinate transformation software, that transforms geospatial coordinates from one coordinate reference system CRS to another. This includes cartographic projections as well as geodetic transformations.

190.2 Versions and Dependencies

- 5.2.0
- **8.1.0**
 1. libtiff/4.0.10

190.3 Module

You can load the modules by:

```
module load proj
```


PROTOBUF

191.1 Description

Googles data interchange format.

191.2 Versions and Dependencies

- 3.0.2

191.3 Module

You can load the modules by:

```
module load protobuf
```


192.1 Description

QEMU is a generic and open source machine emulator and virtualizer.

192.2 Versions and Dependencies

- 2.10.1

192.3 Module

You can load the modules by:

```
module load qemu
```


193.1 Description

Qt is a comprehensive cross-platform C++ application framework.

193.2 Versions and Dependencies

- 5.12.5

193.3 Module

You can load the modules by:

```
module load qt
```


QUANTUMATK

194.1 Description

QuantumATK atomic-scale modeling software enables large-scale and thus more realistic material simulations, integrating multiple simulation methods, ranging from ab initio DFT to semi-empirical and classical force fields analysis, into an easy-to-use platform.

194.2 Versions and Dependencies

- 2020.09

194.3 Module

You can load the modules by:

```
module load quantumatk
```


195.1 Description

R is ‘GNU S’, a freely available language and environment for statistical computing and graphics which provides a wide variety of statistical and graphical techniques: linear and nonlinear modelling, statistical tests, time series analysis, classification, clustering, etc. Please consult the R project homepage for further information.

195.2 Versions and Dependencies

- **3.6.1**

1. gcc/6.3.0

- **3.6.3**

1. gcc/6.3.0
2. tcl/8.6.8
3. tk/8.6.8
4. zlib/1.2.11
5. openblas/0.2.20

- **4.0.0**

1. gcc/6.3.0
2. tcl/8.6.8
3. tk/8.6.8
4. zlib/1.2.11
5. openblas/0.3.7

- **4.1.2**

1. gcc/6.3.0
2. tcl/8.6.8
3. tk/8.6.8
4. libtiff/4.0.10
5. zlib/1.2.11

6. openblas/0.3.7

195.3 Module

You can load the modules by:

```
module load r
```

196.1 Description

Establish recommended development environment for Bell

196.2 Versions and Dependencies

- **20171031**
 1. intel/17.0.1.132
 2. impi/2017.1.132
 3. xalt

196.3 Module

You can load the modules by:

```
module load rcac
```


197.1 Description

This package installs Rstudio desktop from pre-compiled binaries available in the Rstudio website. The installer assumes that you are running on CentOS7/Redhat7/Fedora19. Please fix the download URL for other systems.

197.2 Versions and Dependencies

- **1.2.1335**
 1. r/3.6.1
- **1.3.959**
 1. gcc/6.3.0
 2. r/3.6.3
 3. texlive/20200406
- **2021.09**
 1. gcc/6.3.0
 2. r/4.1.2
 3. texlive/20200406

197.3 Module

You can load the modules by:

```
module load rstudio
```


198.1 Description

Statistical Analysis Software

198.2 Versions and Dependencies

- 9.4

198.3 Module

You can load the modules by:

```
module load sas
```


SENTAURUS

199.1 Description

Sentaurus Device is an advanced multidimensional device simulator capable of simulating electrical, thermal, and optical characteristics of silicon-based and compound semiconductor devices. Sentaurus Device is a new-generation device simulator for designing and optimizing current and future semiconductor devices.

199.2 Versions and Dependencies

- 2017.09
- 2019.03

199.3 Module

You can load the modules by:

```
module load sentaurus
```


200.1 Description

Apache Spark is a fast and general engine for large-scale data processing.

200.2 Versions and Dependencies

- **2.4.4**

1. `hadoop/2.7.7`

200.3 Module

You can load the modules by:

```
module load spark
```


201.1 Description

Stata is a complete, integrated software package that provides all your data science needs—data manipulation, visualization, statistics, and automated reporting.

201.2 Versions and Dependencies

- 17

201.3 Module

You can load the modules by:

```
module load stata
```


202.1 Description

Tcl Tool Command Language is a very powerful but easy to learn dynamic programming language, suitable for a very wide range of uses, including web and desktop applications, networking, administration, testing and many more. Open source and business-friendly, Tcl is a mature yet evolving language that is truly cross platform, easily deployed and highly extensible.

202.2 Versions and Dependencies

- 8.6.8
 1. zlib/1.2.11-generic

202.3 Module

You can load the modules by:

```
module load tcl
```


TECPLOT

203.1 Description

Tecplot 360 is a suite of visualization and analysis tools that can handle large data sets, automate workflows, and visualize parametric results.

203.2 Versions and Dependencies

- 360-2017-R3

203.3 Module

You can load the modules by:

```
module load tecplot
```


204.1 Description

TeX Live is a free software distribution for the TeX typesetting system. Heads up, its is not a reproducible installation. At any point only the most recent version can be installed. Older versions are included for backward compatibility, i.e., if you have that version already installed.

204.2 Versions and Dependencies

- 20200406

204.3 Module

You can load the modules by:

```
module load texlive
```


THERMOCALC

205.1 Description

Thermo-Calc is a thermodynamic calculation software for tackling mineral equilibria problems. It has two main components: the application itself, and the internally-consistent thermodynamic dataset it uses.

