ARC Advanced Research Computing

Intermediate HPC

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Summary of Topics

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2. Array Jobs
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3. Parallel and MPI Workflows
    a. OpenMP vs MPI
    b. Benchmarking and Rightsizing
4. Managing Python Environments
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5. Workflow Optimization Exercises
    a. Understanding Benchmarking Results
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Prerequisites

- Familiarity with command line shells
- Connecting to a system via SSH
- Editing files in terminal
- Experience with scheduling jobs on an HPC system

Array Jobs

- A better way to handle hundreds to thousands of similar jobs
- Submit one job script that walks over a range
- Can be used to vary input parameters or file names for software
- Each sub-job will run independently
- Order of completion is not guaranteed by default

Array Jobs – Examples

- #PBS –J 0-99:3
  - Job will index 34 jobs with ids 0,3,6,9 …, 99
- PBS provides $PBS_ARRAY_INDEX to reference the ID during execution
- Can be used to walk over a directory of input files
- Example script is provided in /scratch/tr-summer-2021/HPC/arrayjobs.sh

Parallel and MPI workflows

- Many scientific software packages support parallel processing
- Allows utilization of multiple core or multiple nodes to speed execution
- Optimizing the number of resources is vital
- Schedulers only consider resources requested not actual utilization

Parallel and MPI workflows – OpenMP vs MPI

- OpenMP uses threaded parallelization or ‘local parallelization’
  - Each thread can run independently on a CPU core
  - Threads share the same memory
  - Tends to be easier to implement on home-grown code than MPI
- MPI distributes work via message passing to MPI threads
  - Biggest advantage is the ability to run on multiple distinct nodes
  - MPI connects over the network and can utilize high speed Infiniband fabrics

Parallel and MPI workflows – Benchmarking and Rightsizing

- Important to fully test your parallel code to make best use of resources
- How software divides the work can lead to various ceilings of parallelism
- Test your software with multiple settings to optimize your future runs
- A better understanding will lead to faster queue times and quicker turnaround

Managing Python Environments

- Python is great for rapid prototyping and has a large variety of packages for scientific computing.
- However, there are many versions of Python and associated packages, which makes keeping track of versions and dependencies difficult.
- Python virtual environments are a way to manage this complexity.

Managing Python Environments

- Anaconda is not well suited for clusters:
  - Installs packages which already exist on the cluster.
  - Installs binaries not optimized for the processor architecture.
  - Makes references to system libraries that are incorrect on clusters.

- Hence it is recommended to use a Python virtual environment instead.

Managing Python Environments - Virtualenv

- Virtualenv is a tool used to create a Python virtual environment.

- Creates a self-contained Python environment with all dependencies that packages can be installed into.

Managing Python Environments - PIP

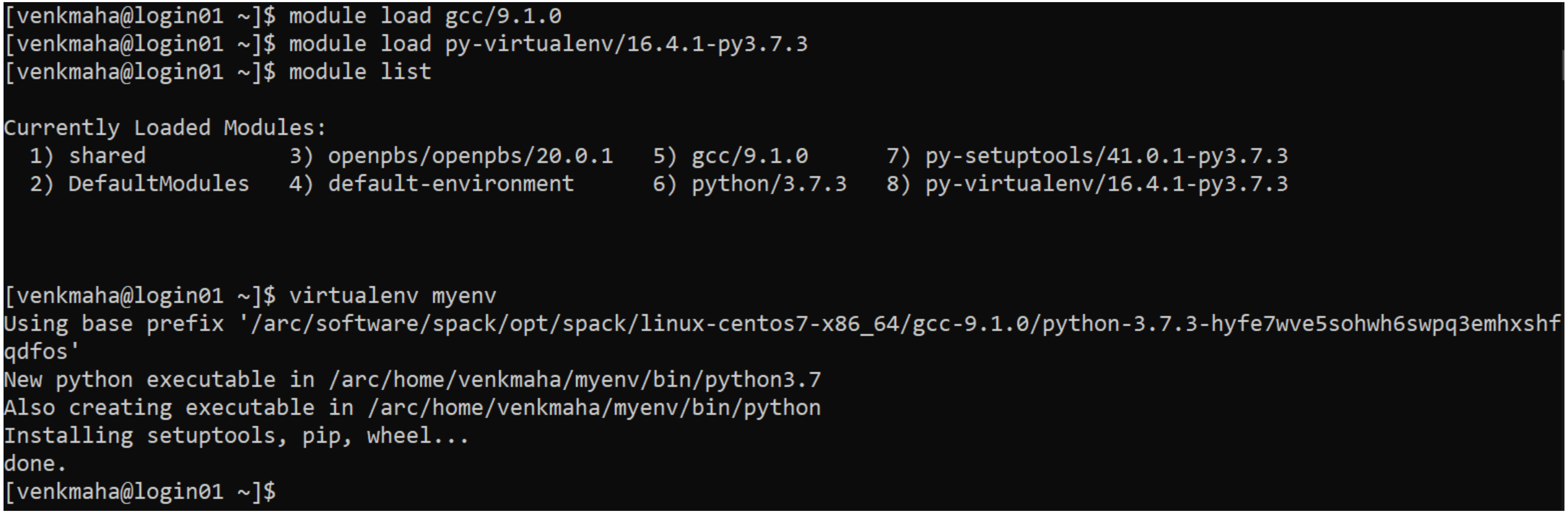
- PIP is the package installer for Python.

- It can be used to install packages from the Python Package Index (PyPI) and other indexes.

- Can be used with virtual environments.

