Enhancing AI/ML Research with HPC Resources:
A Practical Approach

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Outline

- Review of HPC Resources at UK
- Real-World User Challenges
- Software Discovery Service (SDS)
- Singularity Container Composer
- Deploying Custom Containers with Jupyter Notebooks and Open OnDemand
- Questions

Lipscomb & Morgan Compute Clusters

LCC

- 168 compute Intel-based nodes (Skylake/Cascade)

7,168 cores

- 34 NVIDIA GPU nodes

(P100, V100, A100)

128 GPUs VRAM from 12 to80GB

192 GB RAM/node

Last Month – 17.5k Jobs

100 active users

Average wait per job of 2 hrs (GPU)

MCC

- 180 compute AMD-based nodes (Rome)

23,040 cores

512 GB RAM/node

- 2 “Jumbo” nodes

4096 GB RAM/node

Last Month – 181k Jobs

176 active users

Average wait per job of <10 mins

What You Get as a Researcher

Baseline Resource Allocation (Open Access):

- Shared pool of compute time & storage (unallocated resources)
- Access to high-performance CPUs, GPUs, and high-speed parallel storage
- Opportunities to expand allocation with condo model

Storage Quotas:

- $HOME: 10 GB (per user) – persistent storage
- $SCRATCH: 25 TB (per user) – temporary workspace, 90-day deletion policy
- $PROJECT: 1 TB (per project) – persistent
- $PSCRATCH: 50TB (per project) – temprorary workspace, 90-day deletion policy

Software:

- >500 software available within modules
- ~450 applications within containers

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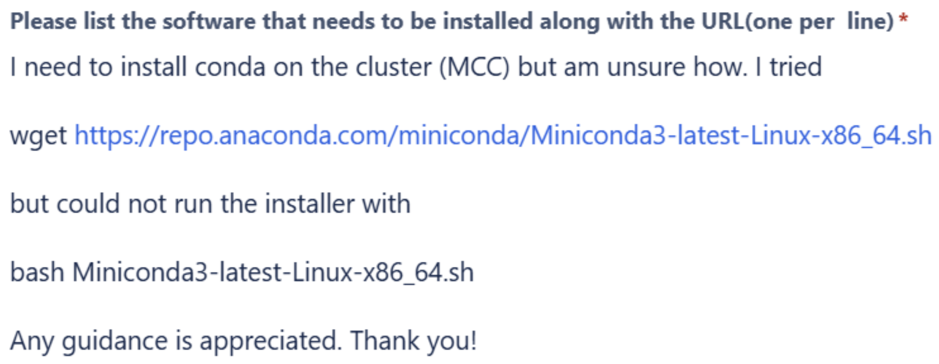
Where is *that* software/package/library etc?

- Software on HPC is not like your local machine
    - Users cannot install system-wide packages (e.g. apt-get … or “make install”)
    - Many different software environments must be available to support a broad range of research
- Two primary ways to access software
    - Modules (LMOD)
        - e.g. module load ccs/Miniforge3 to “load” conda package manager
    - Singularity Containers
        - singularity run --app software /path/to/container.sinf software

Real-World User Challenges



Please list the software that needs to be installed along with the URL(one per line) *

I need to install conda on the cluster (MCC) but am unsure how. I tried

```
wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh
```

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```
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```
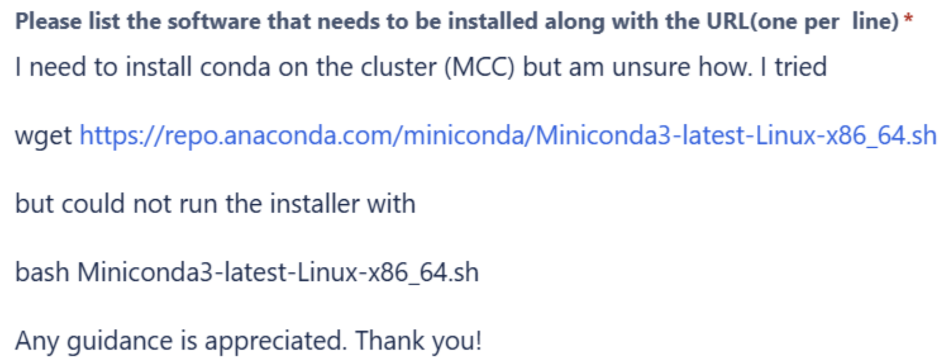

Any guidance is appreciated. Thank you!

Real-World User Challenges



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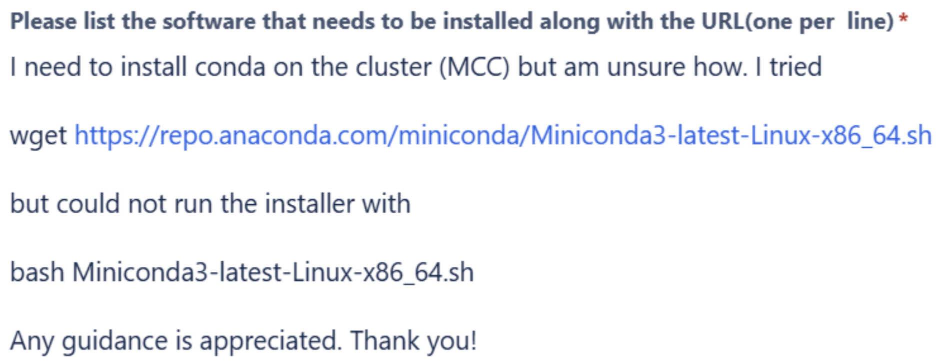
Could you please install “curl” package on node “rome050”

```
sudo apt update
sudo apt install curl
```

Real-World User Challenges



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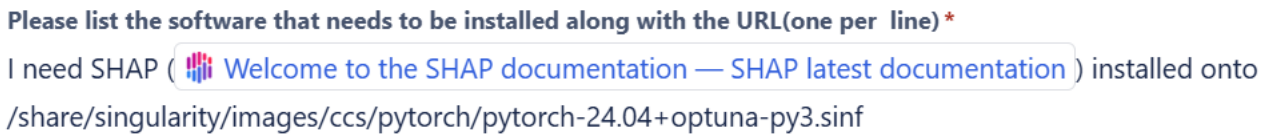


Please list the software that needs to be installed along with the URL(one per line) *

I need SHAP (Welcome to the SHAP documentation — SHAP latest documentation) installed onto /share/singularity/images/ccs/pytorch/pytorch-24.04+optuna-py3.sinf

Software Discovery Service

- Searchable catalog of available software **and containers** on LCC and MCC

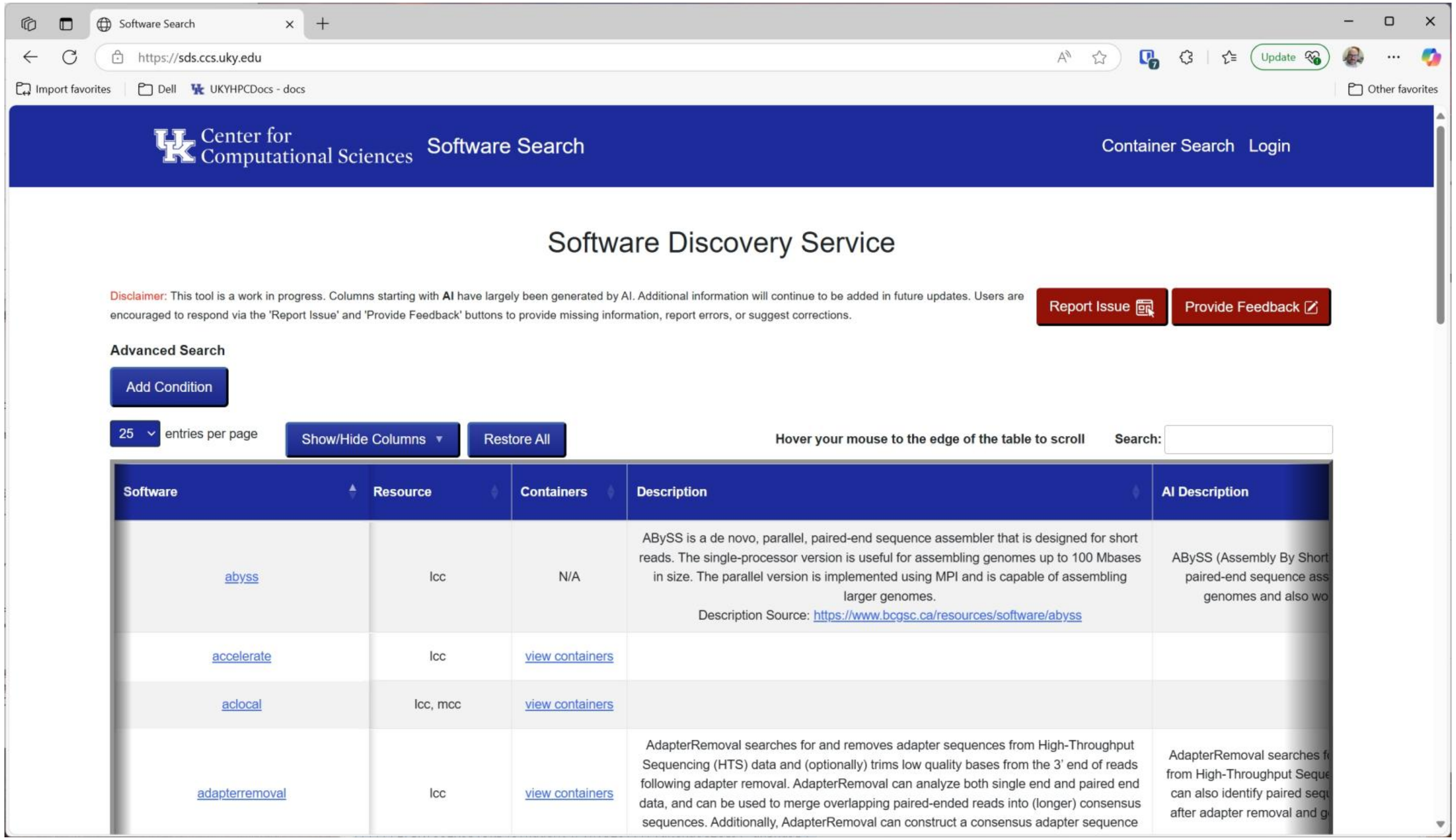
- Software Information – both curated and AI-generated

- Customizable filters for “Software Class”, “Research Discipline”, etc.

https://sds.ccs.uky.edu

Software Discovery Service

Software Search



Software Discovery Service

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Advanced Search

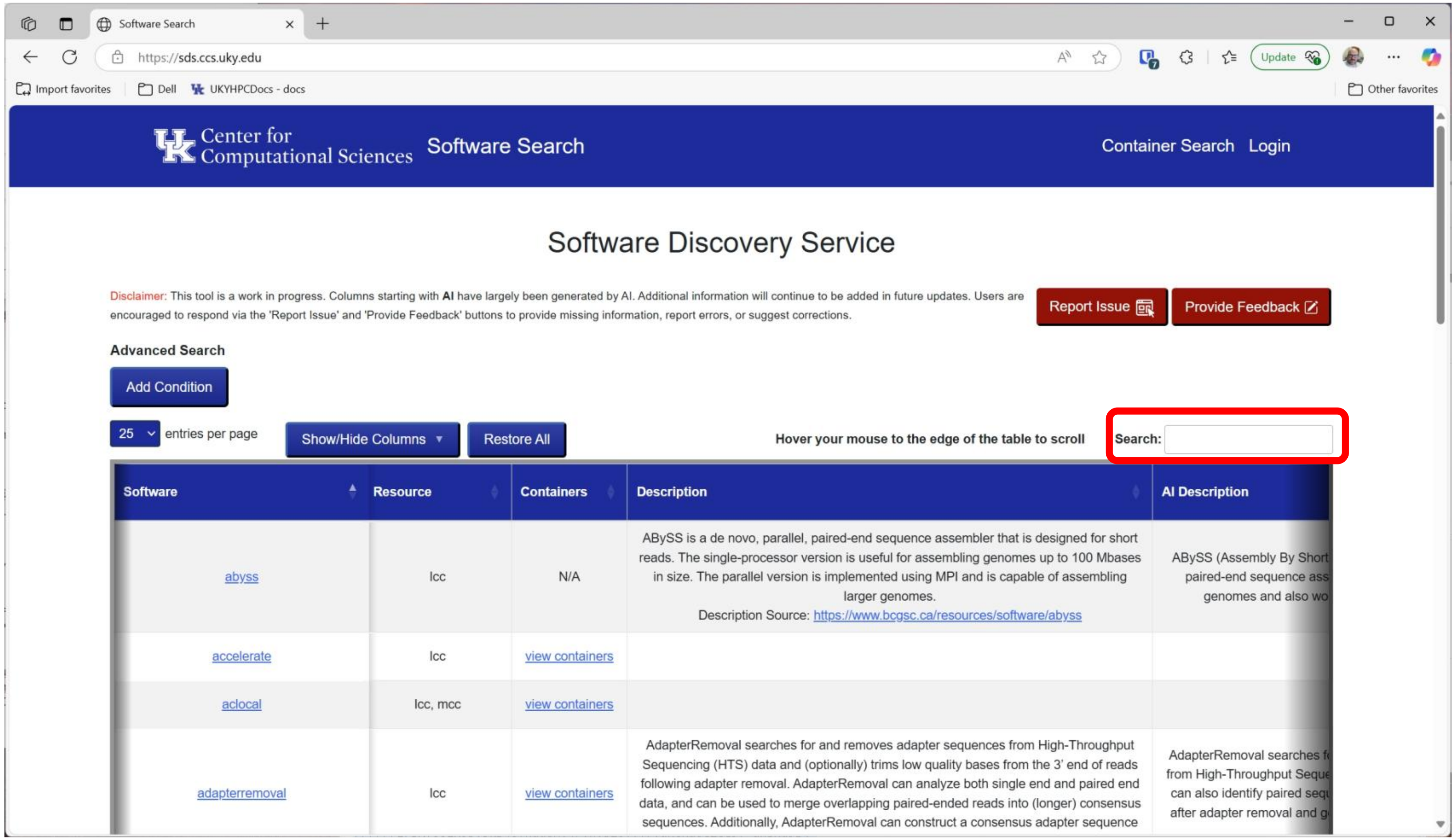
25 entries per page

Hover your mouse to the edge of the table to scroll

Software	Resource	Containers	Description	AI Description
abyss	lcc	N/A	ABySS is a de novo, parallel, paired-end sequence assembler that is designed for short reads. The single-processor version is useful for assembling genomes up to 100 Mbases in size. The parallel version is implemented using MPI and is capable of assembling larger genomes. Description Source: https://www.bcgsc.ca/resources/software/abyss	ABySS (Assembly By Short paired-end sequence ass genomes and also wo
accelerate	lcc	view containers		
aclocal	lcc, mcc	view containers		
adapterremoval	lcc	view containers	AdapterRemoval searches for and removes adapter sequences from High-Throughput Sequencing (HTS) data and (optionally) trims low quality bases from the 3' end of reads following adapter removal. AdapterRemoval can analyze both single end and paired end data, and can be used to merge overlapping paired-ended reads into (longer) consensus sequences. Additionally, AdapterRemoval can construct a consensus adapter sequence	AdapterRemoval searches f from High-Throughput Seque can also identify paired seq after adapter removal and g

Software Discovery Service

Software Search



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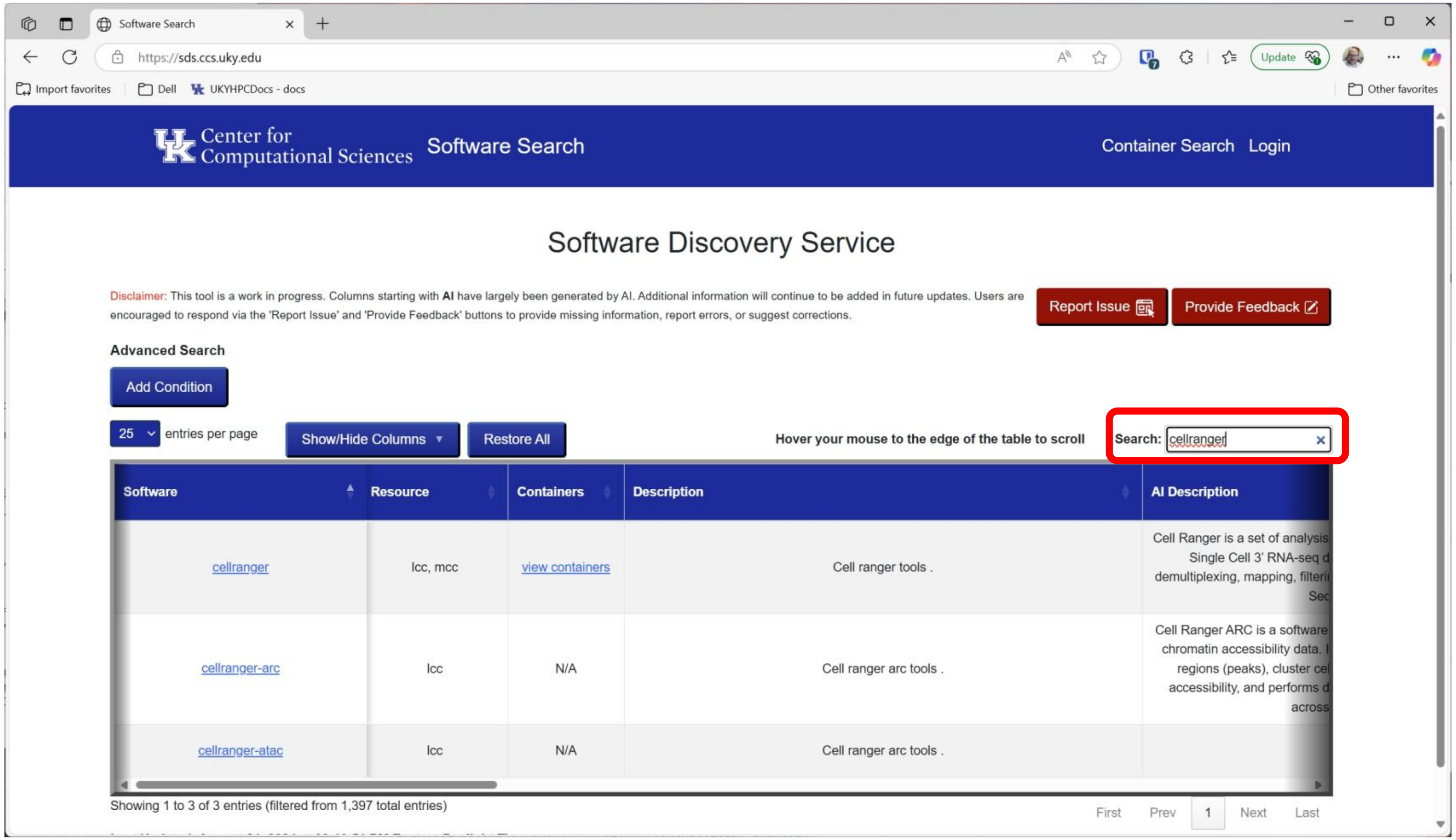

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Search: cellranger

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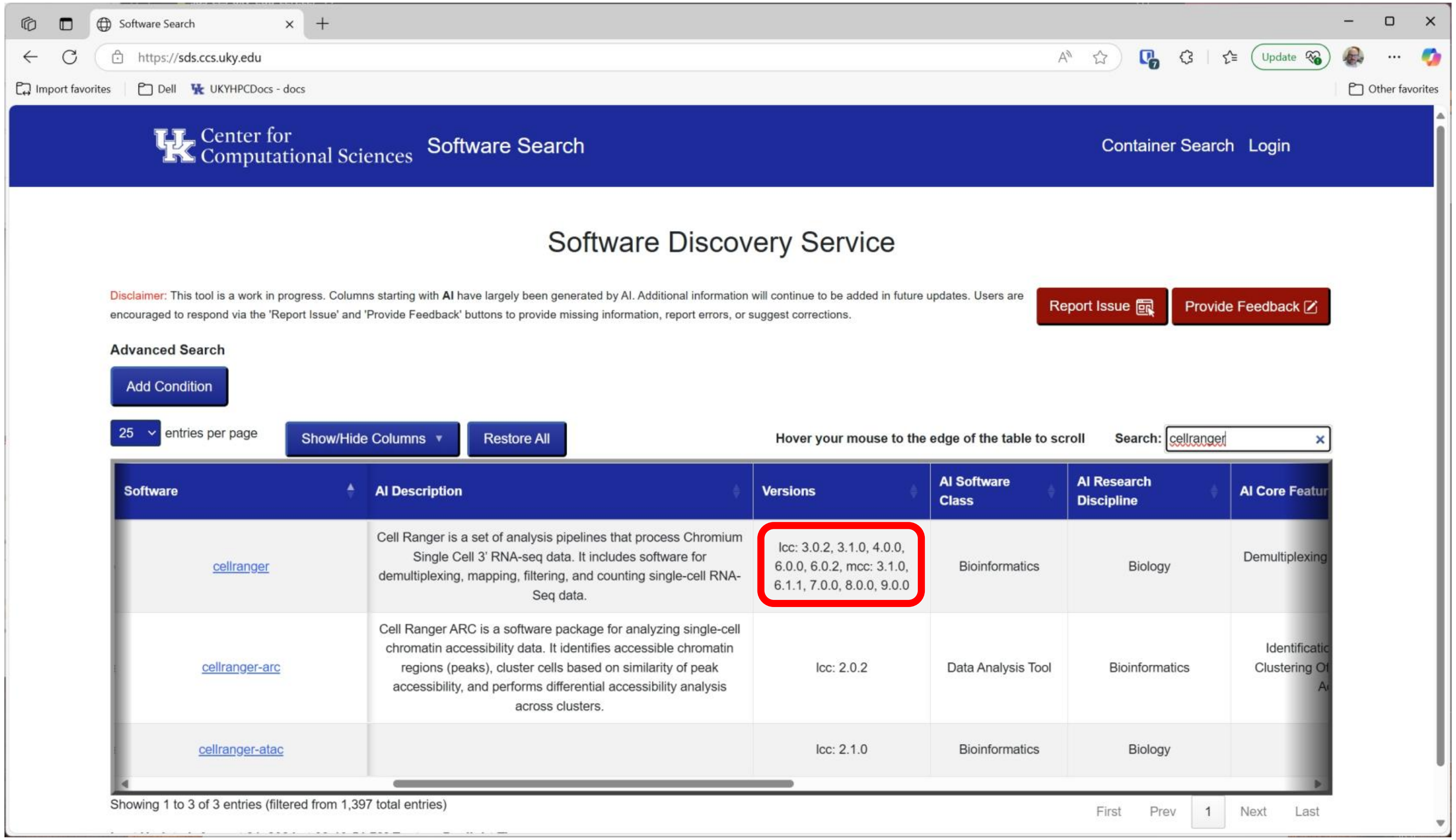
cellranger-arc	lcc	N/A	Cell ranger arc tools .	Cell Ranger ARC is a software chromatin accessibility data. regions (peaks), cluster cel accessibility, and performs d across
cellranger-atac	lcc	N/A	Cell ranger arc tools .	