205.2 Versions and Dependencies

- 2019b
- 2020a
- 2021a
- 2021b

205.3 Module

You can load the modules by:

```
module load thermocalc
```


TOTALVIEW

206.1 Description

RogueWave Totalview software

206.2 Versions and Dependencies

- 2017.0.12
- 2018.2.6
- 2019.1.4
- 2021.4.10

206.3 Module

You can load the modules by:

```
module load totalview
```


UDUNITS2

207.1 Description

Automated units conversion

207.2 Versions and Dependencies

- 2.2.24

207.3 Module

You can load the modules by:

```
module load udunits2
```


USE.OWN

208.1 Description

This module file will add `$HOME/privatemodules` to the list of directories that the `module` command will search for modules. Place your own module files there. This module, when loaded, will create this directory if necessary.

208.2 Module

You can load the modules by:

```
module load use.own
```


UTILITIES

209.1 Module

You can load the modules by:

```
module load utilities
```


VALGRIND

210.1 Description

An instrumentation framework for building dynamic analysis. There are Valgrind tools that can automatically detect many memory management and threading bugs, and profile your programs in detail. You can also use Valgrind to build new tools.

210.2 Versions and Dependencies

- **3.13.0**

1. boost/1.66.0

210.3 Module

You can load the modules by:

```
module load valgrind
```


211.1 Description

Vim is a highly configurable text editor built to enable efficient text editing. It is an improved version of the vi editor distributed with most UNIX systems. Vim is often called a programmers editor, and so useful for programming that many consider it an entire IDE. Its not just for programmers, though. Vim is perfect for all kinds of text editing, from composing email to editing configuration files.

211.2 Versions and Dependencies

- 7.4.2367

211.3 Module

You can load the modules by:

```
module load vim
```


212.1 Description

VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting.

212.2 Versions and Dependencies

- 1.9.3

212.3 Module

You can load the modules by:

```
module load vmd
```


213.1 Description

Visual Studio Code is a streamlined code editor with support for development operations like debugging, task running, and version control. It aims to provide just the tools a developer needs for a quick code-build-debug cycle and leaves more complex workflows to fuller featured IDEs.

213.2 Versions and Dependencies

- **1.56**
 1. gcc/8.3.0
- **1.59**
 1. gcc/8.3.0

213.3 Module

You can load the modules by:

```
module load vscode
```


214.1 Description

XALT is a lightweight software tool for any Linux cluster, workstation, or high-end supercomputer to track executable information and linkage of static shared and dynamically linked libraries. When the code is executed, wrappers intercept both GNU linker (ld) to capture linkage information and environmental variables.

214.2 Versions and Dependencies

- 1.1.2

214.3 Module

You can load the modules by:

```
module load xalt
```


215.1 Description

A free, general-purpose, legally unencumbered lossless data-compression library.

215.2 Versions and Dependencies

- 1.2.11-generic
- 1.2.11

215.3 Module

You can load the modules by:

```
module load zlib
```


ARCHIVEMOUNT

216.1 Description

This module enables the archivemount tool that allows mounting archive files (like .tar, .tar.gz or .zip) as an ordinary filesystem. For more information: <https://www.cybernoia.de/software/archivemount.html>

216.2 Versions and Dependencies

- 0.8.12

216.3 Module

You can load the modules by:

```
module load utilities
module load archivemount
```


217.1 Description

Git is a fast, scalable, distributed revision control system with an unusually rich command set that provides both high-level operations and full access to internals.

217.2 Versions and Dependencies

- 2.19.2

217.3 Module

You can load the modules by:

```
module load utilities  
module load git
```


GRACE

218.1 Description

Grace is a WYSIWYG 2D plotting tool for the X Window System and M*tif.

218.2 Versions and Dependencies

- 5.1.25

218.3 Module

You can load the modules by:

```
module load utilities
module load grace
```


MONITOR

219.1 Description

System resource monitoring tool.

219.2 Versions and Dependencies

- 2.2.0

219.3 Module

You can load the modules by:

```
module load utilities  
module load monitor
```


PARAFLY

220.1 Description

Given a file containing a list of unix commands, multithreading is used to process the commands in parallel on a single server. Success/failure is captured, and failed commands are retained and reported.

220.2 Versions and Dependencies

- r2013-01-21

220.3 Module

You can load the modules by:

```
module load utilities
module load parafly
```


SUBVERSION

221.1 Description

Subversion is a version control system that is designed to be a compelling replacement for CVS in the open source community. It extends and enhances CVS' feature set, while maintaining a similar interface for those already familiar with CVS.

221.2 Versions and Dependencies

- 1.9.7

221.3 Module

You can load the modules by:

```
module load utilities  
module load subversion
```


222.1 Description

Vim is a highly configurable text editor built to make creating and changing any kind of text very efficient. It is included as “vi” with most UNIX systems and with Apple OS X.

222.2 Versions and Dependencies

- 8.1.0301_gcc-6.11.0

222.3 Module

You can load the modules by:

```
module load utilities
module load vim
```


223.1 Description

VisIt is an Open Source, interactive, scalable, visualization, animation and analysis tool. From Unix, Windows or Mac workstations, users can interactively visualize and analyze data ranging in scale from small (<101 core) desktop-sized projects to large (>105 core) leadership-class computing facility simulation campaigns.

223.2 Versions and Dependencies

- 2.13.2

223.3 Module

You can load the modules by:

```
module load utilities  
module load visit
```


VLC

224.1 Description

VLC is a free and open source multimedia player for most multimedia formats.

224.2 Versions and Dependencies

- 3.0.9.2

224.3 Module

You can load the modules by:

```
module load utilities  
module load vlc
```