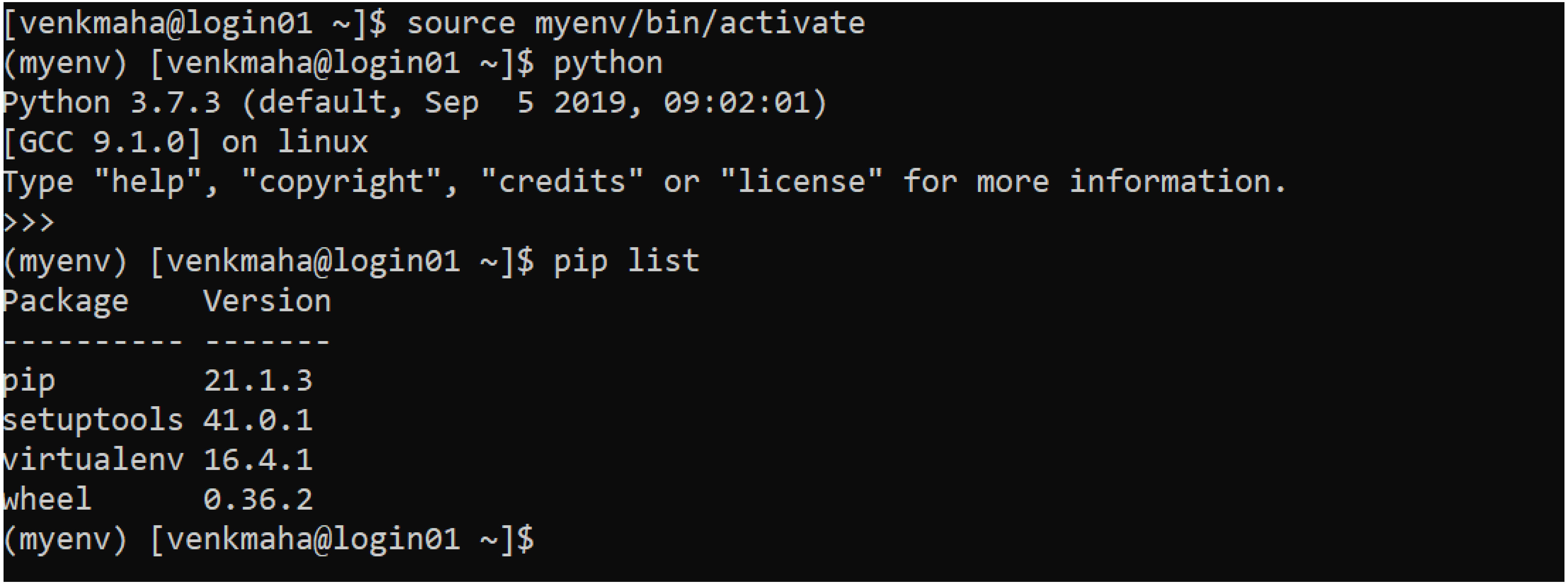
- https://pip.pypa.io/en/stable/cli/

Exercises – create a virtual environment



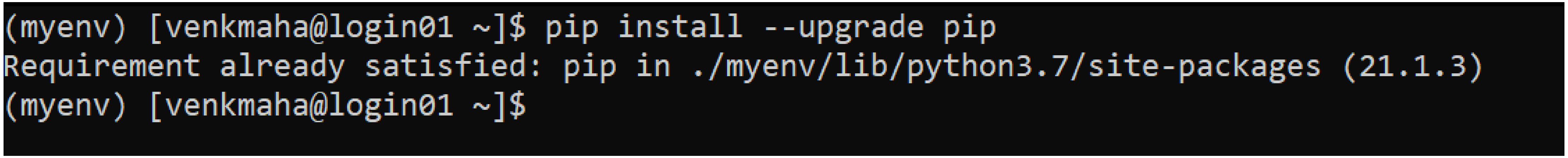
```
[venkmaha@login01 ~]$ module load gcc/9.1.0
[venkmaha@login01 ~]$ module load py-virtualenv/16.4.1-py3.7.3
[venkmaha@login01 ~]$ module list

Currently Loaded Modules:
  1) shared            3) openpbs/openpbs/20.0.1   5) gcc/9.1.0      7) py-setuptools/41.0.1-py3.7.3
  2) DefaultModules    4) default-environment      6) python/3.7.3   8) py-virtualenv/16.4.1-py3.7.3



[venkmaha@login01 ~]$ virtualenv myenv
Using base prefix '/arc/software/spack/opt/spack/linux-centos7-x86_64/gcc-9.1.0/python-3.7.3-hyfe7wve5sohwh6swpq3emhxshf
qdfos'
New python executable in /arc/home/venkmaha/myenv/bin/python3.7
Also creating executable in /arc/home/venkmaha/myenv/bin/python
Installing setuptools, pip, wheel...
done.
[venkmaha@login01 ~]$
```