Showing 1 to 3 of 3 entries (filtered from 1,397 total entries)

Software Discovery Service

Software Search



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Advanced Search

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Search: cellranger

Software	AI Description	Versions	AI Software Class	AI Research Discipline	AI Core Featur
cellranger	Cell Ranger is a set of analysis pipelines that process Chromium Single Cell 3' RNA-seq data. It includes software for demultiplexing, mapping, filtering, and counting single-cell RNA-Seq data.	lcc: 3.0.2, 3.1.0, 4.0.0, 6.0.0, 6.0.2, mcc: 3.1.0, 6.1.1, 7.0.0, 8.0.0, 9.0.0	Bioinformatics	Biology	Demultiplexing
cellranger-arc	Cell Ranger ARC is a software package for analyzing single-cell chromatin accessibility data. It identifies accessible chromatin regions (peaks), cluster cells based on similarity of peak accessibility, and performs differential accessibility analysis across clusters.	lcc: 2.0.2	Data Analysis Tool	Bioinformatics	Identificatic Clustering Of A
cellranger-atac		lcc: 2.1.0	Bioinformatics	Biology	

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Software Discovery Service

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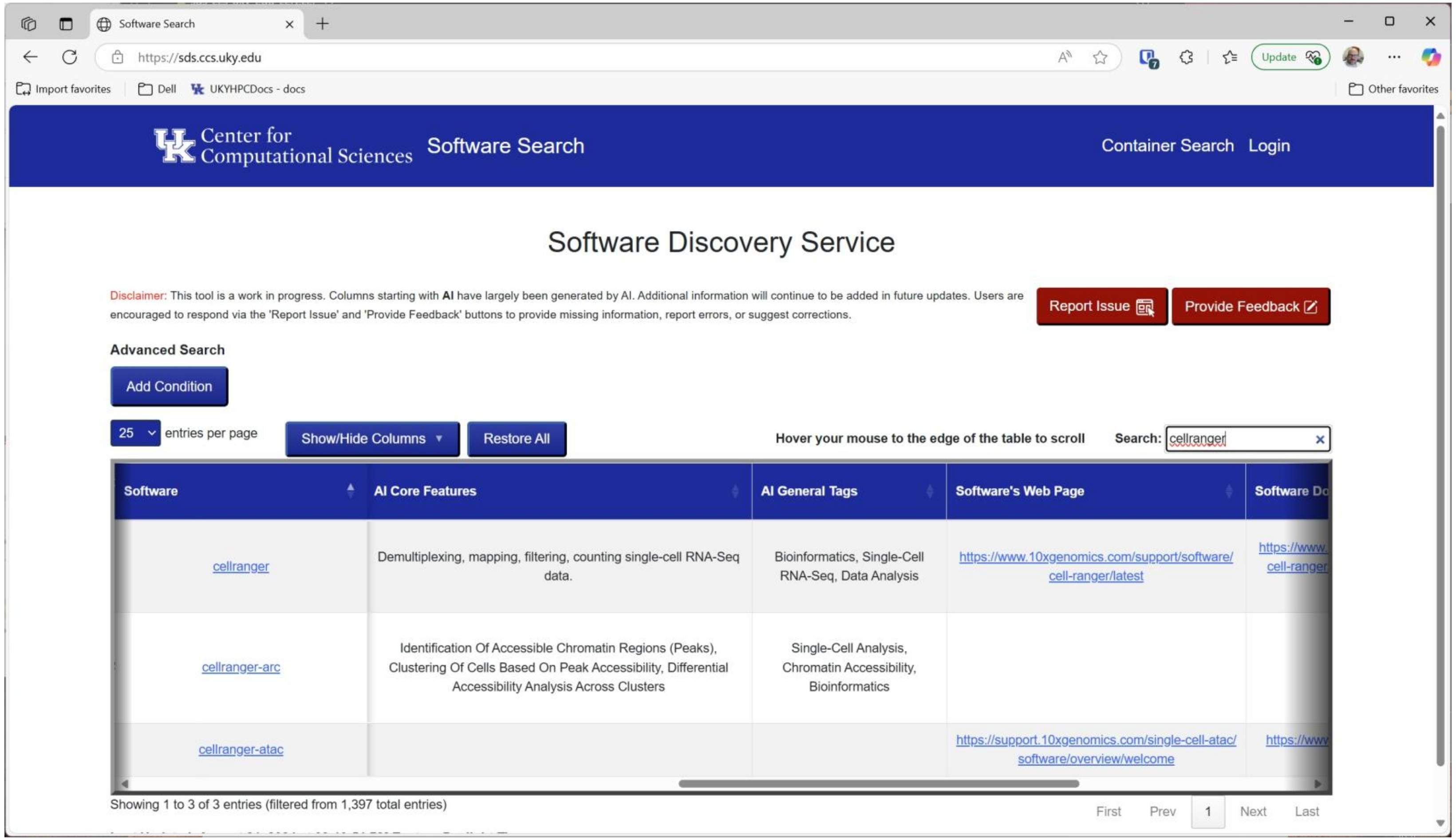

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Advanced Search

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Search: cellranger

Software	AI Core Features	AI General Tags	Software's Web Page	Software Do
cellranger	Demultiplexing, mapping, filtering, counting single-cell RNA-Seq data.	Bioinformatics, Single-Cell RNA-Seq, Data Analysis	https://www.10xgenomics.com/support/software/cell-ranger/latest	https://www. cell-ranger
cellranger-arc	Identification Of Accessible Chromatin Regions (Peaks), Clustering Of Cells Based On Peak Accessibility, Differential Accessibility Analysis Across Clusters	Single-Cell Analysis, Chromatin Accessibility, Bioinformatics		
cellranger-atac			https://support.10xgenomics.com/single-cell-atac/software/overview/welcome	https://www

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Software Discovery Service

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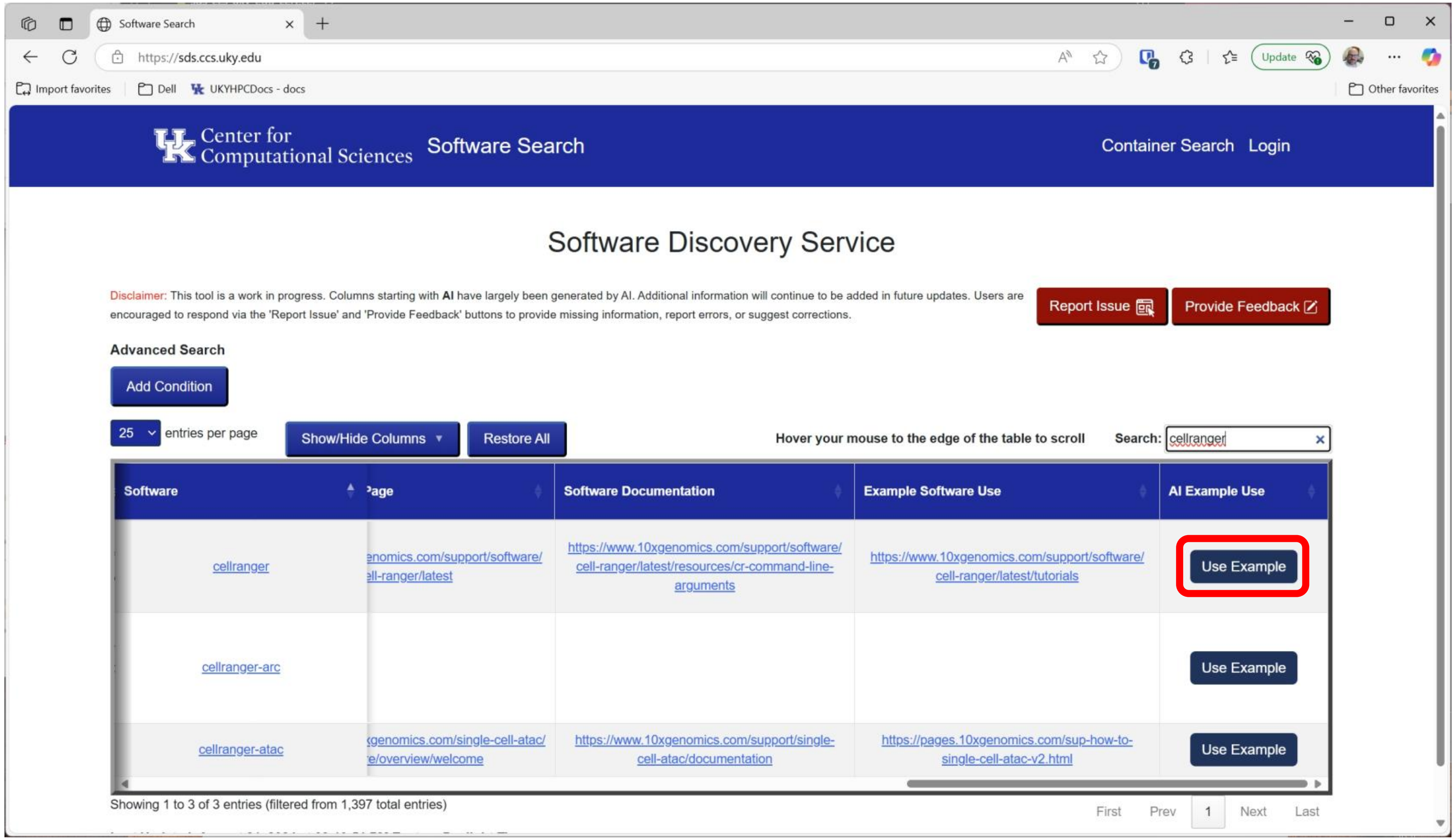

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Software	Page	Software Documentation	Example Software Use	AI Example Use
cellranger	enomics.com/support/software/ ell-ranger/latest	https://www.10xgenomics.com/support/software/cell-ranger/latest/resources/cr-command-line-arguments	https://www.10xgenomics.com/support/software/cell-ranger/latest/tutorials	Use Example
cellranger-arc				Use Example
cellranger-atac	genomics.com/single-cell-atac/ e/overview/welcome	https://www.10xgenomics.com/support/single-cell-atac/documentation	https://pages.10xgenomics.com/sup-how-to-single-cell-atac-v2.html	Use Example

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Software Discovery Service

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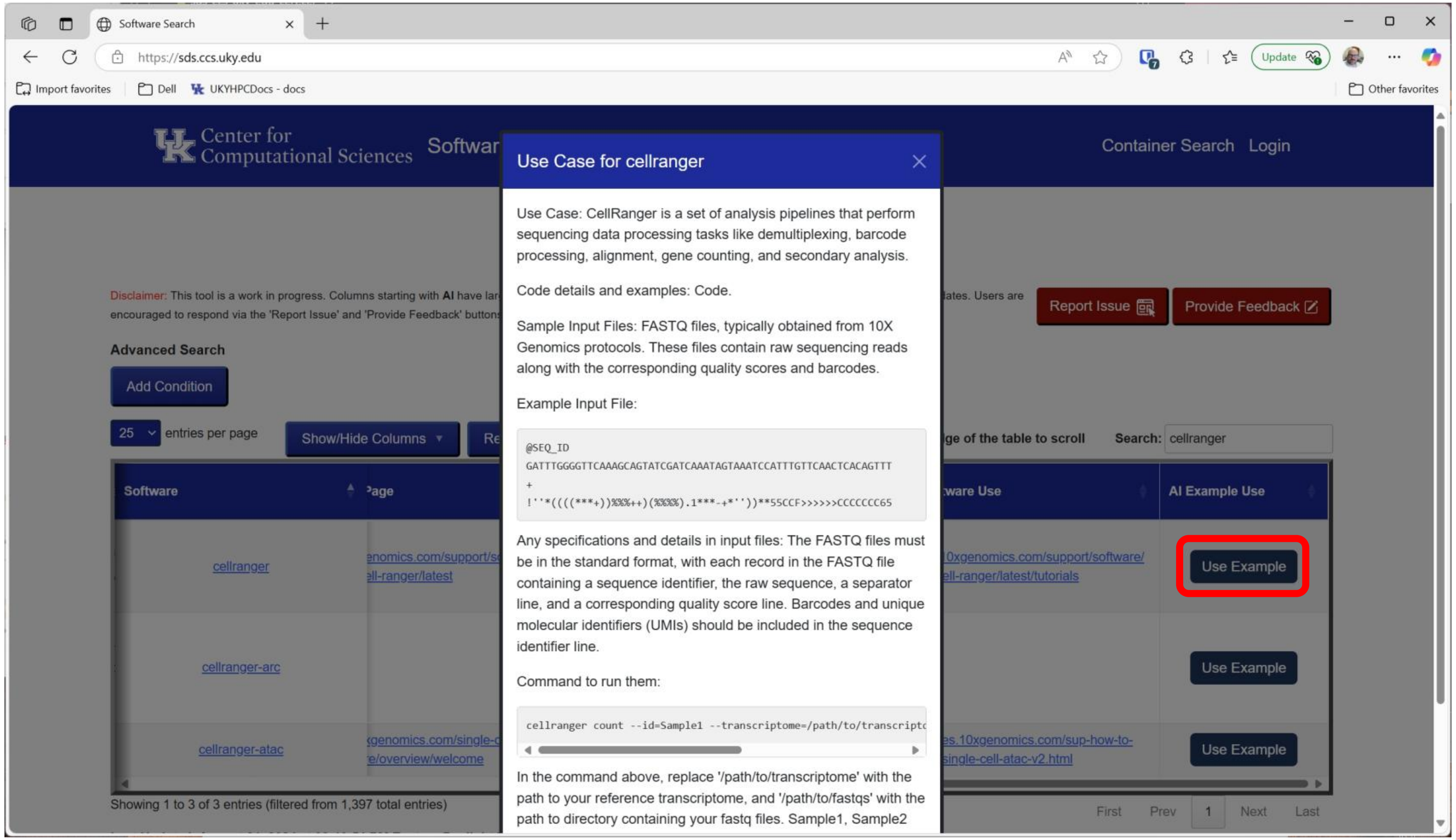

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dates. Users are

Use Case for cellranger

Use Case: CellRanger is a set of analysis pipelines that perform sequencing data processing tasks like demultiplexing, barcode processing, alignment, gene counting, and secondary analysis.

Code details and examples: Code.

Sample Input Files: FASTQ files, typically obtained from 10X Genomics protocols. These files contain raw sequencing reads along with the corresponding quality scores and barcodes.

Example Input File:

```
@SEQ_ID
GATTTGGGGTTCAAAGCAGTATCGATCAAATAGTAAATCCATTTGTTCAACTCACAGTTT
+
!''*((((***+))%%%++)(%%%%).1***-+*''))**55CCF>>>>>>CCCCCCC65
```

Any specifications and details in input files: The FASTQ files must be in the standard format, with each record in the FASTQ file containing a sequence identifier, the raw sequence, a separator line, and a corresponding quality score line. Barcodes and unique molecular identifiers (UMIs) should be included in the sequence identifier line.