Exercises – activate the virtual environment



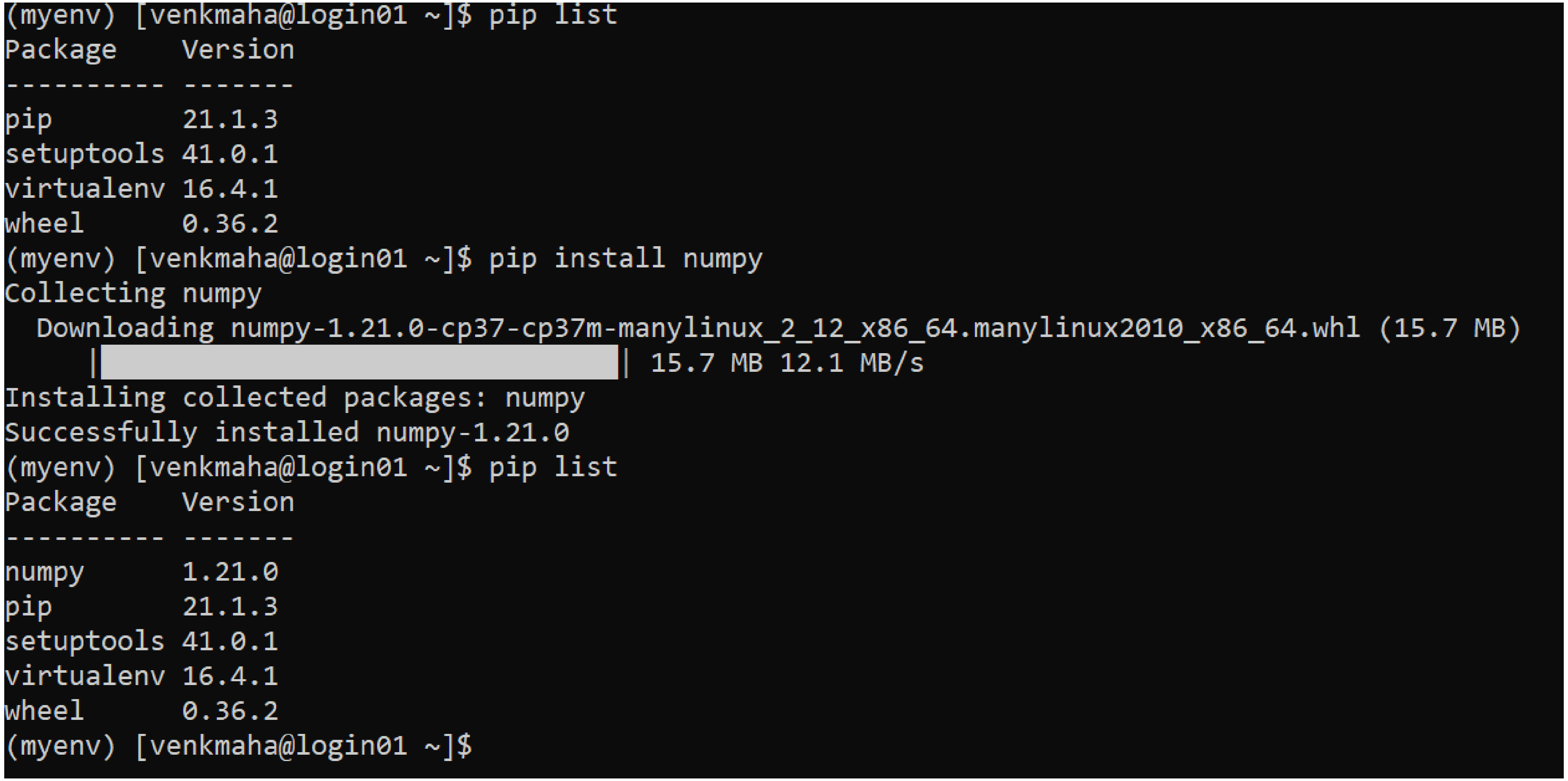
```
[venkmaha@login01 ~]$ source myenv/bin/activate
(myenv) [venkmaha@login01 ~]$ python
Python 3.7.3 (default, Sep  5 2019, 09:02:01)
[GCC 9.1.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>>
(myenv) [venkmaha@login01 ~]$ pip list
Package    Version
---------- -------
pip        21.1.3
setuptools 41.0.1
virtualenv 16.4.1
wheel      0.36.2
(myenv) [venkmaha@login01 ~]$
```

Exercises – upgrade PIP



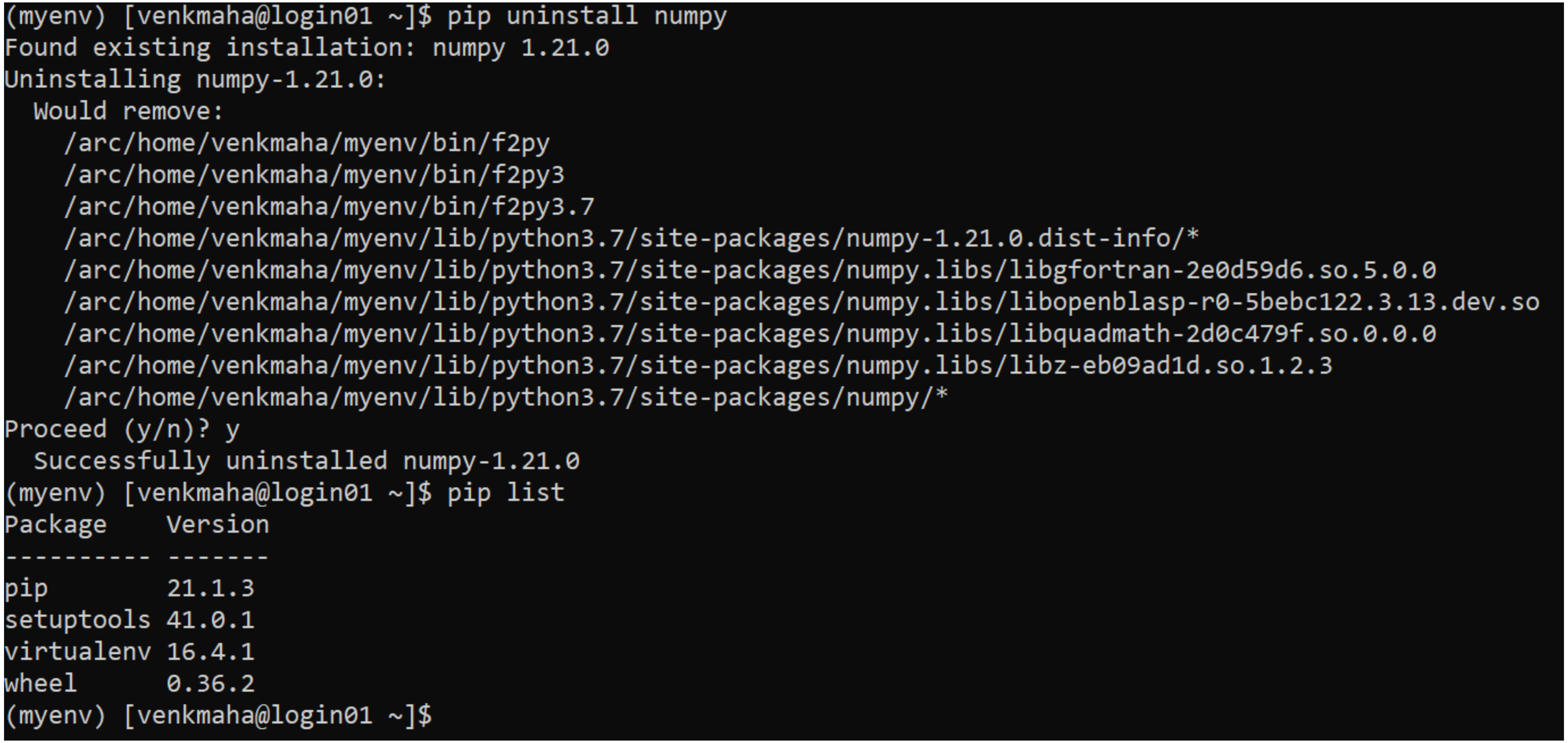
```
(myenv) [venkmaha@login01 ~]$ pip install --upgrade pip
Requirement already satisfied: pip in ./myenv/lib/python3.7/site-packages (21.1.3)
(myenv) [venkmaha@login01 ~]$
```

Exercises – install numpy



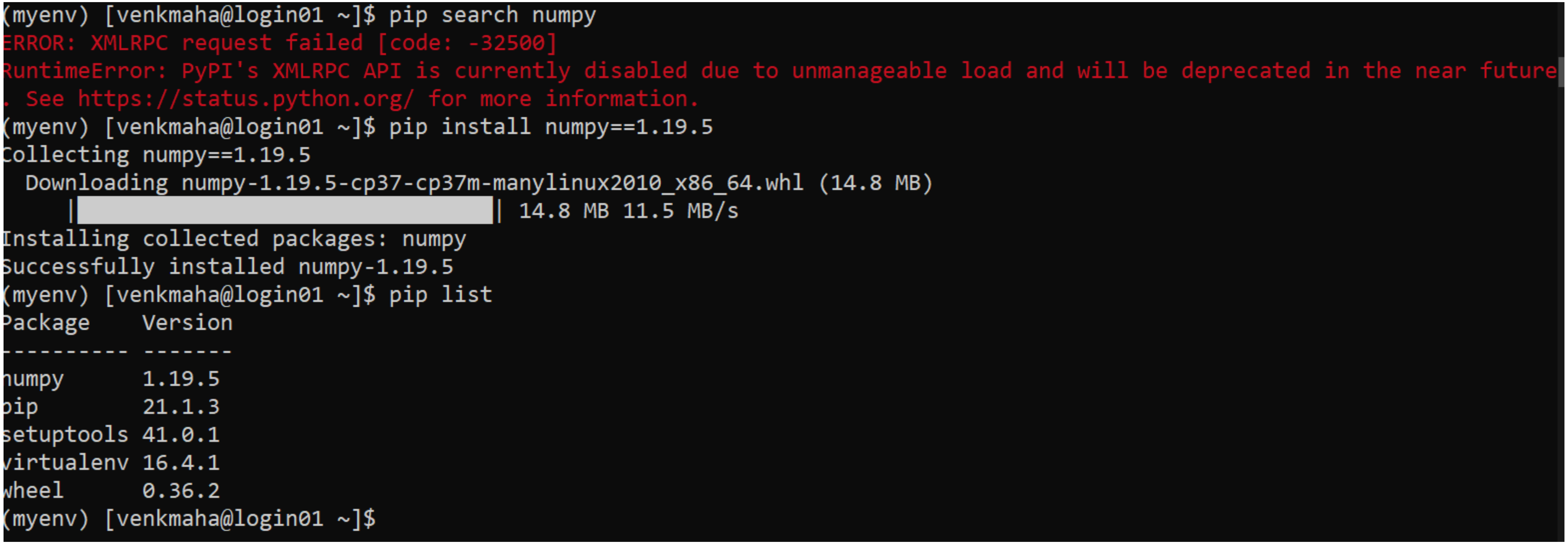
```
(myenv) [venkmaha@login01 ~]$ pip list
Package    Version
---------- -------
pip        21.1.3
setuptools 41.0.1
virtualenv 16.4.1
wheel      0.36.2
(myenv) [venkmaha@login01 ~]$ pip install numpy
Collecting numpy
  Downloading numpy-1.21.0-cp37-cp37m-manylinux_2_12_x86_64.manylinux2010_x86_64.whl (15.7 MB)
     |████████████████████████████████| 15.7 MB 12.1 MB/s
Installing collected packages: numpy
Successfully installed numpy-1.21.0
(myenv) [venkmaha@login01 ~]$ pip list
Package    Version
---------- -------
numpy      1.21.0
pip        21.1.3
setuptools 41.0.1
virtualenv 16.4.1
wheel      0.36.2
(myenv) [venkmaha@login01 ~]$
```