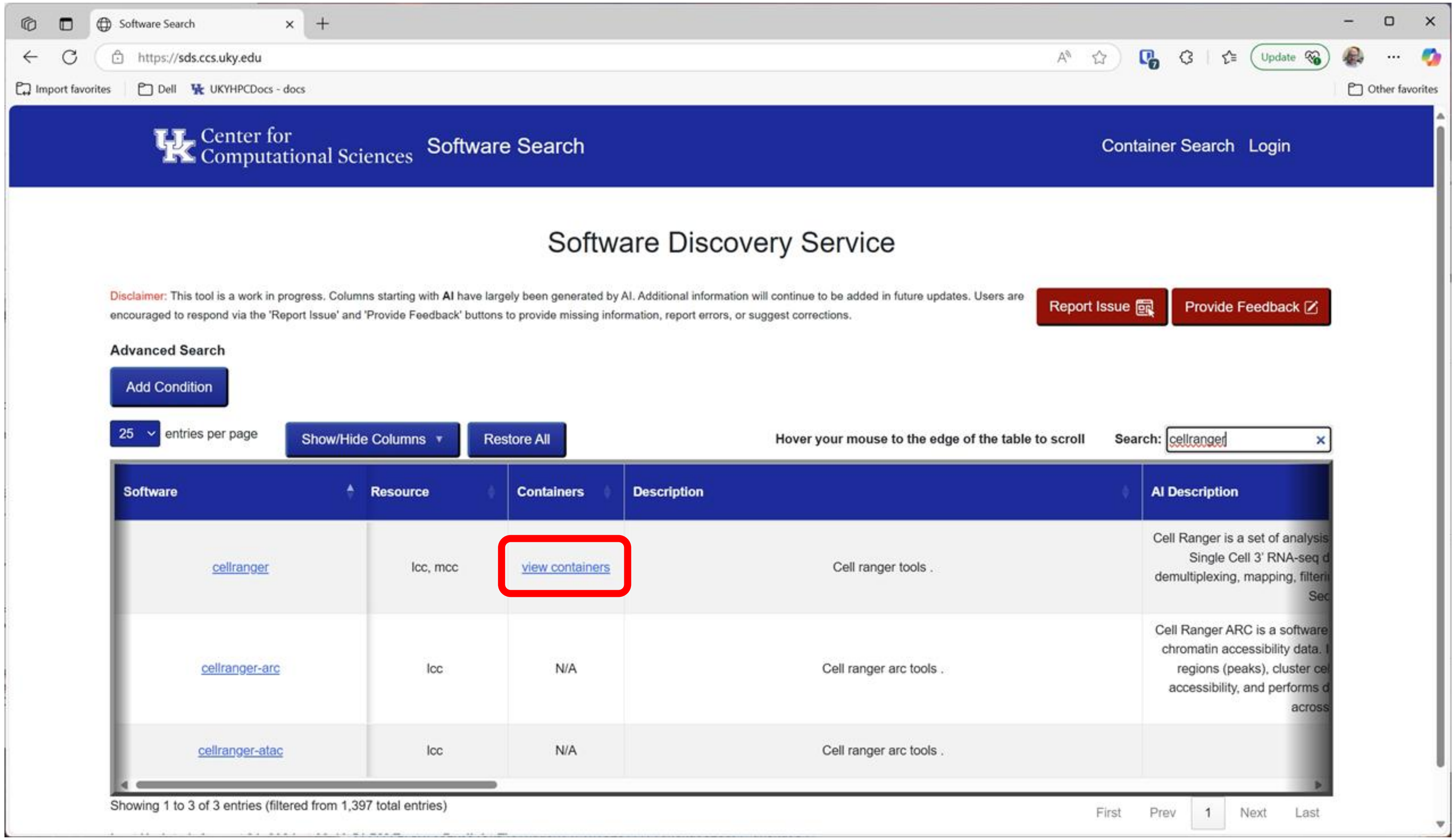
Command to run them:

```
cellranger count --id=Sample1 --transcriptome=/path/to/transcripto
```

In the command above, replace '/path/to/transcriptome' with the path to your reference transcriptome, and '/path/to/fastqs' with the path to directory containing your fastq files. Sample1, Sample2

Software Discovery Service

Software Search



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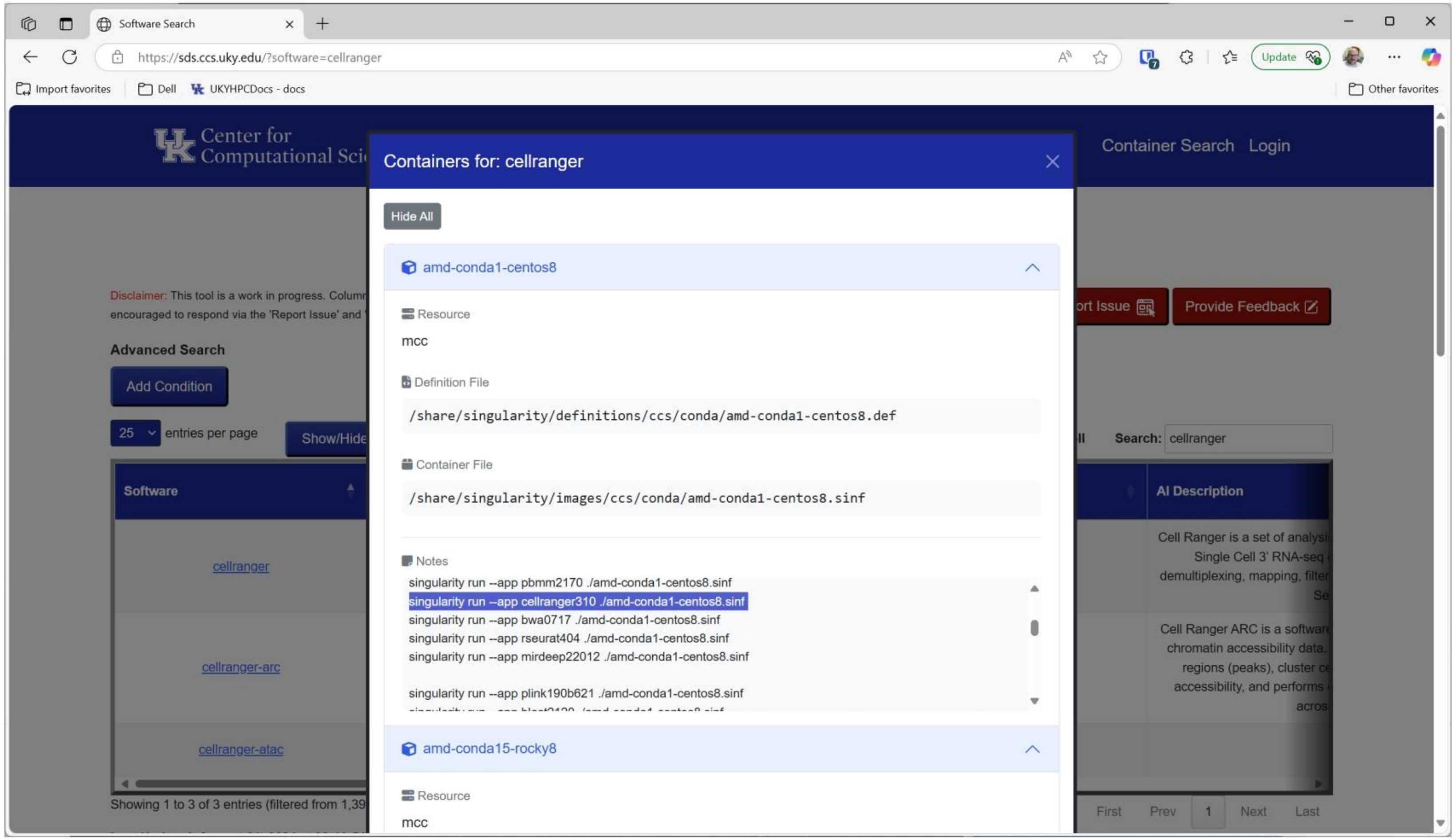
Software Discovery Service

Software Search



Containers for: cellranger

amd-conda1-centos8

Resource

mcc

Definition File

`/share/singularity/definitions/ccs/conda/amd-conda1-centos8.def`

Container File

`/share/singularity/images/ccs/conda/amd-conda1-centos8.sinf`

Notes

```
singularity run --app pbmm2170 ./amd-conda1-centos8.sinf
singularity run --app cellranger310 ./amd-conda1-centos8.sinf
singularity run --app bwa0717 ./amd-conda1-centos8.sinf
singularity run --app rseurat404 ./amd-conda1-centos8.sinf
singularity run --app mirdeep22012 ./amd-conda1-centos8.sinf

singularity run --app plink190b621 ./amd-conda1-centos8.sinf
```

amd-conda15-rocky8

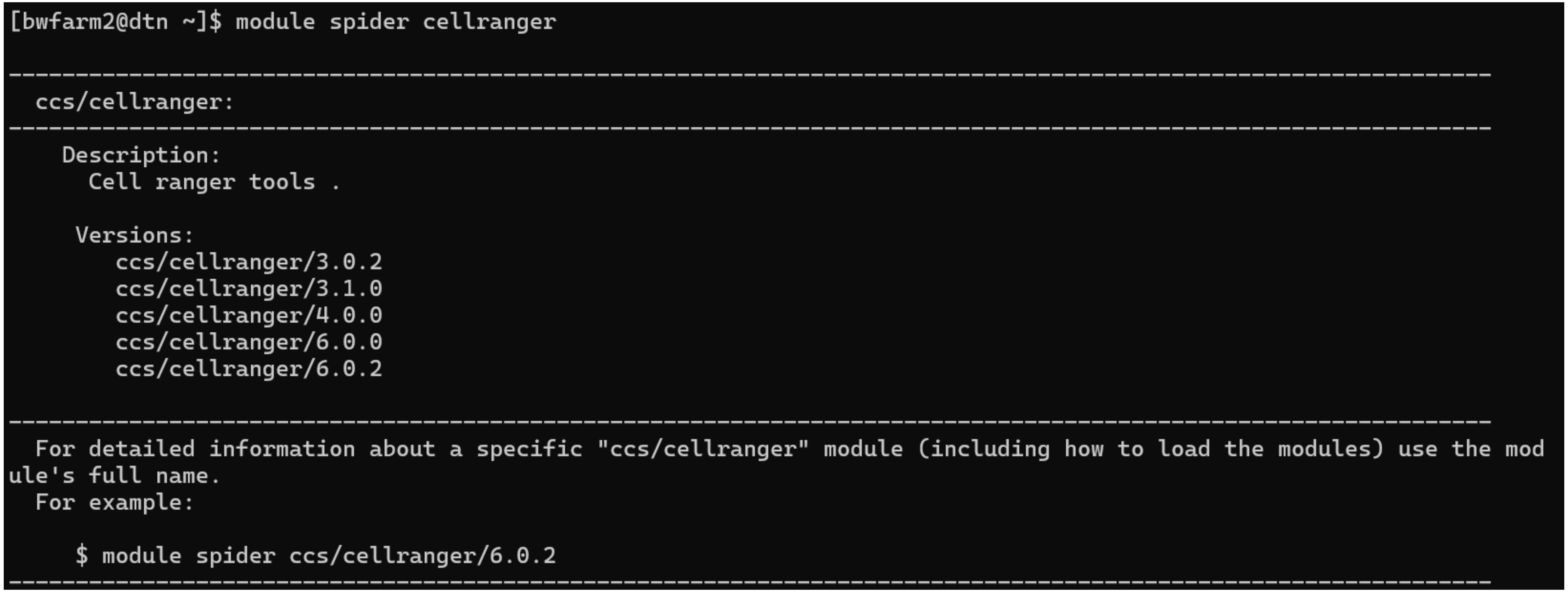
Resource

mcc

Software Discovery Service

Software Search

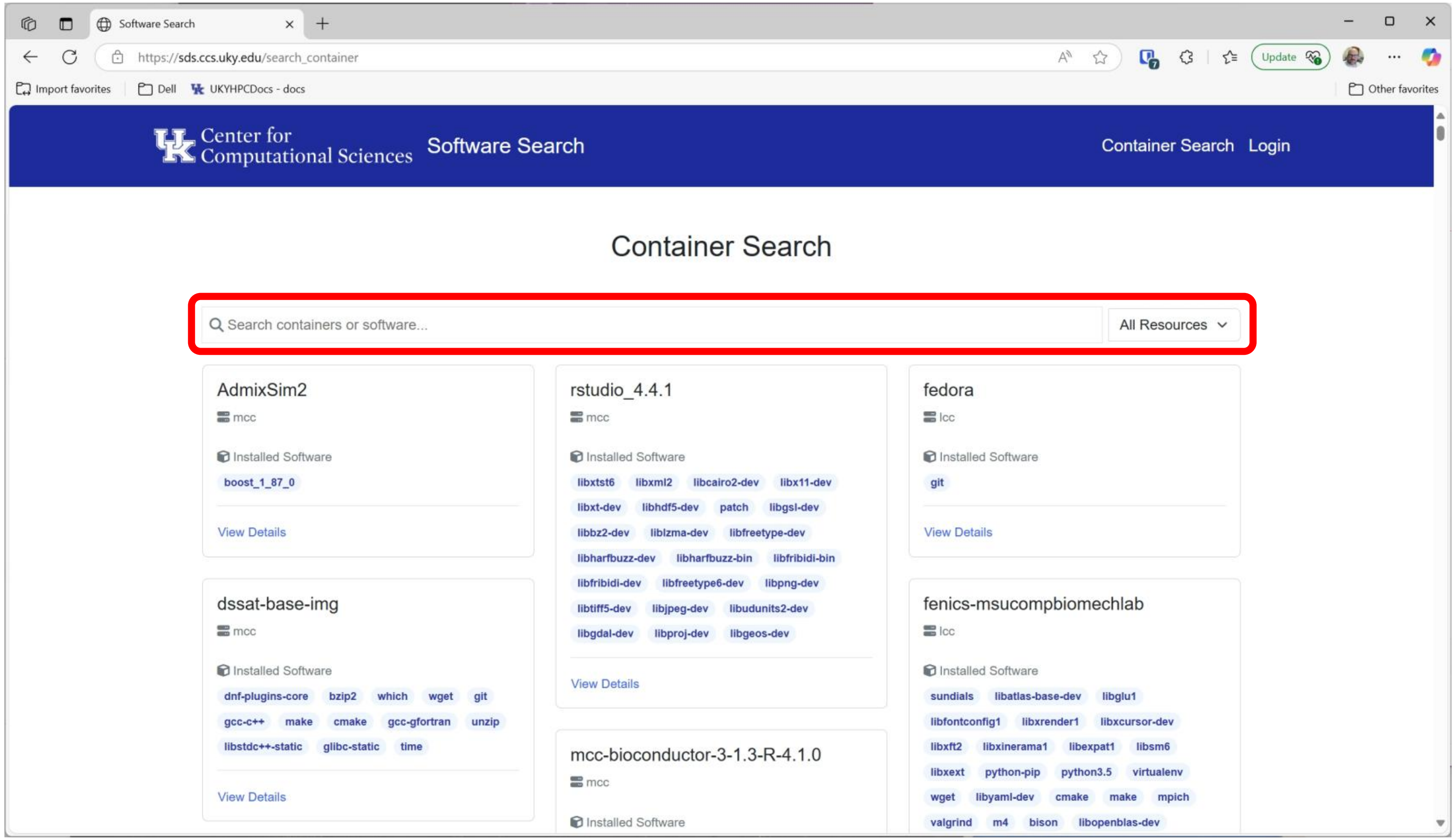
LMOD (module spider)



```
[bwfarm2@dtn ~]$ module spider cellranger

---------------------------------------------------------------------------------------------------------------
  ccs/cellranger:
---------------------------------------------------------------------------------------------------------------
    Description:
      Cell ranger tools .

     Versions:
        ccs/cellranger/3.0.2
        ccs/cellranger/3.1.0
        ccs/cellranger/4.0.0
        ccs/cellranger/6.0.0
        ccs/cellranger/6.0.2


---------------------------------------------------------------------------------------------------------------
  For detailed information about a specific "ccs/cellranger" module (including how to load the modules) use the mod
ule's full name.
  For example:

     $ module spider ccs/cellranger/6.0.2
---------------------------------------------------------------------------------------------------------------
```

Software Discovery Service

Container Search



Container Search

Search containers or software...

All Resources

AdmixSim2

mcc

Installed Software

boost_1_87_0

View Details

dssat-base-img

mcc

Installed Software

dnf-plugins-core bzip2 which wget git gcc-c++ make cmake gcc-gfortran unzip libstdc++-static glibc-static time

View Details

rstudio_4.4.1

mcc

Installed Software

libxtst6 libxml2 libcairo2-dev libx11-dev libxt-dev libhdf5-dev patch libgsl-dev libbz2-dev liblzma-dev libfreetype-dev libharfbuzz-dev libharfbuzz-bin libfribidi-bin libfribidi-dev libfreetype6-dev libpng-dev libtiff5-dev libjpeg-dev libudunits2-dev libgdal-dev libproj-dev libgeos-dev

View Details

mcc-bioconductor-3-1.3-R-4.1.0

mcc

Installed Software

fedora

lcc

Installed Software

git

View Details

fenics-msucompbiomechlab

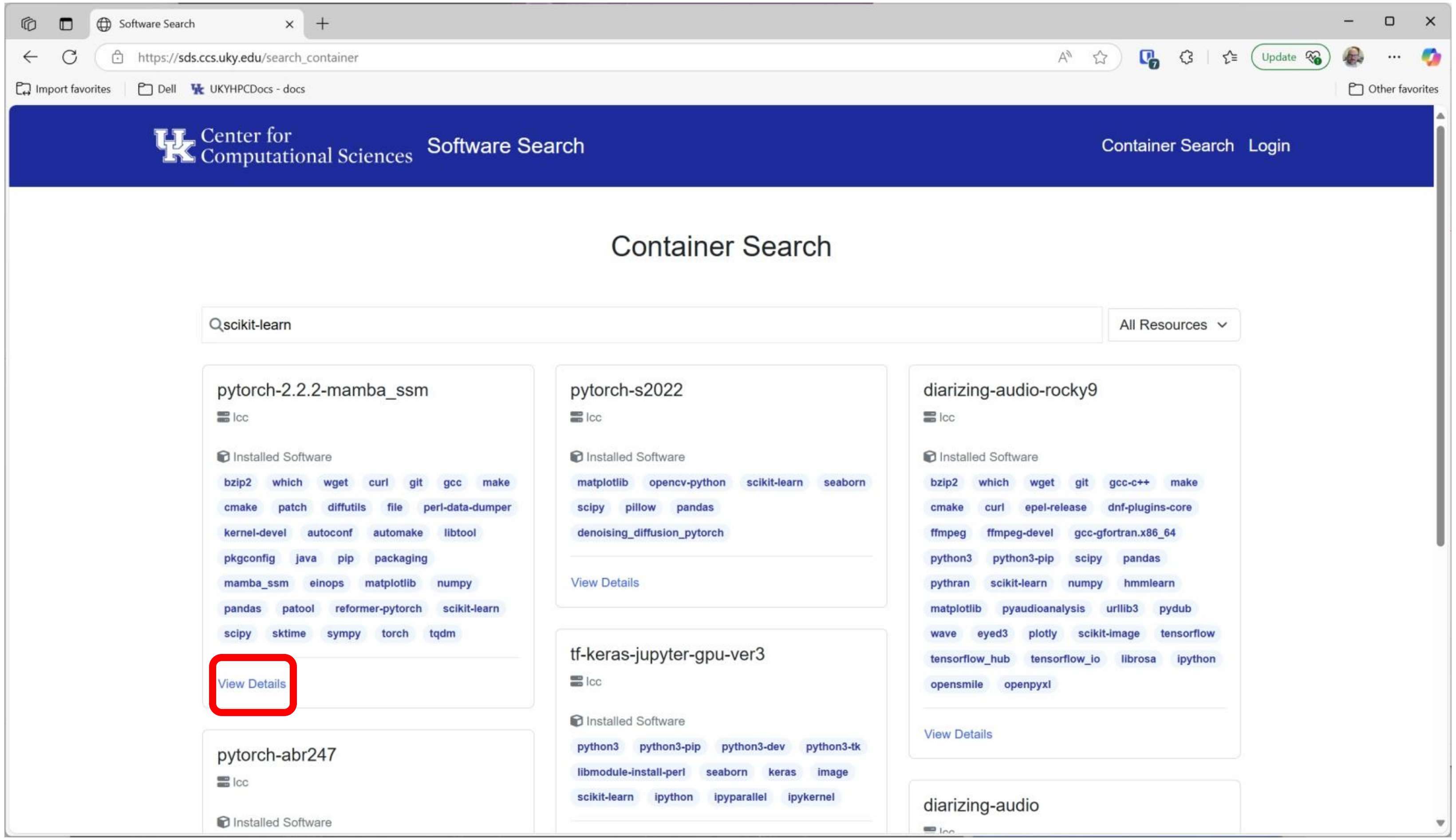
lcc

Installed Software

sundials libatlas-base-dev libglu1 libfontconfig1 libxrender1 libxcursor-dev libxft2 libxinerama1 libexpat1 libsm6 libxext python-pip python3.5 virtualenv wget libyaml-dev cmake make mpich valgrind m4 bison libopenblas-dev

Software Discovery Service

Container Search



Container Search

scikit-learn | All Resources

pytorch-2.2.2-mamba_ssm

lcc

Installed Software

bzip2, which, wget, curl, git, gcc, make, cmake, patch, diffutils, file, perl-data-dumper, kernel-devel, autoconf, automake, libtool, pkgconfig, java, pip, packaging, mamba_ssm, einops, matplotlib, numpy, pandas, patool, reformer-pytorch, scikit-learn, scipy, sktime, sympy, torch, tqdm

View Details

pytorch-abr247

lcc

Installed Software

pytorch-s2022

lcc

Installed Software

matplotlib, opencv-python, scikit-learn, seaborn, scipy, pillow, pandas, denoising_diffusion_pytorch

View Details

tf-keras-jupyter-gpu-ver3

lcc

Installed Software

python3, python3-pip, python3-dev, python3-tk, libmodule-install-perl, seaborn, keras, image, scikit-learn, ipython, ipyparallel, ipykernel

diarizing-audio-rocky9

lcc

Installed Software

bzip2, which, wget, git, gcc-c++, make, cmake, curl, epel-release, dnf-plugins-core, ffmpeg, ffmpeg-devel, gcc-gfortran.x86_64, python3, python3-pip, scipy, pandas, pythran, scikit-learn, numpy, hmmlearn, matplotlib, pyaudioanalysis, urllib3, pydub, wave, eyed3, plotly, scikit-image, tensorflow, tensorflow_hub, tensorflow_io, librosa, ipython, opensmile, openpyxl

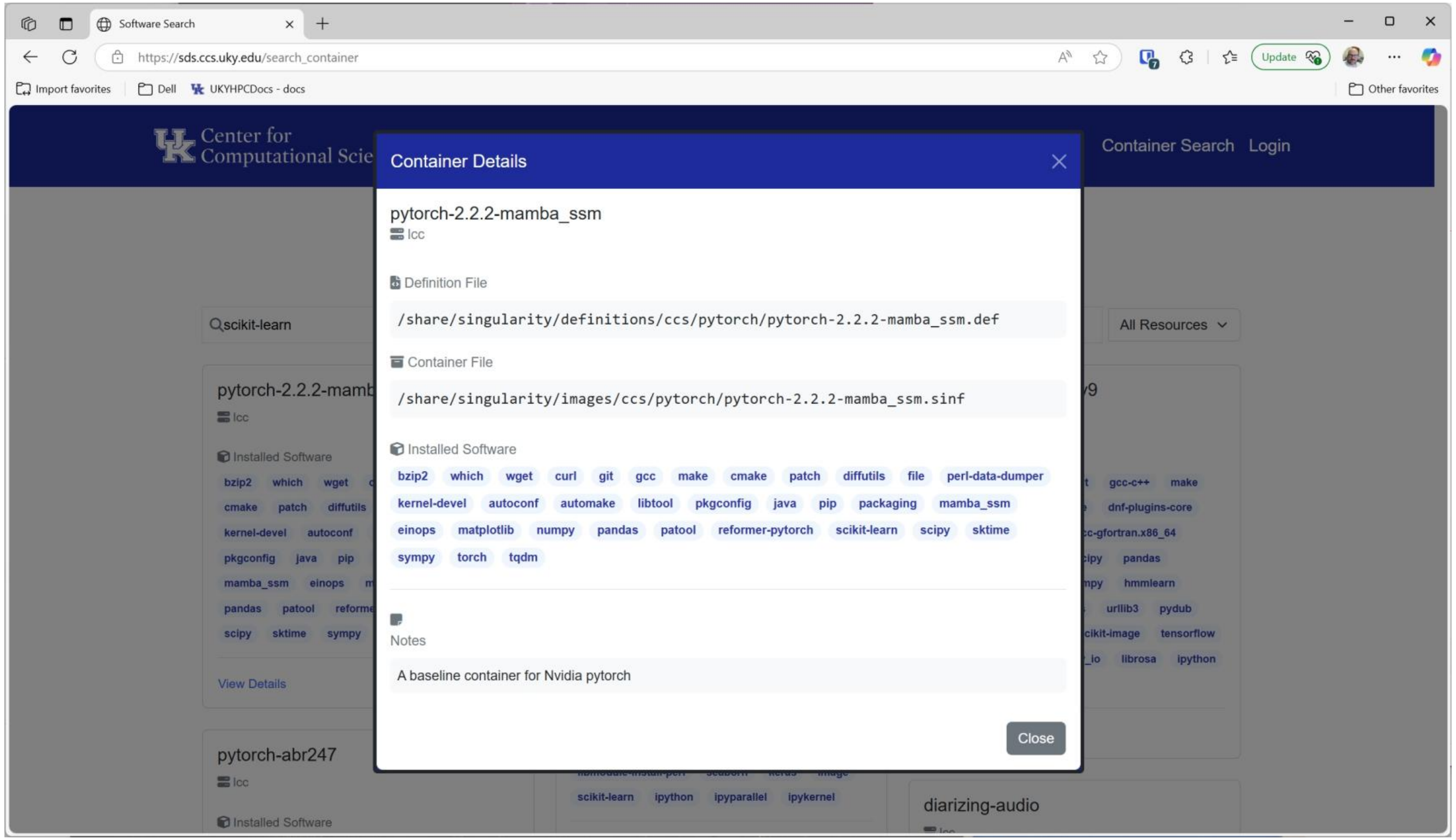
View Details

diarizing-audio

lcc

Software Discovery Service

Container Search



Container Details

pytorch-2.2.2-mamba_ssm

lcc

Definition File

`/share/singularity/definitions/ccs/pytorch/pytorch-2.2.2-mamba_ssm.def`

Container File

`/share/singularity/images/ccs/pytorch/pytorch-2.2.2-mamba_ssm.sinf`

Installed Software

bzip2 which wget curl git gcc make cmake patch diffutils file perl-data-dumper kernel-devel autoconf automake libtool pkgconfig java pip packaging mamba_ssm einops matplotlib numpy pandas patool reformer-pytorch scikit-learn scipy sktime sympy torch tqdm

Notes

A baseline container for Nvidia pytorch

Benefits of Containerized Software

- Reproducibility
    - Same environment everywhere you run it.
    - Consistent software behavior, easy to share.
- Portability
    - Move between systems without compatibility issues.
    - Work across environments without reconfiguring.
- Isolation
    - Keeps software and dependencies separate from the host system.
    - Run multiple versions or projects without conflicts.
- Flexibility and Customization
    - Tailor containers to your needs.
    - Experiment without affecting other environments.

Singularity Container Composer

- Template-Based Singularity Container Creation
    - Use pre-made templates to quickly set up your environment.

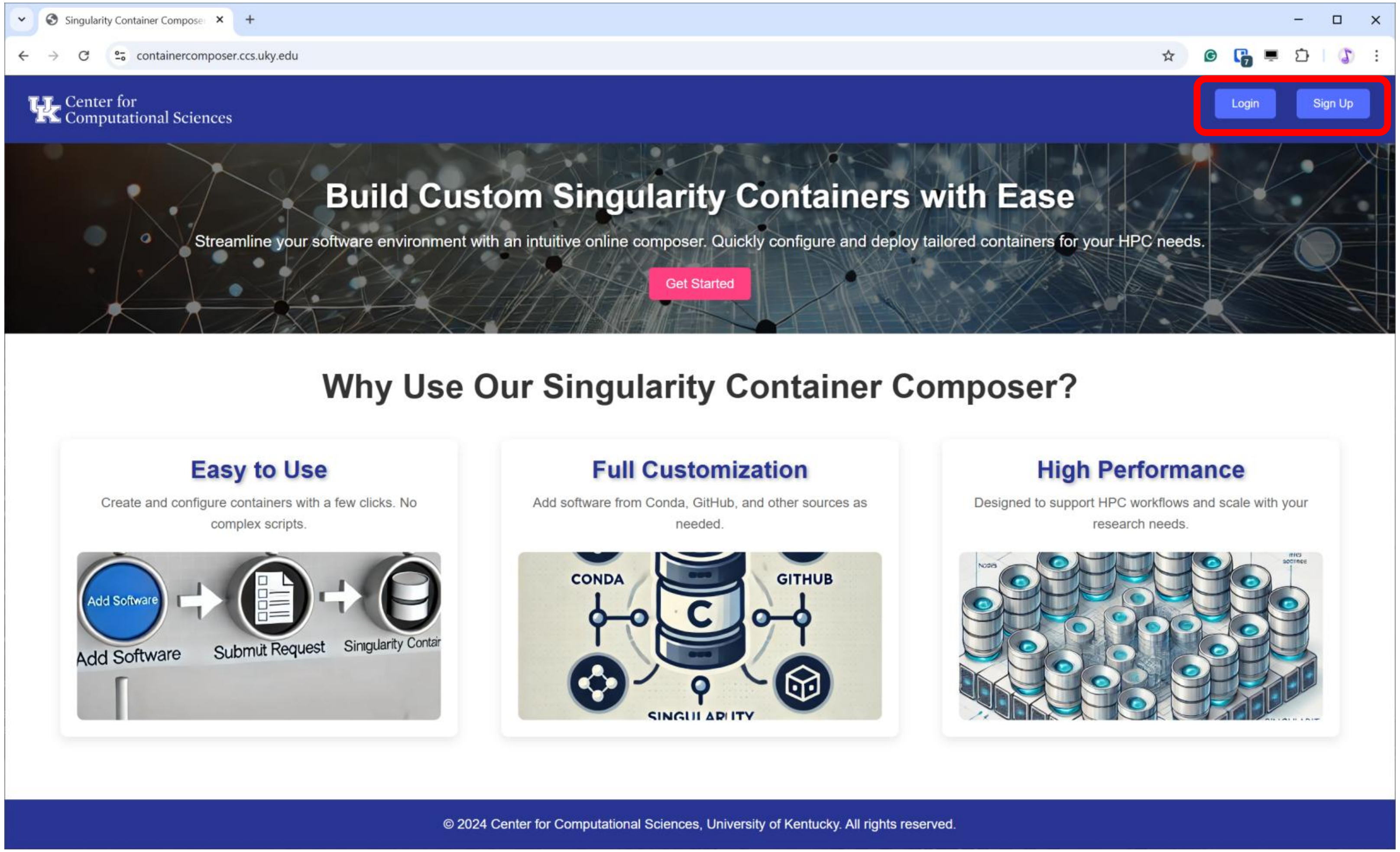
- Automated Build and Download Link
    - Containers built automatically and delivered via email.
    - Download your container ready for use on LCC or MCC.

- Customized Containers with Admin Approval

https://containercomposer.ccs.uky.edu

Documentation

Singularity Container Composer



Build Custom Singularity Containers with Ease

Streamline your software environment with an intuitive online composer. Quickly configure and deploy tailored containers for your HPC needs.

Why Use Our Singularity Container Composer?

Easy to Use

Create and configure containers with a few clicks. No complex scripts.

Full Customization

Add software from Conda, GitHub, and other sources as needed.

High Performance

Designed to support HPC workflows and scale with your research needs.

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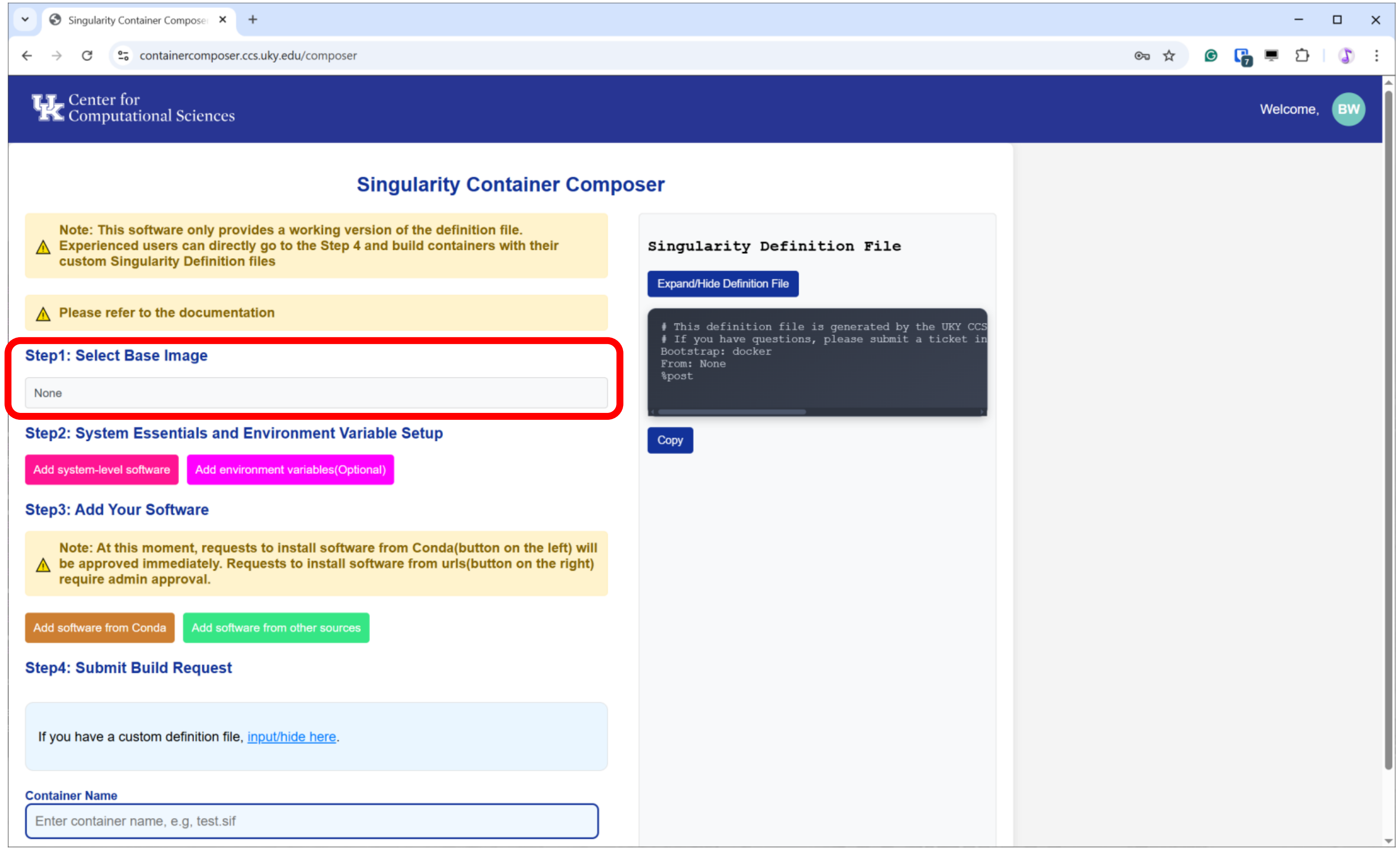
Singularity Container Composer



Singularity Container Composer

⚠ Note: This software only provides a working version of the definition file. Experienced users can directly go to the Step 4 and build containers with their custom Singularity Definition files

⚠ Please refer to the documentation

Step1: Select Base Image

None

Step2: System Essentials and Environment Variable Setup

Step3: Add Your Software

⚠ Note: At this moment, requests to install software from Conda(button on the left) will be approved immediately. Requests to install software from urls(button on the right) require admin approval.

Step4: Submit Build Request

If you have a custom definition file, input/hide here.

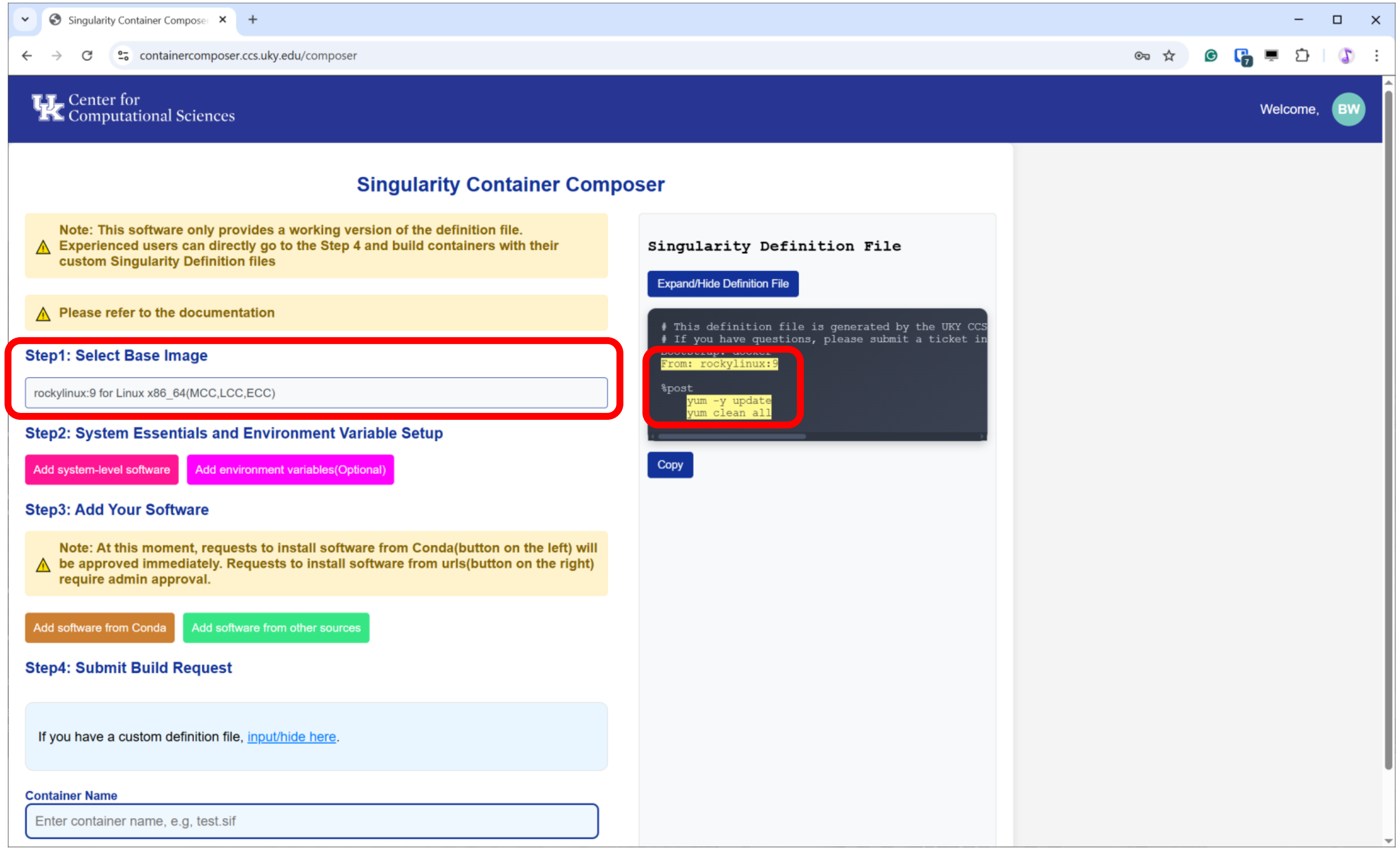
Container Name

Enter container name, e.g, test.sif

Singularity Definition File

```
# This definition file is generated by the UKY CCS
# If you have questions, please submit a ticket in
Bootstrap: docker
From: None
%post
```

Singularity Container Composer



Singularity Container Composer

⚠ Note: This software only provides a working version of the definition file. Experienced users can directly go to the Step 4 and build containers with their custom Singularity Definition files

⚠ Please refer to the documentation

Step1: Select Base Image

rockylinux:9 for Linux x86_64(MCC,LCC,ECC)

Step2: System Essentials and Environment Variable Setup

Step3: Add Your Software

⚠ Note: At this moment, requests to install software from Conda(button on the left) will be approved immediately. Requests to install software from urls(button on the right) require admin approval.

Step4: Submit Build Request

If you have a custom definition file, input/hide here.