Exercises – uninstall numpy



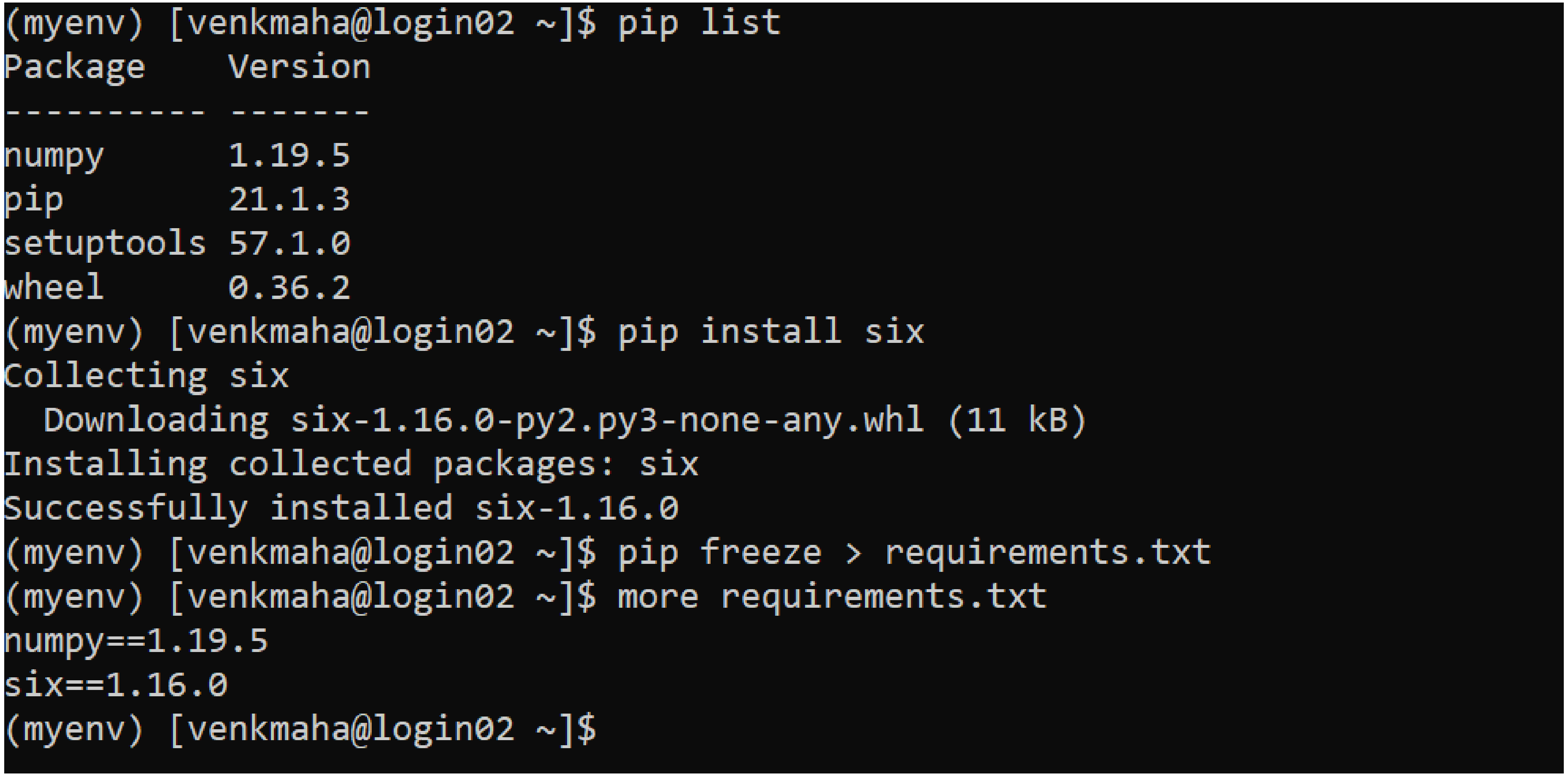
```
(myenv) [venkmaha@login01 ~]$ pip uninstall numpy
Found existing installation: numpy 1.21.0
Uninstalling numpy-1.21.0:
  Would remove:
    /arc/home/venkmaha/myenv/bin/f2py
    /arc/home/venkmaha/myenv/bin/f2py3
    /arc/home/venkmaha/myenv/bin/f2py3.7
    /arc/home/venkmaha/myenv/lib/python3.7/site-packages/numpy-1.21.0.dist-info/*
    /arc/home/venkmaha/myenv/lib/python3.7/site-packages/numpy.libs/libgfortran-2e0d59d6.so.5.0.0
    /arc/home/venkmaha/myenv/lib/python3.7/site-packages/numpy.libs/libopenblasp-r0-5bebc122.3.13.dev.so
    /arc/home/venkmaha/myenv/lib/python3.7/site-packages/numpy.libs/libquadmath-2d0c479f.so.0.0.0
    /arc/home/venkmaha/myenv/lib/python3.7/site-packages/numpy.libs/libz-eb09ad1d.so.1.2.3
    /arc/home/venkmaha/myenv/lib/python3.7/site-packages/numpy/*
Proceed (y/n)? y
  Successfully uninstalled numpy-1.21.0
(myenv) [venkmaha@login01 ~]$ pip list
Package    Version
---------- -------
pip        21.1.3
setuptools 41.0.1
virtualenv 16.4.1
wheel      0.36.2
(myenv) [venkmaha@login01 ~]$
```