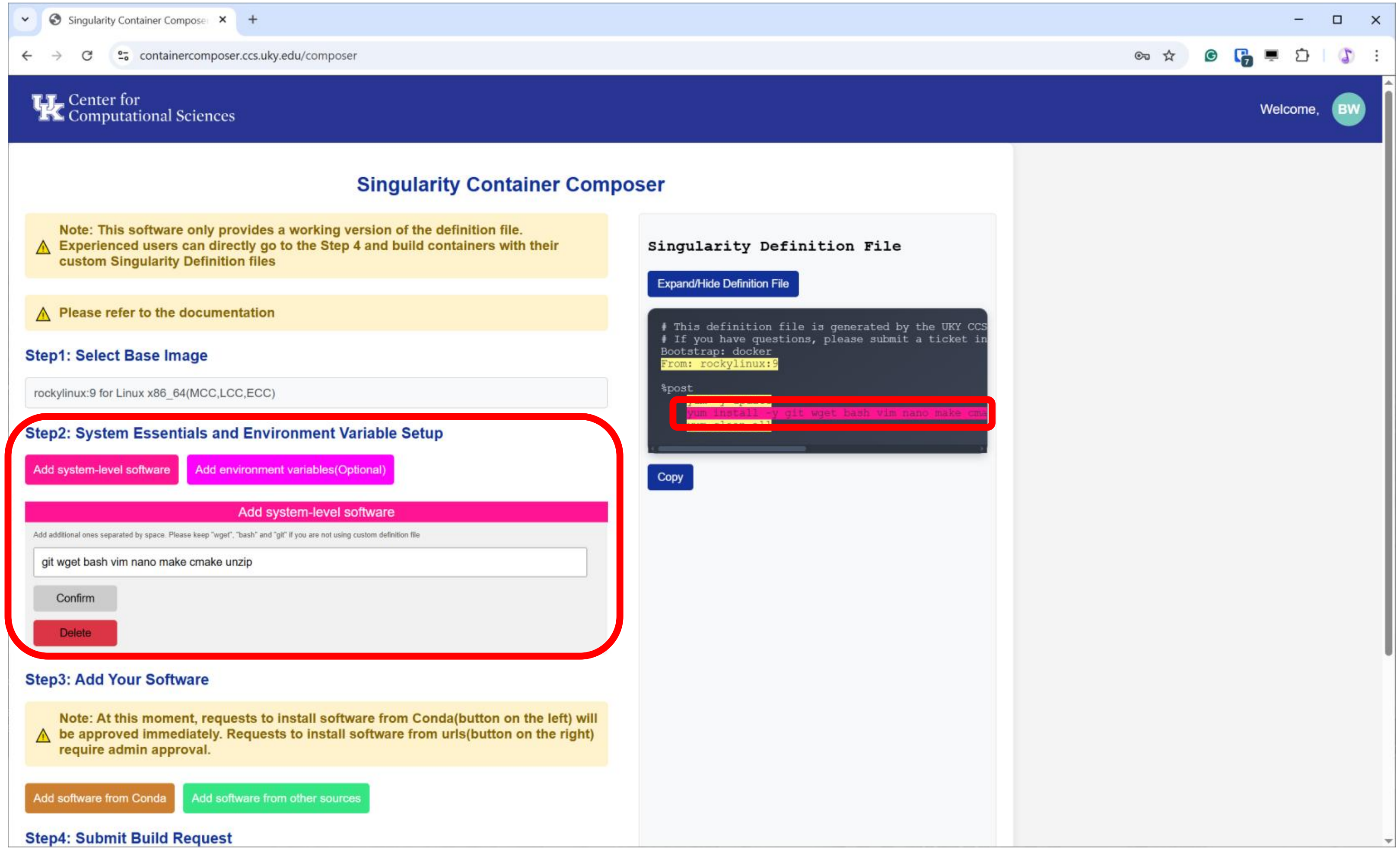
Container Name

Enter container name, e.g, test.sif

Singularity Definition File

```
# This definition file is generated by the UKY CCS
# If you have questions, please submit a ticket in
Bootstrap: docker
From: rockylinux:9

%post
    yum -y update
    yum clean all
```

Singularity Container Composer



Singularity Container Composer

⚠ Note: This software only provides a working version of the definition file. Experienced users can directly go to the Step 4 and build containers with their custom Singularity Definition files

⚠ Please refer to the documentation

Step1: Select Base Image

rockylinux:9 for Linux x86_64(MCC,LCC,ECC)

Step2: System Essentials and Environment Variable Setup

Add additional ones separated by space. Please keep "wget", "bash" and "git" if you are not using custom definition file

git wget bash vim nano make cmake unzip

Step3: Add Your Software

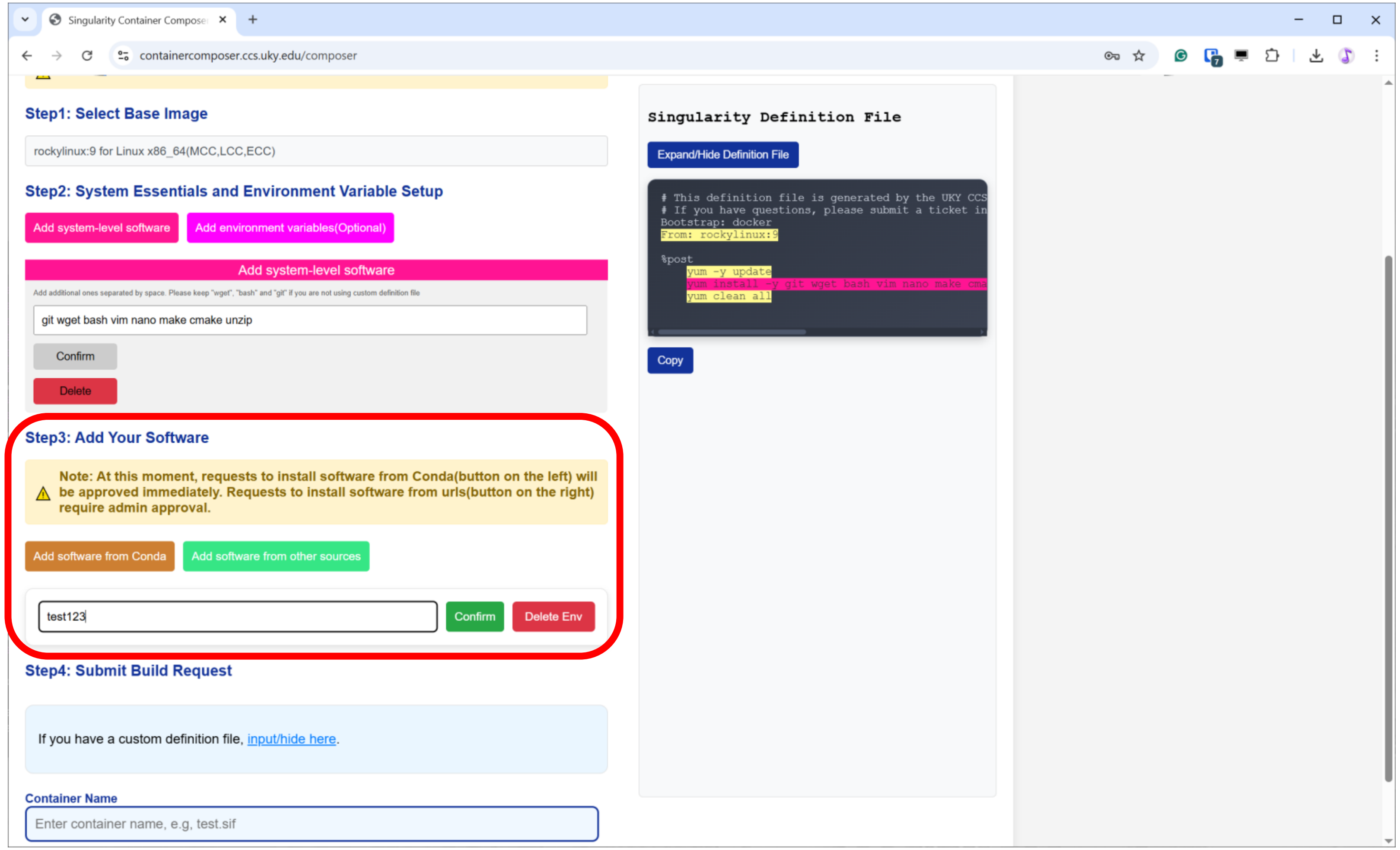
⚠ Note: At this moment, requests to install software from Conda(button on the left) will be approved immediately. Requests to install software from urls(button on the right) require admin approval.

Step4: Submit Build Request

Singularity Definition File

```
# This definition file is generated by the UKY CCS
# If you have questions, please submit a ticket in
Bootstrap: docker
From: rockylinux:9

%post
    yum -y update
    yum install -y git wget bash vim nano make cma
    yum clean all
```

Singularity Container Composer



Step1: Select Base Image

rockylinux:9 for Linux x86_64(MCC,LCC,ECC)

Step2: System Essentials and Environment Variable Setup

Add additional ones separated by space. Please keep "wget", "bash" and "git" if you are not using custom definition file

git wget bash vim nano make cmake unzip

Step3: Add Your Software

⚠ Note: At this moment, requests to install software from Conda(button on the left) will be approved immediately. Requests to install software from urls(button on the right) require admin approval.

test123

Step4: Submit Build Request

If you have a custom definition file, input/hide here.

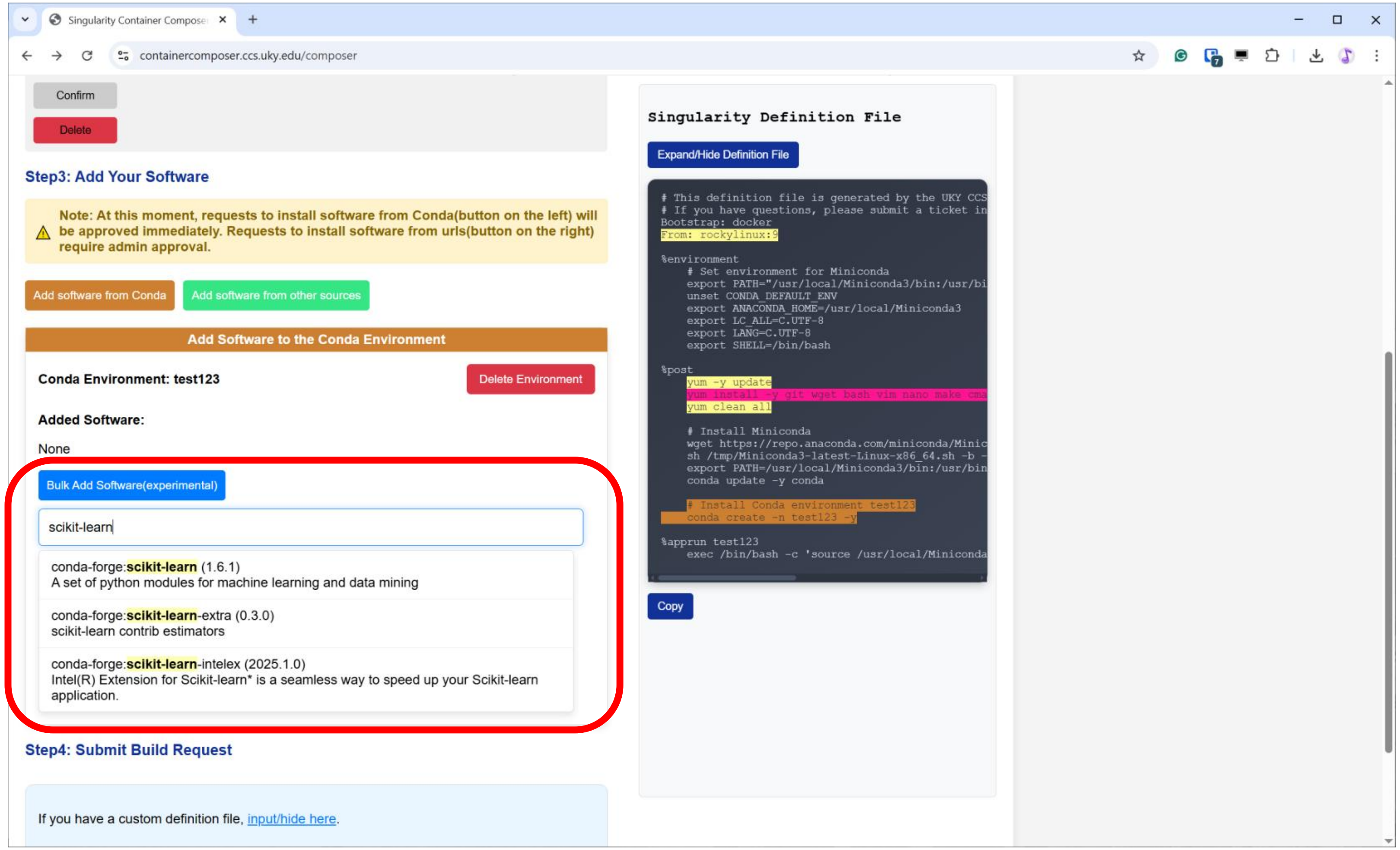
Container Name

Enter container name, e.g, test.sif

Singularity Definition File

```
# This definition file is generated by the UKY CCS
# If you have questions, please submit a ticket in
Bootstrap: docker
From: rockylinux:9

%post
    yum -y update
    yum install -y git wget bash vim nano make cma
    yum clean all
```

Singularity Container Composer



Step3: Add Your Software

⚠ Note: At this moment, requests to install software from Conda(button on the left) will be approved immediately. Requests to install software from urls(button on the right) require admin approval.

Add Software to the Conda Environment

Conda Environment: test123

Added Software:

None

scikit-learn

conda-forge:**scikit-learn** (1.6.1)
A set of python modules for machine learning and data mining

conda-forge:**scikit-learn**-extra (0.3.0)
scikit-learn contrib estimators

conda-forge:**scikit-learn**-intelex (2025.1.0)
Intel(R) Extension for Scikit-learn* is a seamless way to speed up your Scikit-learn application.

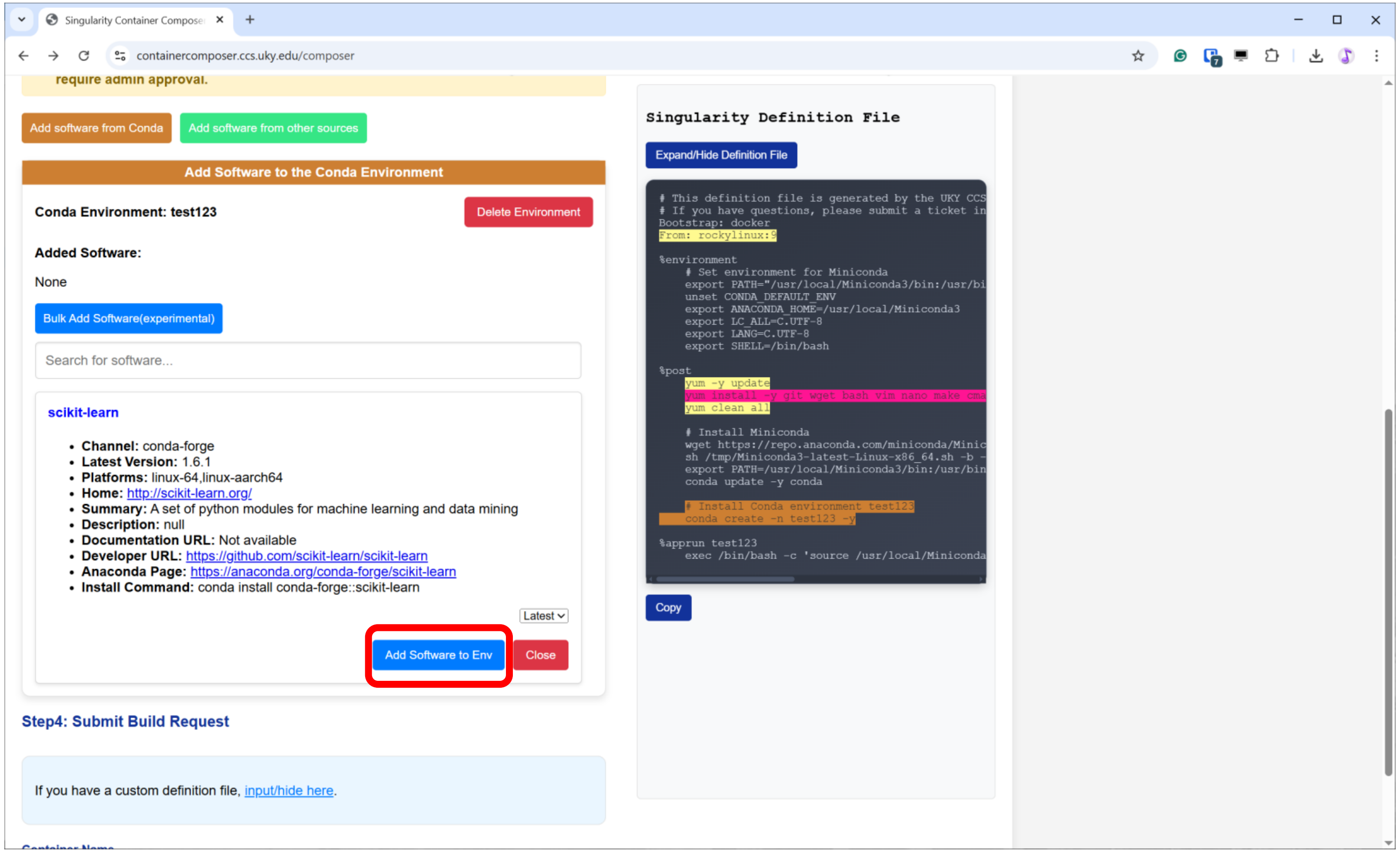
Step4: Submit Build Request

If you have a custom definition file, input/hide here.

Singularity Definition File

```
# This definition file is generated by the UKY CCS
# If you have questions, please submit a ticket in
Bootstrap: docker
From: rockylinux:9

%environment
    # Set environment for Miniconda
    export PATH="/usr/local/Miniconda3/bin:/usr/bi
    unset CONDA_DEFAULT_ENV
    export ANACONDA_HOME=/usr/local/Miniconda3
    export LC_ALL=C.UTF-8
    export LANG=C.UTF-8
    export SHELL=/bin/bash

%post
    yum -y update
    yum install -y git wget bash vim nano make cma
    yum clean all

    # Install Miniconda
    wget https://repo.anaconda.com/miniconda/Minic
    sh /tmp/Miniconda3-latest-Linux-x86_64.sh -b -
    export PATH=/usr/local/Miniconda3/bin:/usr/bin
    conda update -y conda

    # Install Conda environment test123
    conda create -n test123 -y

%apprun test123
    exec /bin/bash -c 'source /usr/local/Miniconda
```

Singularity Container Composer



require admin approval.

Add Software to the Conda Environment

Conda Environment: test123

Added Software:

None

scikit-learn

- **Channel:** conda-forge
- **Latest Version:** 1.6.1
- **Platforms:** linux-64,linux-aarch64
- **Home:** http://scikit-learn.org/
- **Summary:** A set of python modules for machine learning and data mining
- **Description:** null
- **Documentation URL:** Not available
- **Developer URL:** https://github.com/scikit-learn/scikit-learn
- **Anaconda Page:** https://anaconda.org/conda-forge/scikit-learn
- **Install Command:** conda install conda-forge::scikit-learn

Step4: Submit Build Request

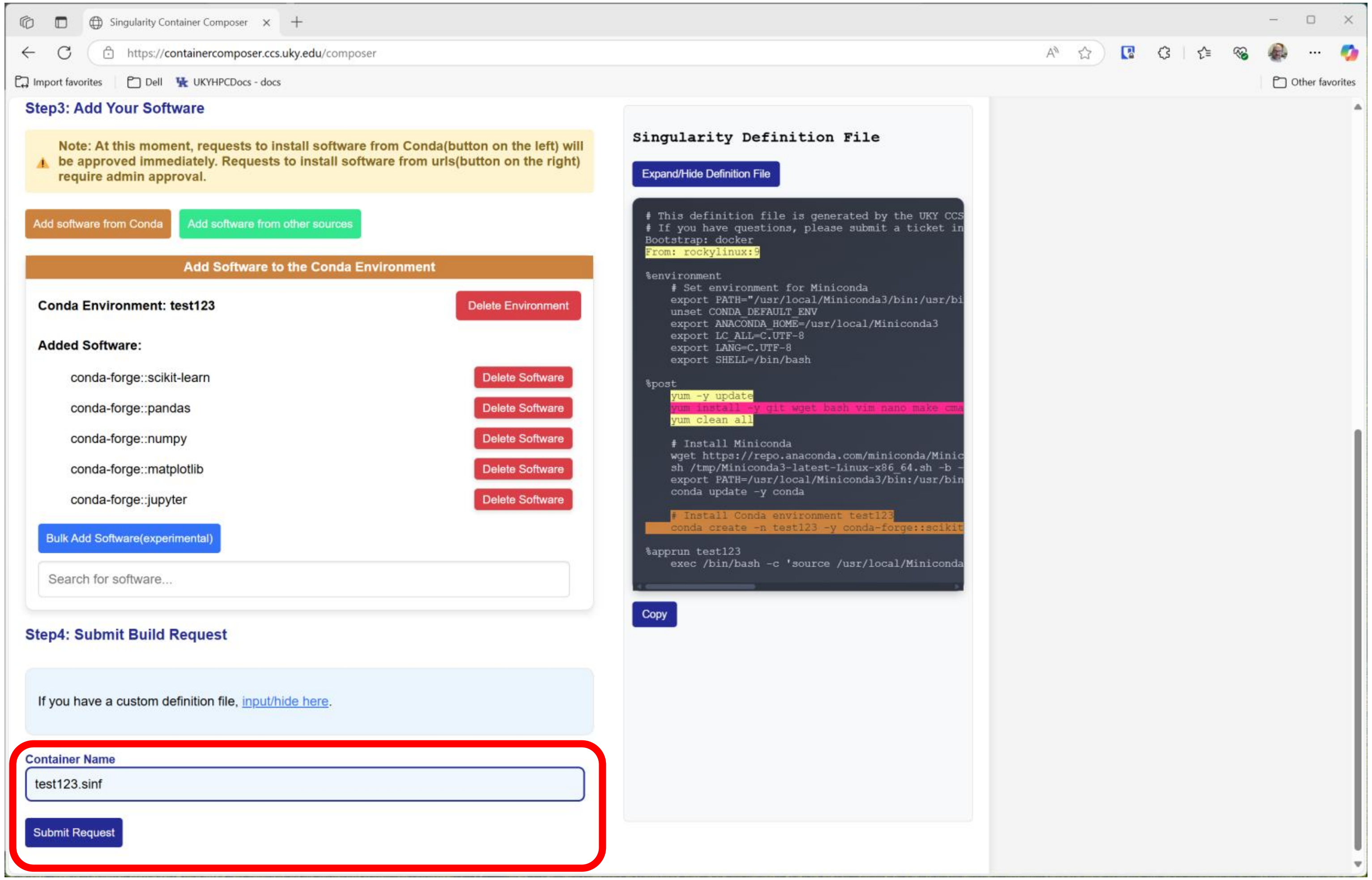
If you have a custom definition file, input/hide here.