Exercises – install a specific version of numpy



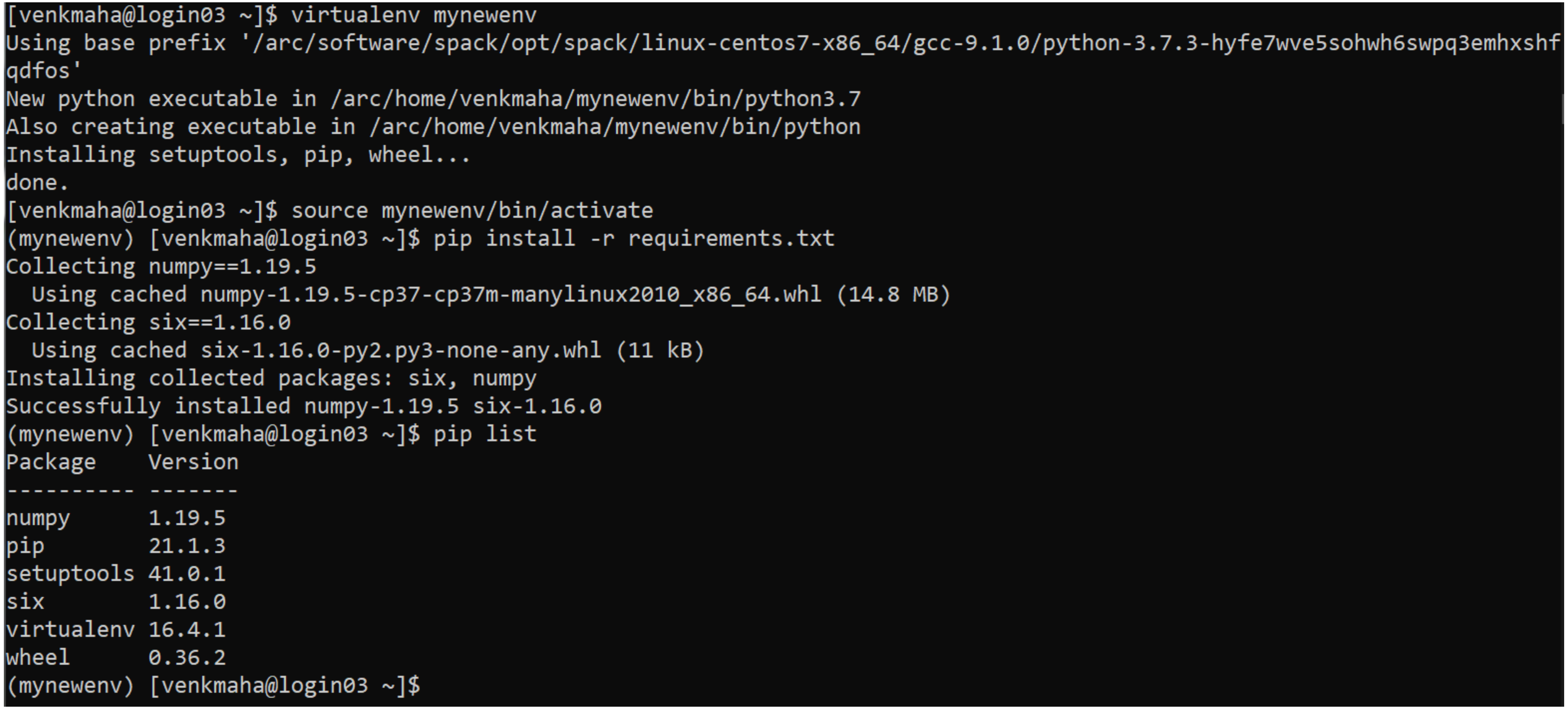
```
(myenv) [venkmaha@login01 ~]$ pip search numpy
ERROR: XMLRPC request failed [code: -32500]
RuntimeError: PyPI's XMLRPC API is currently disabled due to unmanageable load and will be deprecated in the near future
. See https://status.python.org/ for more information.
(myenv) [venkmaha@login01 ~]$ pip install numpy==1.19.5
Collecting numpy==1.19.5
  Downloading numpy-1.19.5-cp37-cp37m-manylinux2010_x86_64.whl (14.8 MB)
     |████████████████████████████████| 14.8 MB 11.5 MB/s
Installing collected packages: numpy
Successfully installed numpy-1.19.5
(myenv) [venkmaha@login01 ~]$ pip list
Package    Version
---------- -------
numpy      1.19.5
pip        21.1.3
setuptools 41.0.1
virtualenv 16.4.1
wheel      0.36.2
(myenv) [venkmaha@login01 ~]$
```

Exercises – freeze a list of requirements



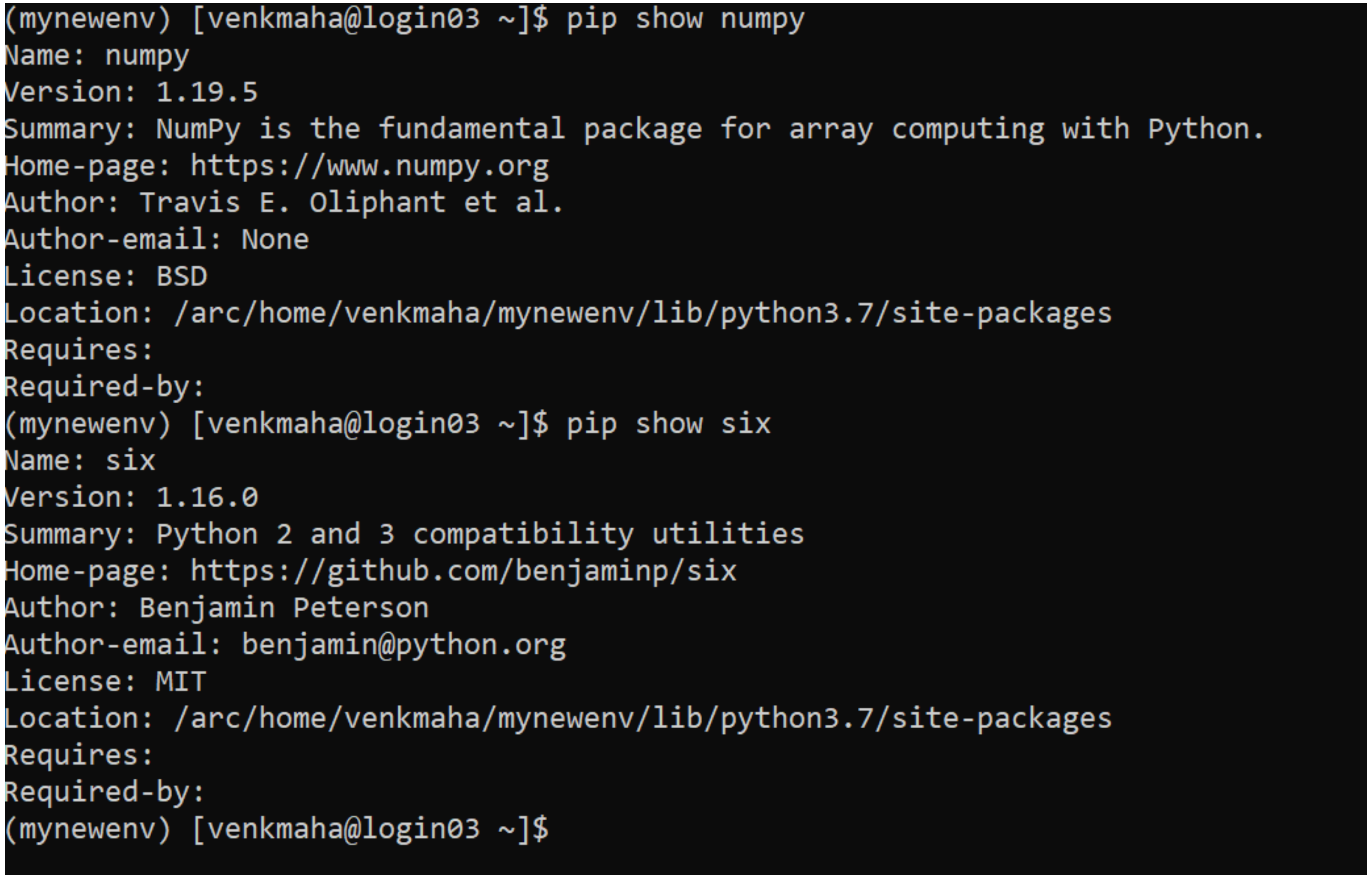
```
(myenv) [venkmaha@login02 ~]$ pip list
Package    Version
---------- -------
numpy      1.19.5
pip        21.1.3
setuptools 57.1.0
wheel      0.36.2
(myenv) [venkmaha@login02 ~]$ pip install six
Collecting six
  Downloading six-1.16.0-py2.py3-none-any.whl (11 kB)
Installing collected packages: six
Successfully installed six-1.16.0
(myenv) [venkmaha@login02 ~]$ pip freeze > requirements.txt
(myenv) [venkmaha@login02 ~]$ more requirements.txt
numpy==1.19.5
six==1.16.0
(myenv) [venkmaha@login02 ~]$
```