Singularity Definition File

```
# This definition file is generated by the UKY CCS
# If you have questions, please submit a ticket in
Bootstrap: docker
From: rockylinux:9

%environment
    # Set environment for Miniconda
    export PATH="/usr/local/Miniconda3/bin:/usr/bi
    unset CONDA_DEFAULT_ENV
    export ANACONDA_HOME=/usr/local/Miniconda3
    export LC_ALL=C.UTF-8
    export LANG=C.UTF-8
    export SHELL=/bin/bash

%post
    yum -y update
    yum install -y git wget bash vim nano make cma
    yum clean all

    # Install Miniconda
    wget https://repo.anaconda.com/miniconda/Minic
    sh /tmp/Miniconda3-latest-Linux-x86_64.sh -b -
    export PATH=/usr/local/Miniconda3/bin:/usr/bin
    conda update -y conda

    # Install Conda environment test123
    conda create -n test123 -y

%apprun test123
    exec /bin/bash -c 'source /usr/local/Miniconda
```

University of Kentucky

Singularity Container Composer



Step3: Add Your Software

Note: At this moment, requests to install software from Conda(button on the left) will be approved immediately. Requests to install software from urls(button on the right) require admin approval.

Conda Environment: test123

Added Software:

- conda-forge::scikit-learn
- conda-forge::pandas
- conda-forge::numpy
- conda-forge::matplotlib
- conda-forge::jupyter

Step4: Submit Build Request

If you have a custom definition file, input/hide here.

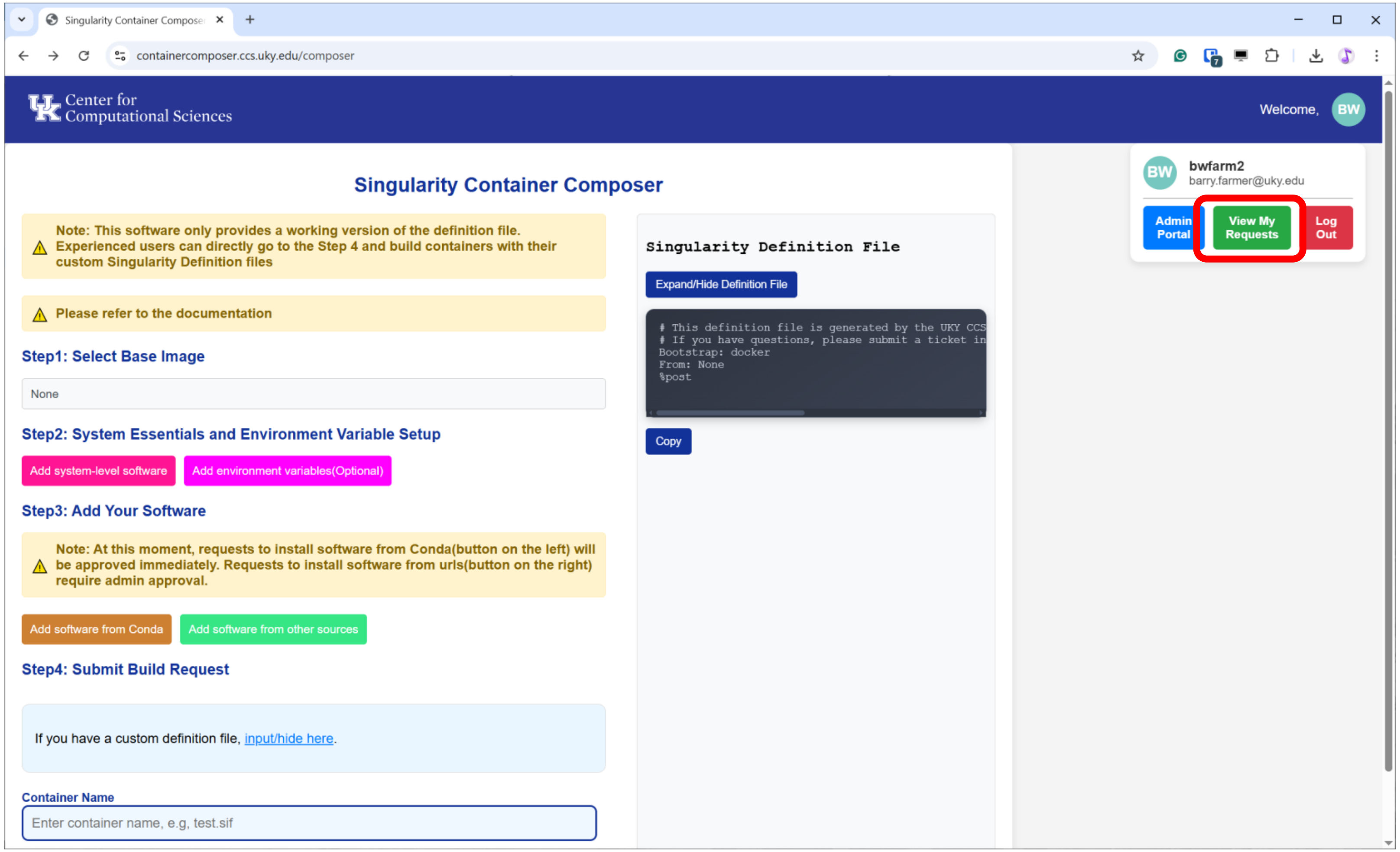
Container Name

test123.sinf

Singularity Definition File

```
# This definition file is generated by the UKY CCS
# If you have questions, please submit a ticket in
Bootstrap: docker
From: rockylinux:9

%environment
    # Set environment for Miniconda
    export PATH="/usr/local/Miniconda3/bin:/usr/bi
    unset CONDA_DEFAULT_ENV
    export ANACONDA_HOME=/usr/local/Miniconda3
    export LC_ALL=C.UTF-8
    export LANG=C.UTF-8
    export SHELL=/bin/bash

%post
    yum -y update
    yum install -y git wget bash vim nano make cma
    yum clean all

    # Install Miniconda
    wget https://repo.anaconda.com/miniconda/Minic
    sh /tmp/Miniconda3-latest-Linux-x86_64.sh -b -
    export PATH=/usr/local/Miniconda3/bin:/usr/bin
    conda update -y conda

    # Install Conda environment test123
    conda create -n test123 -y conda-forge::scikit

%apprun test123
    exec /bin/bash -c 'source /usr/local/Miniconda
```

Singularity Container Composer



bwfarm2
barry.farmer@uky.edu

Singularity Container Composer

⚠ **Note: This software only provides a working version of the definition file. Experienced users can directly go to the Step 4 and build containers with their custom Singularity Definition files**

⚠ **Please refer to the documentation**

Step1: Select Base Image

None

Step2: System Essentials and Environment Variable Setup

Step3: Add Your Software

⚠ **Note: At this moment, requests to install software from Conda(button on the left) will be approved immediately. Requests to install software from urls(button on the right) require admin approval.**

Step4: Submit Build Request

If you have a custom definition file, input/hide here.

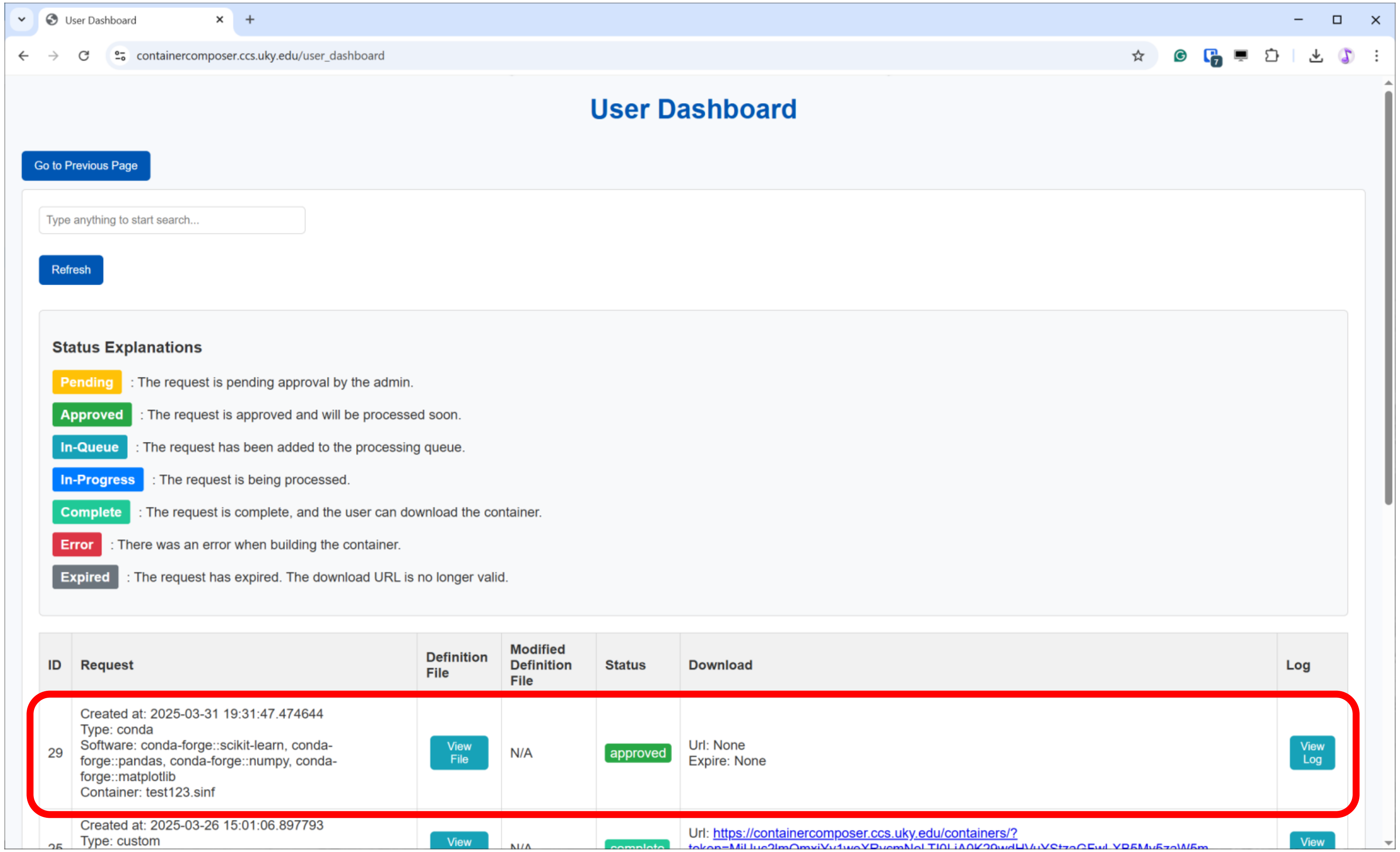
Container Name

Enter container name, e.g, test.sif

Singularity Definition File

```
# This definition file is generated by the UKY CCS
# If you have questions, please submit a ticket in
Bootstrap: docker
From: None
%post
```

Singularity Container Composer



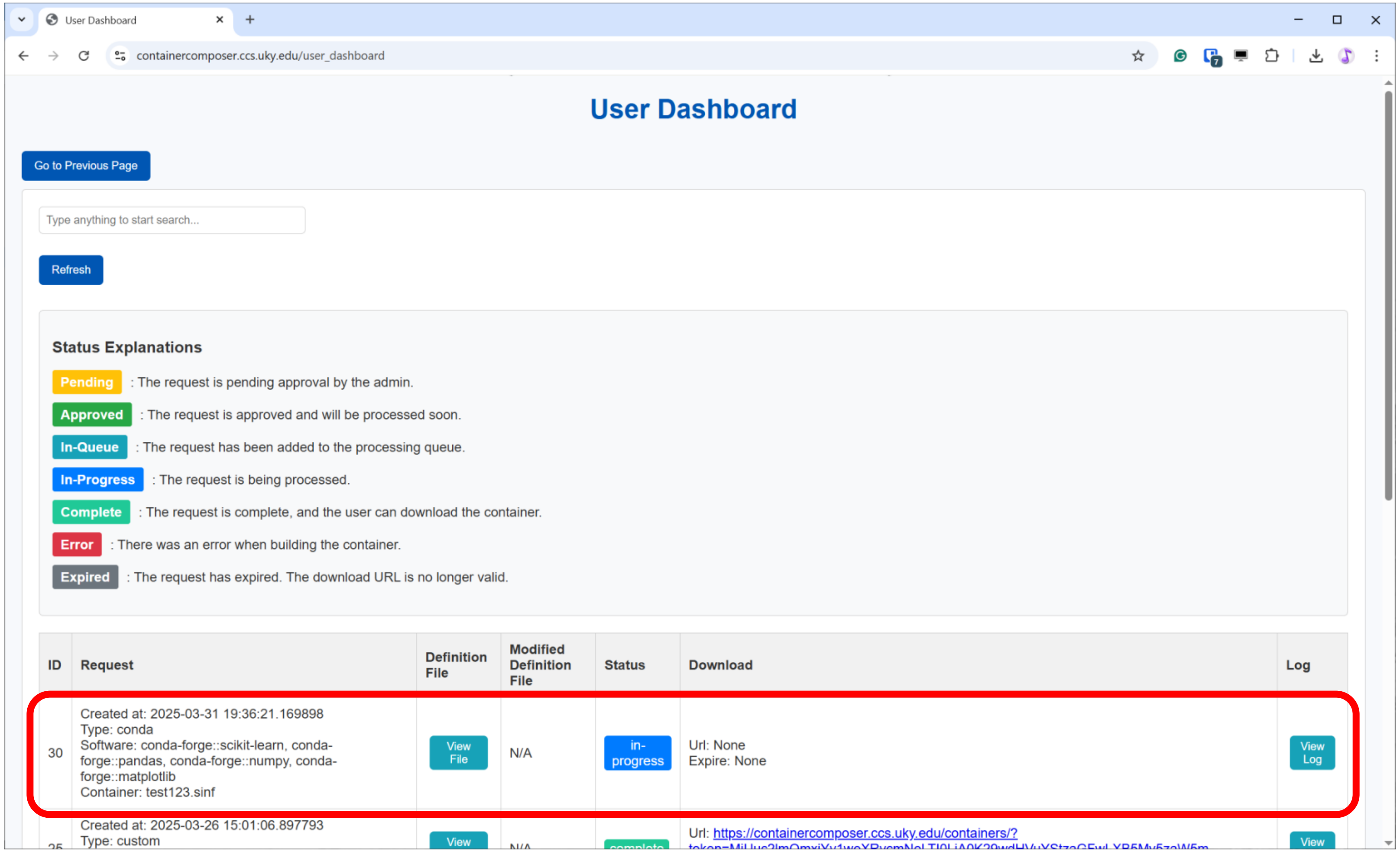
User Dashboard

Status Explanations

- **Pending** : The request is pending approval by the admin.
- **Approved** : The request is approved and will be processed soon.
- **In-Queue** : The request has been added to the processing queue.
- **In-Progress** : The request is being processed.
- **Complete** : The request is complete, and the user can download the container.
- **Error** : There was an error when building the container.
- **Expired** : The request has expired. The download URL is no longer valid.

ID	Request	Definition File	Modified Definition File	Status	Download	Log
29	Created at: 2025-03-31 19:31:47.474644 Type: conda Software: conda-forge::scikit-learn, conda-forge::pandas, conda-forge::numpy, conda-forge::matplotlib Container: test123.sinf	View File	N/A	approved	Url: None Expire: None	View Log
	Created at: 2025-03-26 15:01:06.897793 Type: custom	View			Url: https://containercomposer.ccs.uky.edu/containers/?	View

Singularity Container Composer



User Dashboard

Go to Previous Page

Type anything to start search...

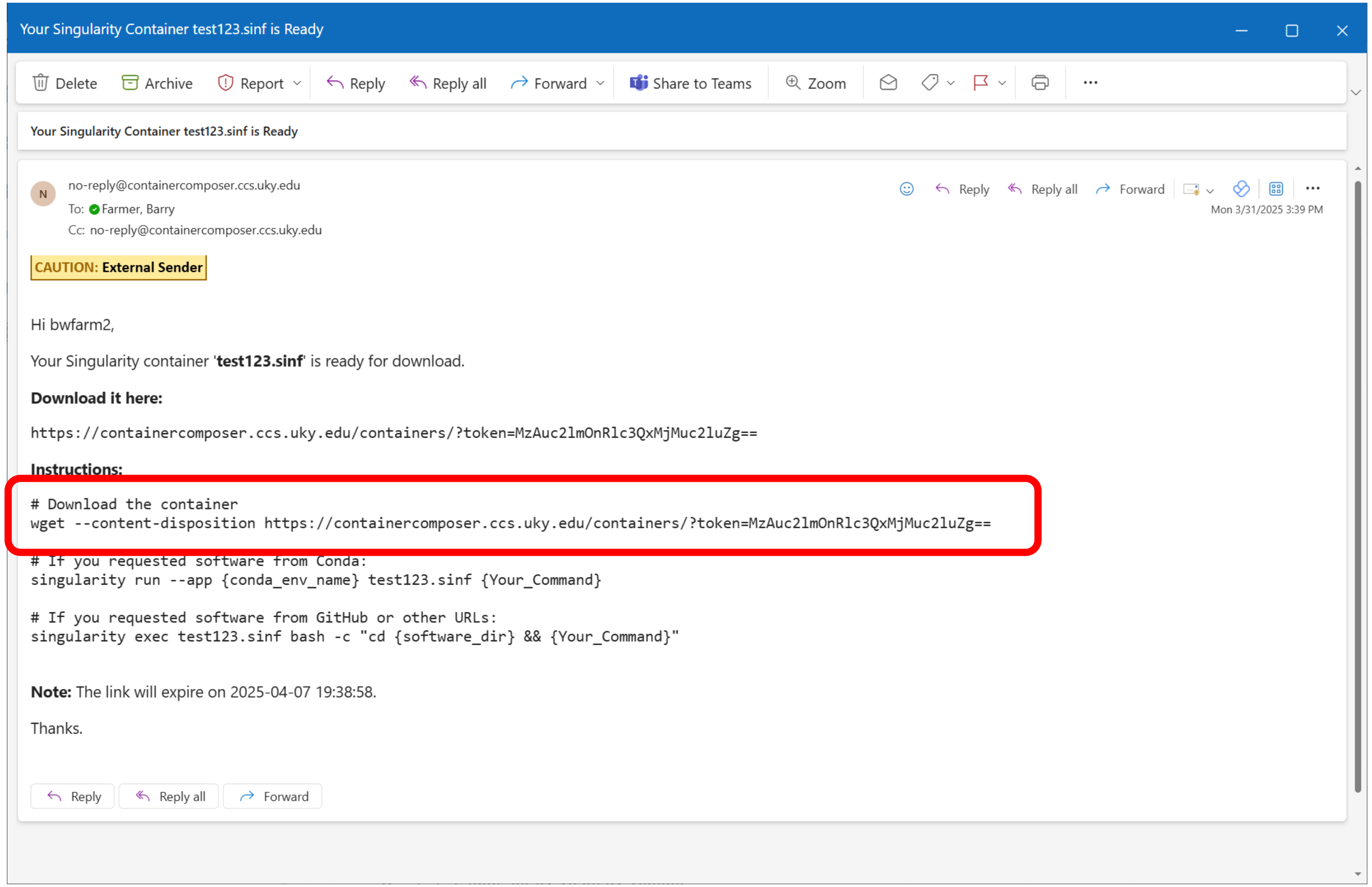
Refresh

Status Explanations

Pending : The request is pending approval by the admin.
Approved : The request is approved and will be processed soon.
In-Queue : The request has been added to the processing queue.
In-Progress : The request is being processed.
Complete : The request is complete, and the user can download the container.
Error : There was an error when building the container.
Expired : The request has expired. The download URL is no longer valid.

ID	Request	Definition File	Modified Definition File	Status	Download	Log
30	Created at: 2025-03-31 19:36:21.169898 Type: conda Software: conda-forge::scikit-learn, conda-forge::pandas, conda-forge::numpy, conda-forge::matplotlib Container: test123.sinf	View File	N/A	in-progress	Url: None Expire: None	View Log
	Created at: 2025-03-26 15:01:06.897793 Type: custom	View			Url: https://containercomposer.ccs.uky.edu/containers/?	View

Singularity Container Composer



Your Singularity Container test123.sinf is Ready

N no-reply@containercomposer.ccs.uky.edu
To: Farmer, Barry
Cc: no-reply@containercomposer.ccs.uky.edu
Mon 3/31/2025 3:39 PM

CAUTION: External Sender

Hi bwfarm2,

Your Singularity container '**test123.sinf**' is ready for download.