Exercises – build and install requirements



```
[venkmaha@login03 ~]$ virtualenv mynewenv
Using base prefix '/arc/software/spack/opt/spack/linux-centos7-x86_64/gcc-9.1.0/python-3.7.3-hyfe7wve5sohwh6swpq3emhxshf
qdfos'
New python executable in /arc/home/venkmaha/mynewenv/bin/python3.7
Also creating executable in /arc/home/venkmaha/mynewenv/bin/python
Installing setuptools, pip, wheel...
done.
[venkmaha@login03 ~]$ source mynewenv/bin/activate
(mynewenv) [venkmaha@login03 ~]$ pip install -r requirements.txt
Collecting numpy==1.19.5
  Using cached numpy-1.19.5-cp37-cp37m-manylinux2010_x86_64.whl (14.8 MB)
Collecting six==1.16.0
  Using cached six-1.16.0-py2.py3-none-any.whl (11 kB)
Installing collected packages: six, numpy
Successfully installed numpy-1.19.5 six-1.16.0
(mynewenv) [venkmaha@login03 ~]$ pip list
Package    Version
---------- -------
numpy      1.19.5
pip        21.1.3
setuptools 41.0.1
six        1.16.0
virtualenv 16.4.1
wheel      0.36.2
(mynewenv) [venkmaha@login03 ~]$
```

Exercises – show package details



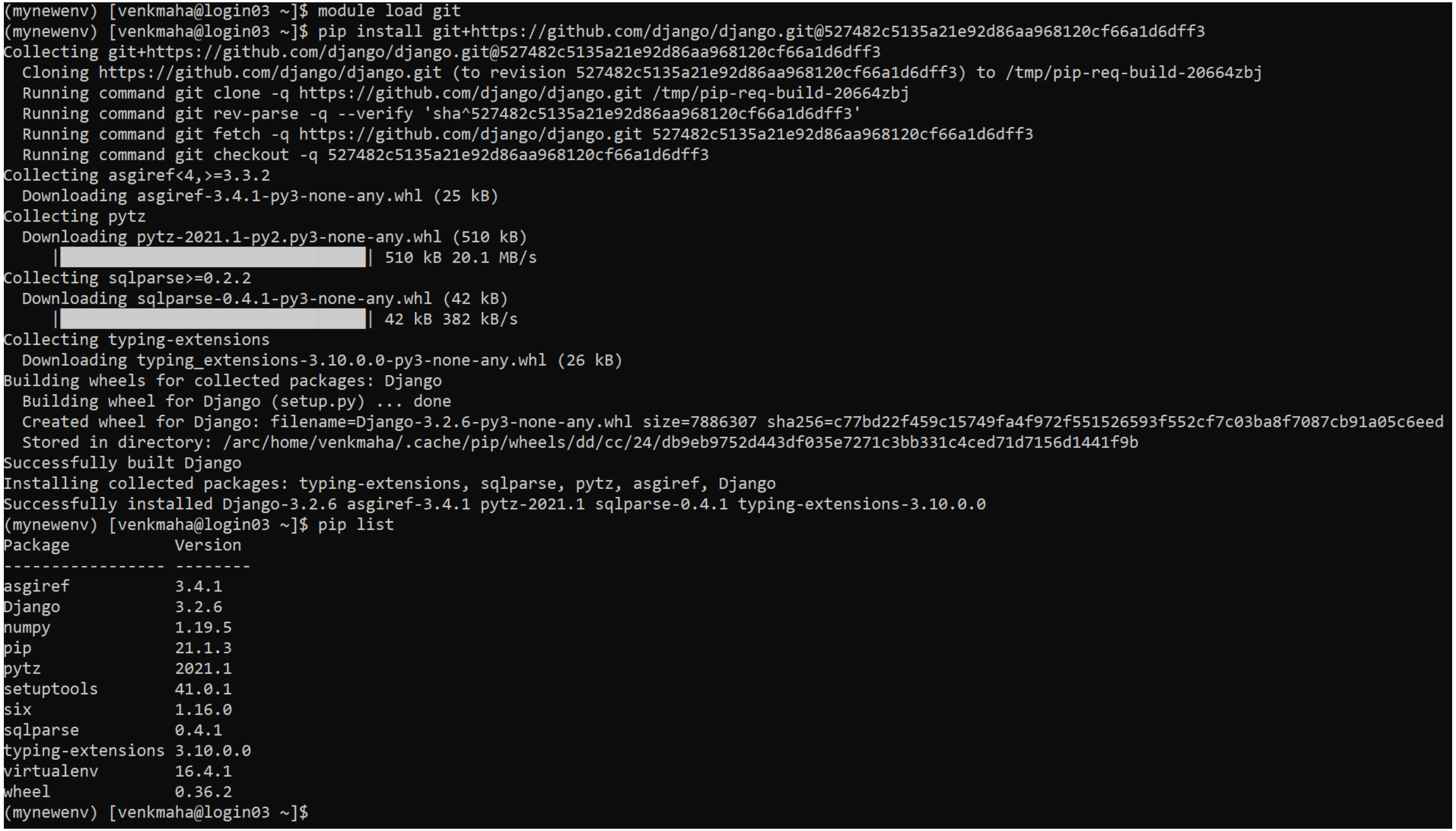
```
(mynewenv) [venkmaha@login03 ~]$ pip show numpy
Name: numpy
Version: 1.19.5
Summary: NumPy is the fundamental package for array computing with Python.
Home-page: https://www.numpy.org
Author: Travis E. Oliphant et al.
Author-email: None
License: BSD
Location: /arc/home/venkmaha/mynewenv/lib/python3.7/site-packages
Requires:
Required-by:
(mynewenv) [venkmaha@login03 ~]$ pip show six
Name: six
Version: 1.16.0
Summary: Python 2 and 3 compatibility utilities
Home-page: https://github.com/benjaminp/six
Author: Benjamin Peterson
Author-email: benjamin@python.org
License: MIT
Location: /arc/home/venkmaha/mynewenv/lib/python3.7/site-packages
Requires:
Required-by:
(mynewenv) [venkmaha@login03 ~]$
```

Exercises – install from Git repo

- module load git

- pip install git+https://github.com/django/django.git@527482c5135a21e92d86aa968120cf66a1d6dff3

Exercises – install from Git repo



```
(mynewenv) [venkmaha@login03 ~]$ module load git
(mynewenv) [venkmaha@login03 ~]$ pip install git+https://github.com/django/django.git@527482c5135a21e92d86aa968120cf66a1d6dff3
Collecting git+https://github.com/django/django.git@527482c5135a21e92d86aa968120cf66a1d6dff3
  Cloning https://github.com/django/django.git (to revision 527482c5135a21e92d86aa968120cf66a1d6dff3) to /tmp/pip-req-build-20664zbj
  Running command git clone -q https://github.com/django/django.git /tmp/pip-req-build-20664zbj
  Running command git rev-parse -q --verify 'sha^527482c5135a21e92d86aa968120cf66a1d6dff3'
  Running command git fetch -q https://github.com/django/django.git 527482c5135a21e92d86aa968120cf66a1d6dff3
  Running command git checkout -q 527482c5135a21e92d86aa968120cf66a1d6dff3
Collecting asgiref<4,>=3.3.2
  Downloading asgiref-3.4.1-py3-none-any.whl (25 kB)
Collecting pytz
  Downloading pytz-2021.1-py2.py3-none-any.whl (510 kB)
     |████████████████████████████████| 510 kB 20.1 MB/s
Collecting sqlparse>=0.2.2
  Downloading sqlparse-0.4.1-py3-none-any.whl (42 kB)
     |████████████████████████████████| 42 kB 382 kB/s
Collecting typing-extensions
  Downloading typing_extensions-3.10.0.0-py3-none-any.whl (26 kB)
Building wheels for collected packages: Django
  Building wheel for Django (setup.py) ... done
  Created wheel for Django: filename=Django-3.2.6-py3-none-any.whl size=7886307 sha256=c77bd22f459c15749fa4f972f551526593f552cf7c03ba8f7087cb91a05c6eed
  Stored in directory: /arc/home/venkmaha/.cache/pip/wheels/dd/cc/24/db9eb9752d443df035e7271c3bb331c4ced71d7156d1441f9b
Successfully built Django
Installing collected packages: typing-extensions, sqlparse, pytz, asgiref, Django
Successfully installed Django-3.2.6 asgiref-3.4.1 pytz-2021.1 sqlparse-0.4.1 typing-extensions-3.10.0.0
(mynewenv) [venkmaha@login03 ~]$ pip list
Package           Version
----------------- --------
asgiref           3.4.1
Django            3.2.6
numpy             1.19.5
pip               21.1.3
pytz              2021.1
setuptools        41.0.1
six               1.16.0
sqlparse          0.4.1
typing-extensions 3.10.0.0
virtualenv        16.4.1
wheel             0.36.2
(mynewenv) [venkmaha@login03 ~]$
```

Workflow Optimization Exercises

- Files for exercises are in /scratch/tr-summer-2021/HPC/workflow
- Job scripts will write out to /scratch/tr-summer-2021/HPC/output/JOB_ID_output.txt
- Find your previous jobs with `qstat –xu USERNAME’ and full job info with `qstat –xf JOB_ID’

Workflow Optimization Exercises – Benchmarking Results

- Utilizing the LAMMPS script benchmarking_exercise.sh determine the optimal number of cores and nodes to run a large number of similar jobs in the future.
- Options are 8 CPUS, 16 CPUs, 32CPUs, and 2 nodes with 32CPUs.
- To save on system load we will present the 16, 32 and multi-node examples and give job ids to inspect the total load.
- Use `qstat –xf JOB_ID’ after completion to look at actual runtime.
- Consider what point adding more processing power provides minimal speedup

Workflow Optimization Exercises – Storage Optimization

- Utilizing the script [[insert script name.sh]] edit it to point the output to $PBS_TMPDIR and copy the file JOB_ID_final.txt to /scratch/tr-summer-2021/HPC/output/ before the job script exits.
- Due to the local nature of the $TMPDIR writes of files are much better performing for frequent file output.
- Once your job is completed move the file from /scratch/tr-summer-2021/HPC/output/ to /arc/project/tr-summer-2021/HPC/StorageOp
- Final results should not be stored on /scratch and should instead be moved to your project space

Workflow Optimization Exercises – ??

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