Download it here:

`https://containercomposer.ccs.uky.edu/containers/?token=MzAuc2lmOnRlc3QxMjMuc2luZg==`

Instructions:

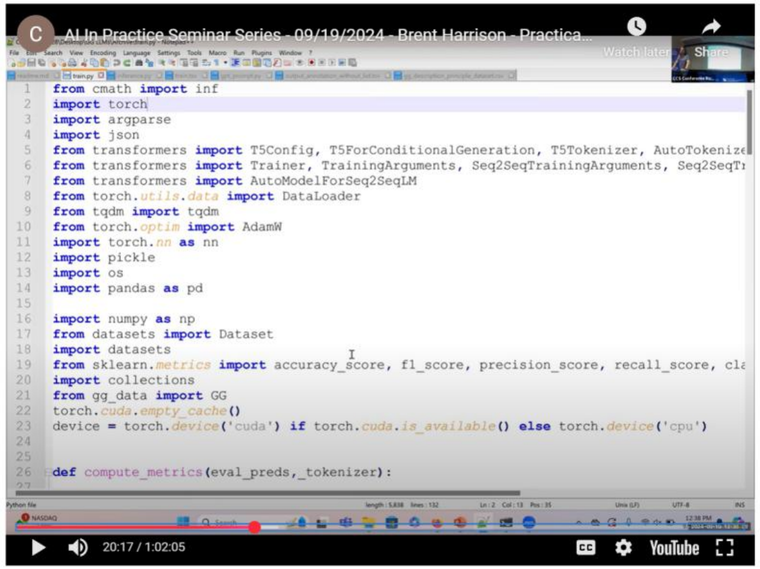
```
# Download the container
wget --content-disposition https://containercomposer.ccs.uky.edu/containers/?token=MzAuc2lmOnRlc3QxMjMuc2luZg==

# If you requested software from Conda:
singularity run --app {conda_env_name} test123.sinf {Your_Command}

# If you requested software from GitHub or other URLs:
singularity exec test123.sinf bash -c "cd {software_dir} && {Your_Command}"
```

Note: The link will expire on 2025-04-07 19:38:58.

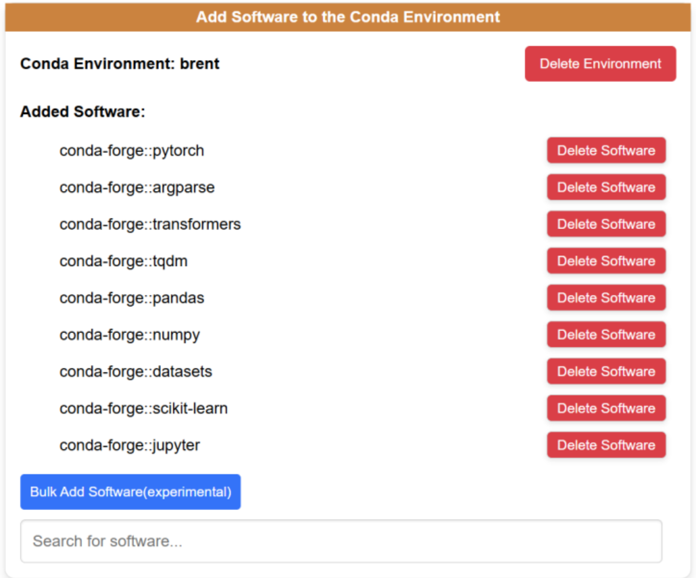
Thanks.

Containers for previous AI In Practice Seminars

- September 19, 2024
    - Brent Harrison, Computer Science, UK
        - Python Environment with:
            - cmath torch argparse json transformers tqdm pickle os pandas numpy datasets scikit-learn collections gg_data



```python
from cmath import inf
import torch
import argparse
import json
from transformers import T5Config, T5ForConditionalGeneration, T5Tokenizer, AutoTokenize
from transformers import Trainer, TrainingArguments, Seq2SeqTrainingArguments, Seq2SeqTr
from transformers import AutoModelForSeq2SeqLM
from torch.utils.data import DataLoader
from tqdm import tqdm
from torch.optim import AdamW
import torch.nn as nn
import pickle
import os
import pandas as pd

import numpy as np
from datasets import Dataset
import datasets
from sklearn.metrics import accuracy_score, f1_score, precision_score, recall_score, cla
import collections
from gg_data import GG
torch.cuda.empty_cache()
device = torch.device('cuda') if torch.cuda.is_available() else torch.device('cpu')


def compute_metrics(eval_preds,_tokenizer):
```


Add Software to the Conda Environment

Conda Environment: brent

Added Software:

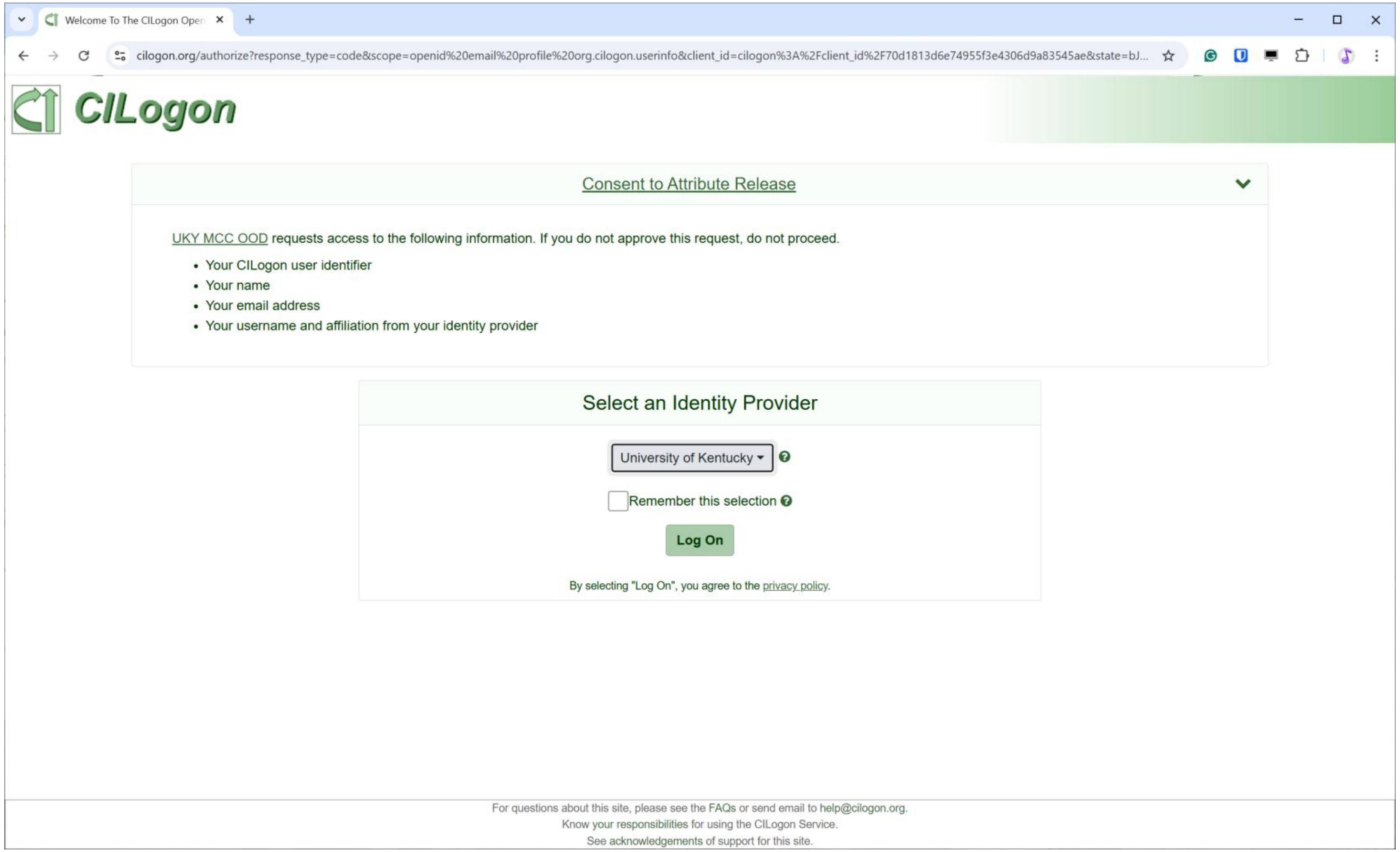
conda-forge::pytorch
conda-forge::argparse
conda-forge::transformers
conda-forge::tqdm
conda-forge::pandas
conda-forge::numpy
conda-forge::datasets
conda-forge::scikit-learn
conda-forge::jupyter

Open OnDemand

- Web Based Access to HPC Resources
- Interactive App Launchers
- Remote Desktop Access

LCC	MCC
https://ood.ccs.uky.edu	https://mcc-ood.ccs.uky.edu

Open OnDemand



Consent to Attribute Release

UKY MCC OOD requests access to the following information. If you do not approve this request, do not proceed.

- Your CILogon user identifier
- Your name
- Your email address
- Your username and affiliation from your identity provider

Select an Identity Provider

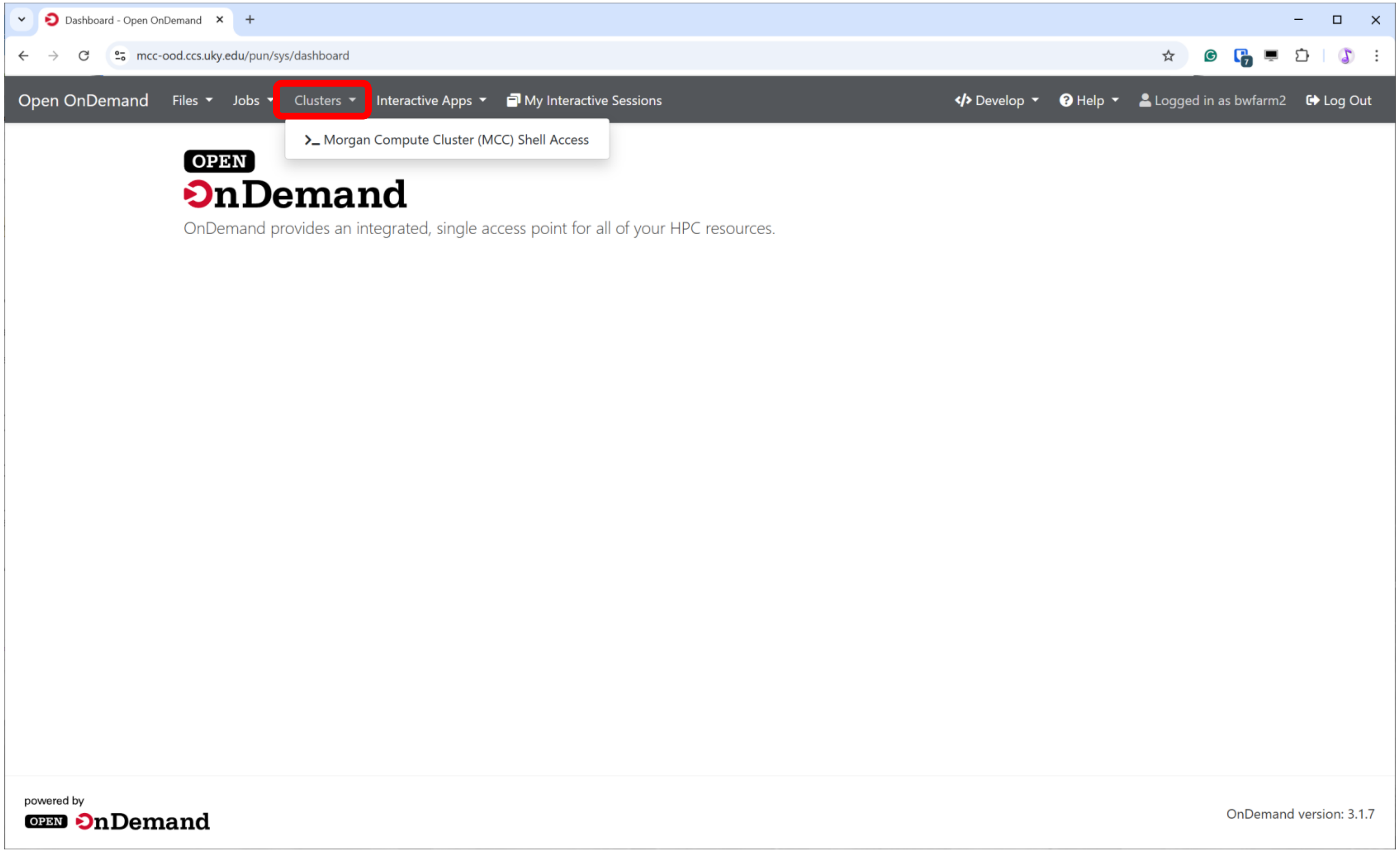
University of Kentucky

☐ Remember this selection

By selecting "Log On", you agree to the privacy policy.

For questions about this site, please see the FAQs or send email to help@cilogon.org.
Know your responsibilities for using the CILogon Service.
See acknowledgements of support for this site.

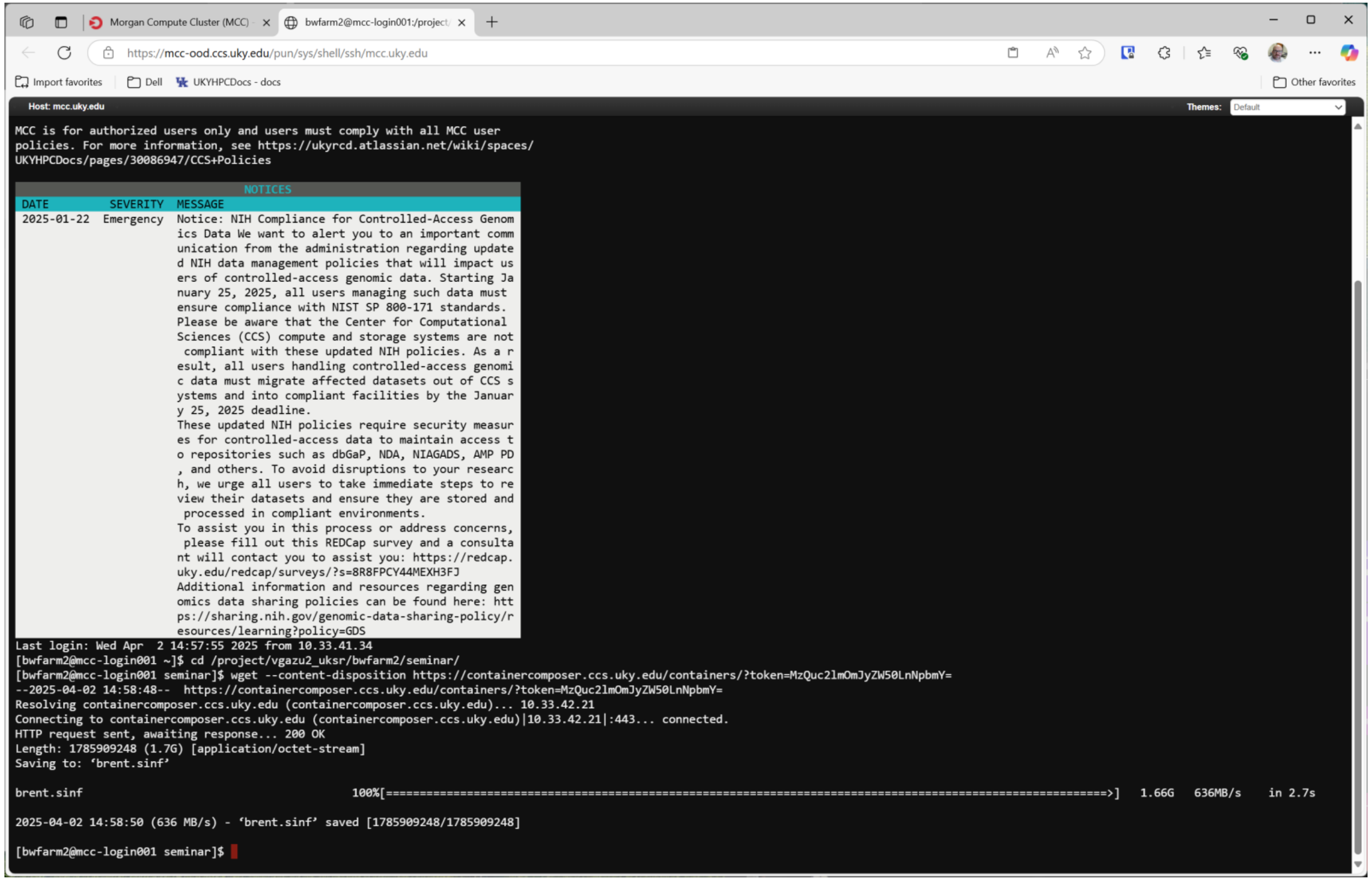
Open OnDemand



OnDemand provides an integrated, single access point for all of your HPC resources.

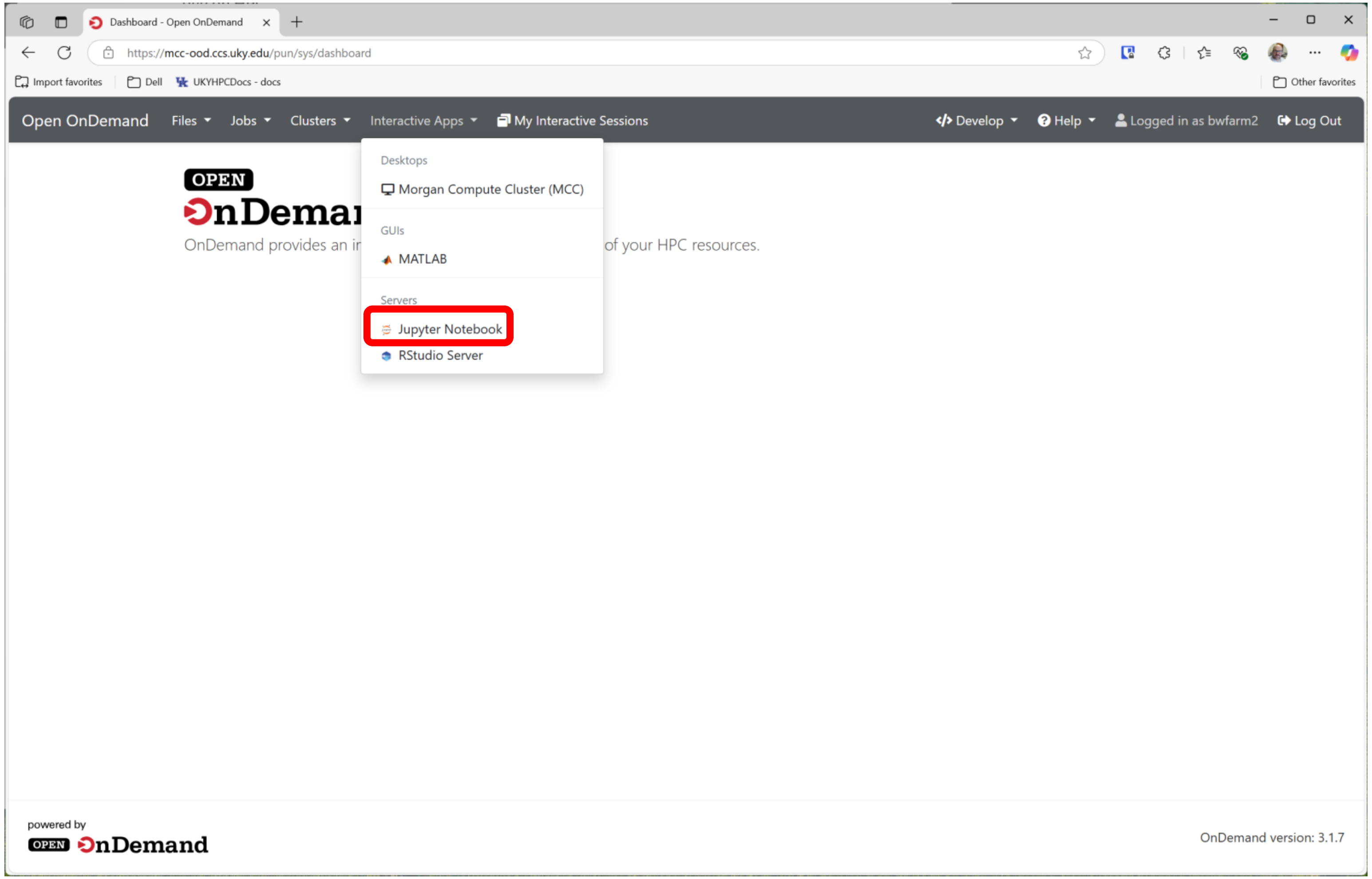
OnDemand version: 3.1.7

Open OnDemand

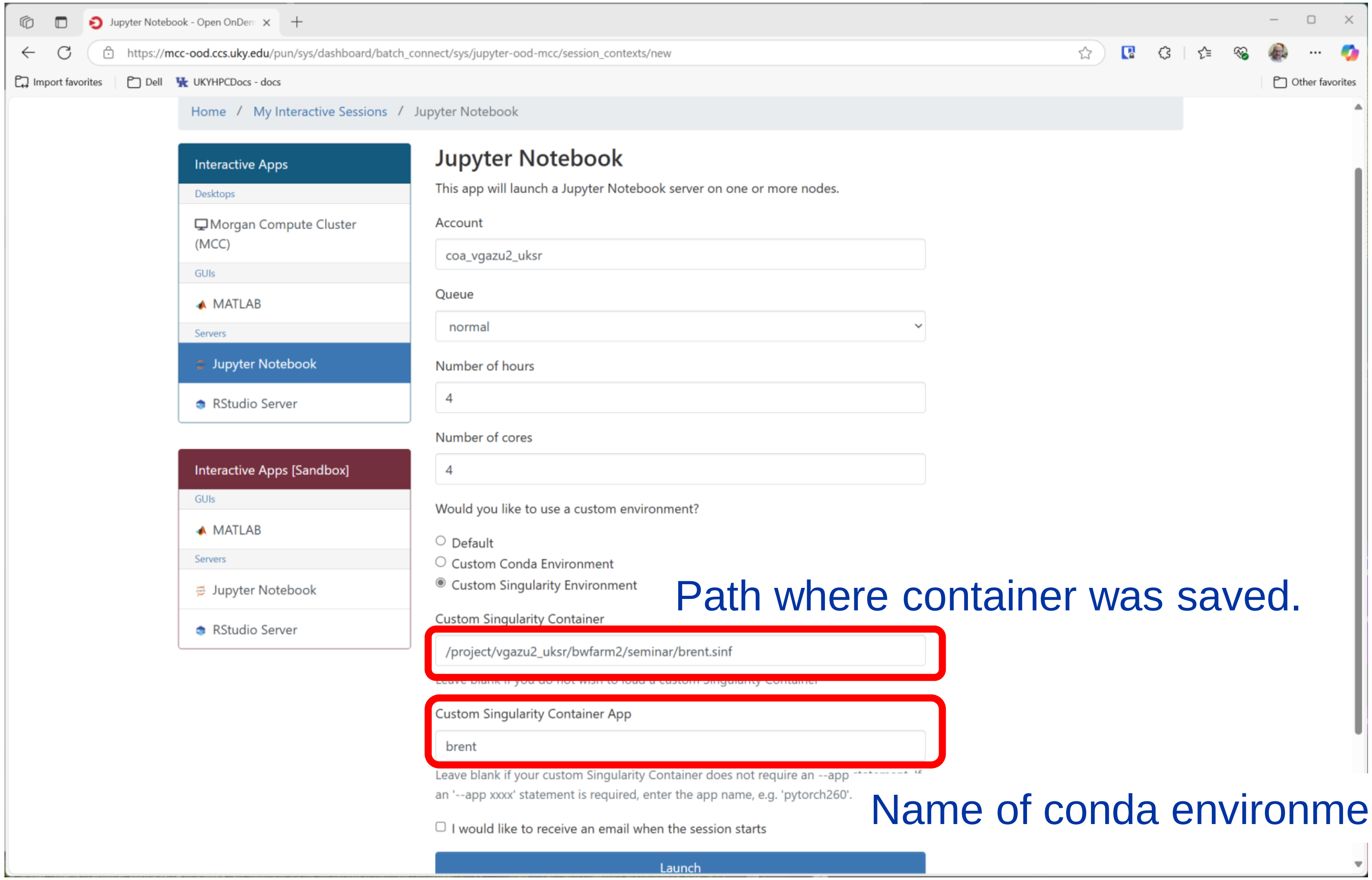


```
MCC is for authorized users only and users must comply with all MCC user
policies. For more information, see https://ukyrcd.atlassian.net/wiki/spaces/
UKYHPCDocs/pages/30086947/CCS+Policies

                                  NOTICES
 DATE         SEVERITY  MESSAGE
 2025-01-22  Emergency  Notice: NIH Compliance for Controlled-Access Genom
                        ics Data We want to alert you to an important comm
                        unication from the administration regarding update
                        d NIH data management policies that will impact us
                        ers of controlled-access genomic data. Starting Ja
                        nuary 25, 2025, all users managing such data must
                        ensure compliance with NIST SP 800-171 standards.
                        Please be aware that the Center for Computational
                        Sciences (CCS) compute and storage systems are not
                         compliant with these updated NIH policies. As a r
                        esult, all users handling controlled-access genomi
                        c data must migrate affected datasets out of CCS s
                        ystems and into compliant facilities by the Januar
                        y 25, 2025 deadline.
                        These updated NIH policies require security measur
                        es for controlled-access data to maintain access t
                        o repositories such as dbGaP, NDA, NIAGADS, AMP PD
                        , and others. To avoid disruptions to your researc
                        h, we urge all users to take immediate steps to re
                        view their datasets and ensure they are stored and
                         processed in compliant environments.
                        To assist you in this process or address concerns,
                         please fill out this REDCap survey and a consulta
                        nt will contact you to assist you: https://redcap.
                        uky.edu/redcap/surveys/?s=8R8FPCY44MEXH3FJ
                        Additional information and resources regarding gen
                        omics data sharing policies can be found here: htt
                        ps://sharing.nih.gov/genomic-data-sharing-policy/r
                        esources/learning?policy=GDS
Last login: Wed Apr  2 14:57:55 2025 from 10.33.41.34
[bwfarm2@mcc-login001 ~]$ cd /project/vgazu2_uksr/bwfarm2/seminar/
[bwfarm2@mcc-login001 seminar]$ wget --content-disposition https://containercomposer.ccs.uky.edu/containers/?token=MzQuc2lmOmJyZW50LnNpbmY=
--2025-04-02 14:58:48--  https://containercomposer.ccs.uky.edu/containers/?token=MzQuc2lmOmJyZW50LnNpbmY=
Resolving containercomposer.ccs.uky.edu (containercomposer.ccs.uky.edu)... 10.33.42.21
Connecting to containercomposer.ccs.uky.edu (containercomposer.ccs.uky.edu)|10.33.42.21|:443... connected.
HTTP request sent, awaiting response... 200 OK
Length: 1785909248 (1.7G) [application/octet-stream]
Saving to: ‘brent.sinf’

brent.sinf                                        100%[=========================================================================================================>]   1.66G   636MB/s    in 2.7s

2025-04-02 14:58:50 (636 MB/s) - ‘brent.sinf’ saved [1785909248/1785909248]

[bwfarm2@mcc-login001 seminar]$ 
```

Open OnDemand



Open OnDemand



Jupyter Notebook

This app will launch a Jupyter Notebook server on one or more nodes.

Account: coa_vgazu2_uksr

Queue: normal

Number of hours: 4

Number of cores: 4

Would you like to use a custom environment?

○ Default
○ Custom Conda Environment
● Custom Singularity Environment

Custom Singularity Container: /project/vgazu2_uksr/bwfarm2/seminar/brent.sinf

Leave blank if you do not wish to load a custom Singularity Container

Custom Singularity Container App: brent

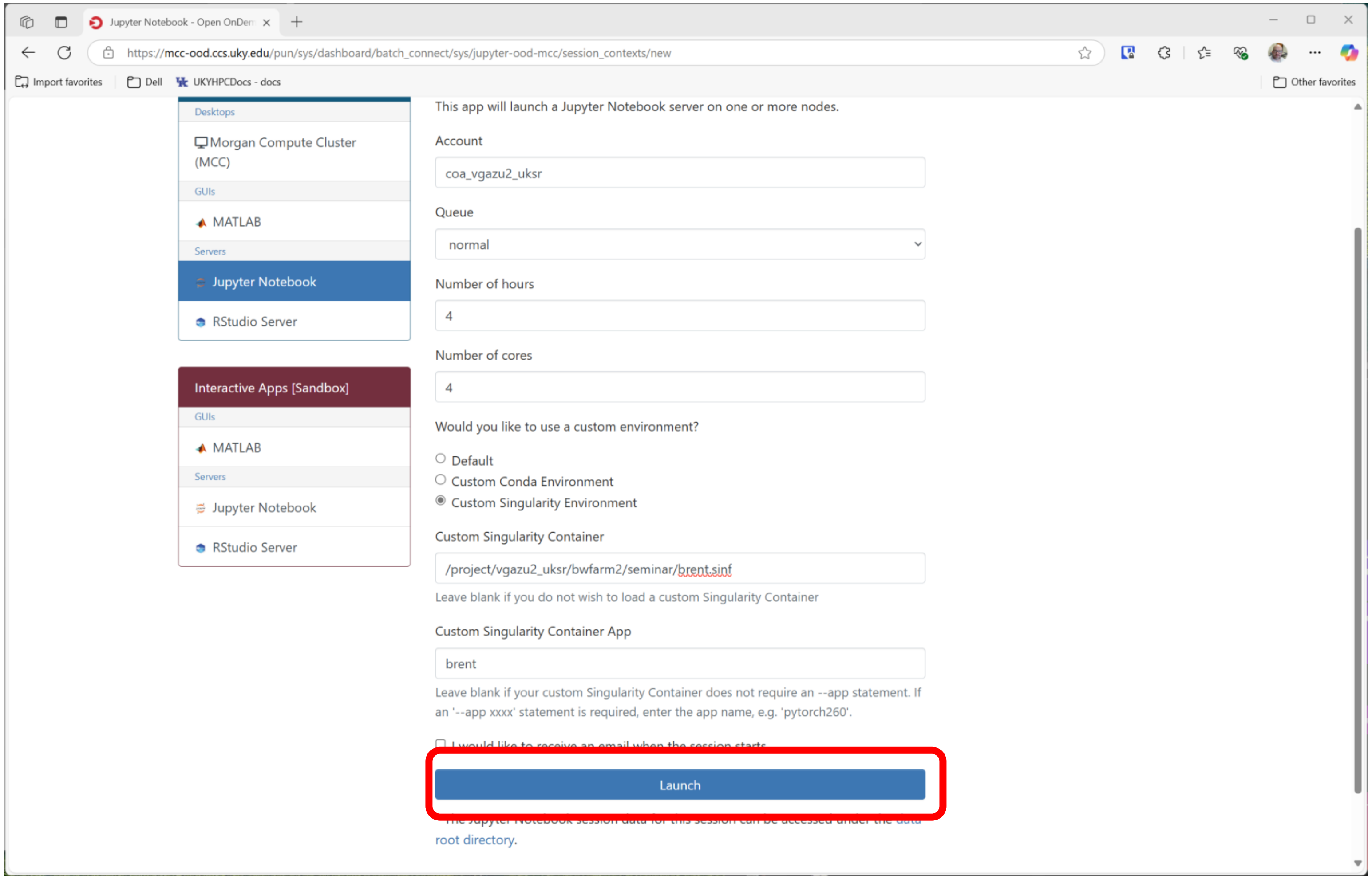
Leave blank if your custom Singularity Container does not require an --app statement. If an '--app xxxx' statement is required, enter the app name, e.g. 'pytorch260'.

☐ I would like to receive an email when the session starts

Path where container was saved.

Name of conda environment.

Open OnDemand



This app will launch a Jupyter Notebook server on one or more nodes.

Account: coa_vgazu2_uksr

Queue: normal

Number of hours: 4

Number of cores: 4

Would you like to use a custom environment?

○ Default
○ Custom Conda Environment
● Custom Singularity Environment

Custom Singularity Container: /project/vgazu2_uksr/bwfarm2/seminar/brent.sinf

Leave blank if you do not wish to load a custom Singularity Container

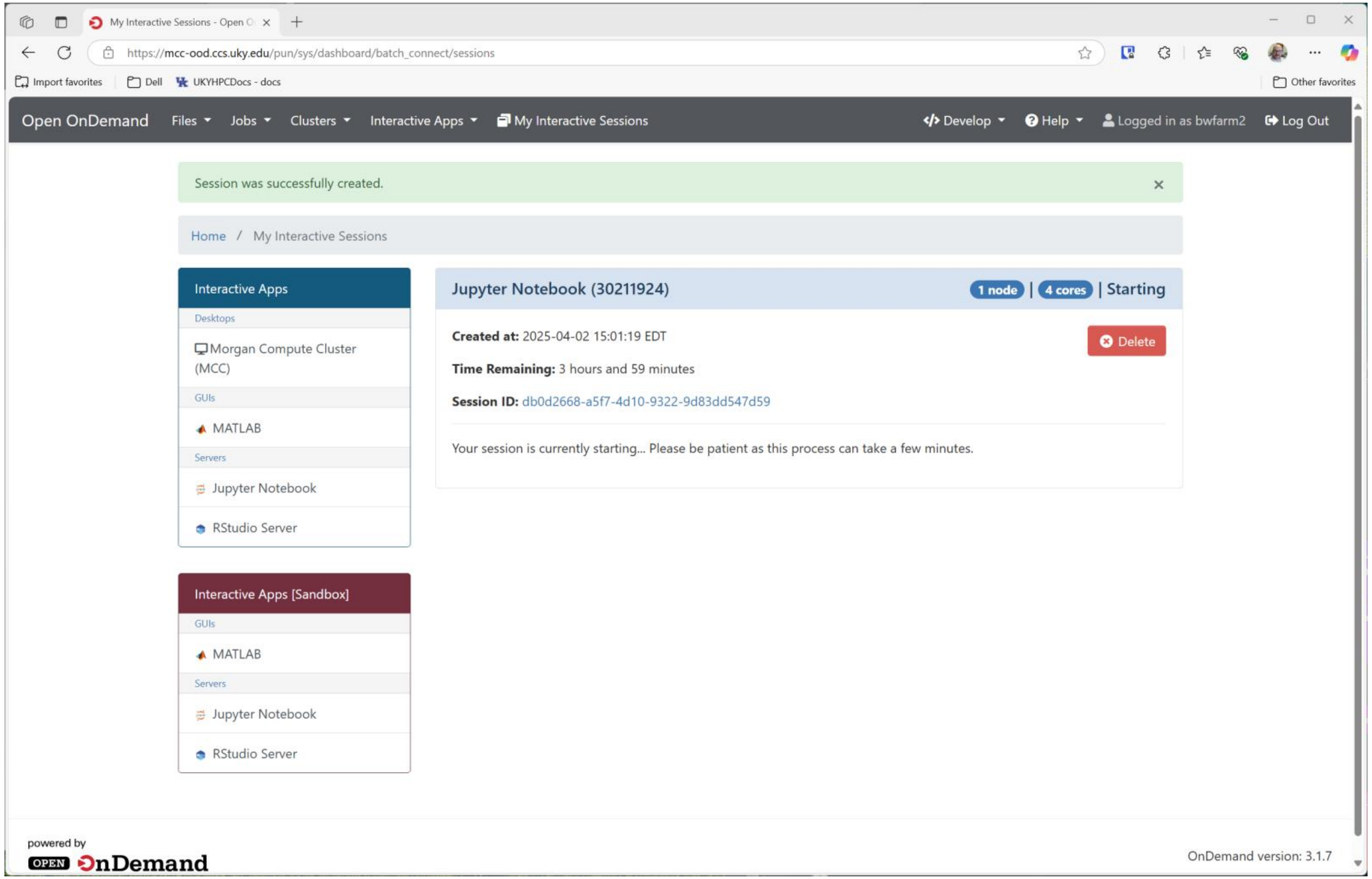
Custom Singularity Container App: brent

Leave blank if your custom Singularity Container does not require an --app statement. If an '--app xxxx' statement is required, enter the app name, e.g. 'pytorch260'.

☐ I would like to receive an email when the session starts

The Jupyter Notebook session data for this session can be accessed under the data root directory.

Open OnDemand



Session was successfully created.

Jupyter Notebook (30211924) | 1 node | 4 cores | Starting

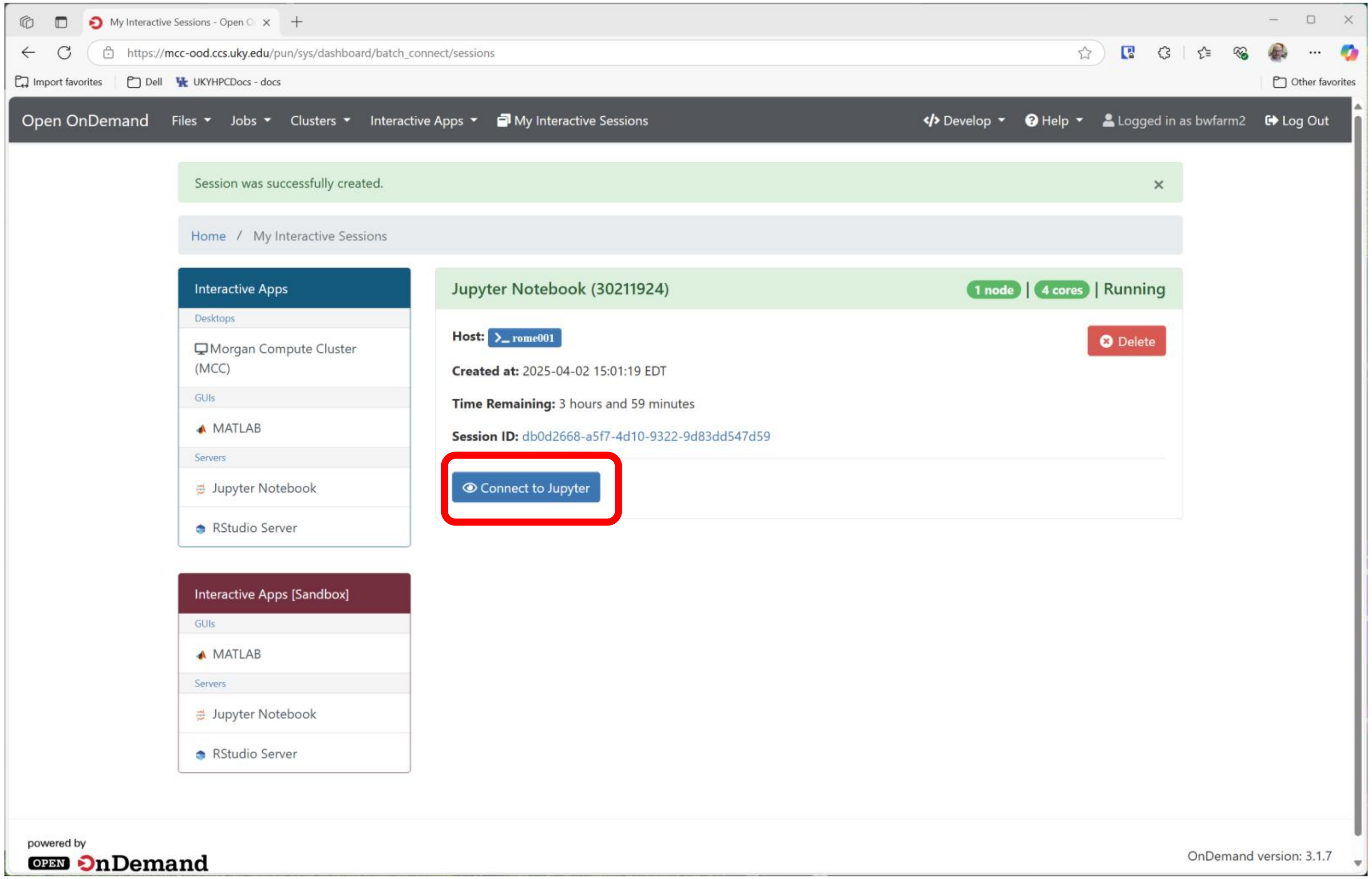
Created at: 2025-04-02 15:01:19 EDT

Time Remaining: 3 hours and 59 minutes

Session ID: db0d2668-a5f7-4d10-9322-9d83dd547d59

Your session is currently starting... Please be patient as this process can take a few minutes.

Open OnDemand



Session was successfully created.

Jupyter Notebook (30211924) 1 node | 4 cores | Running

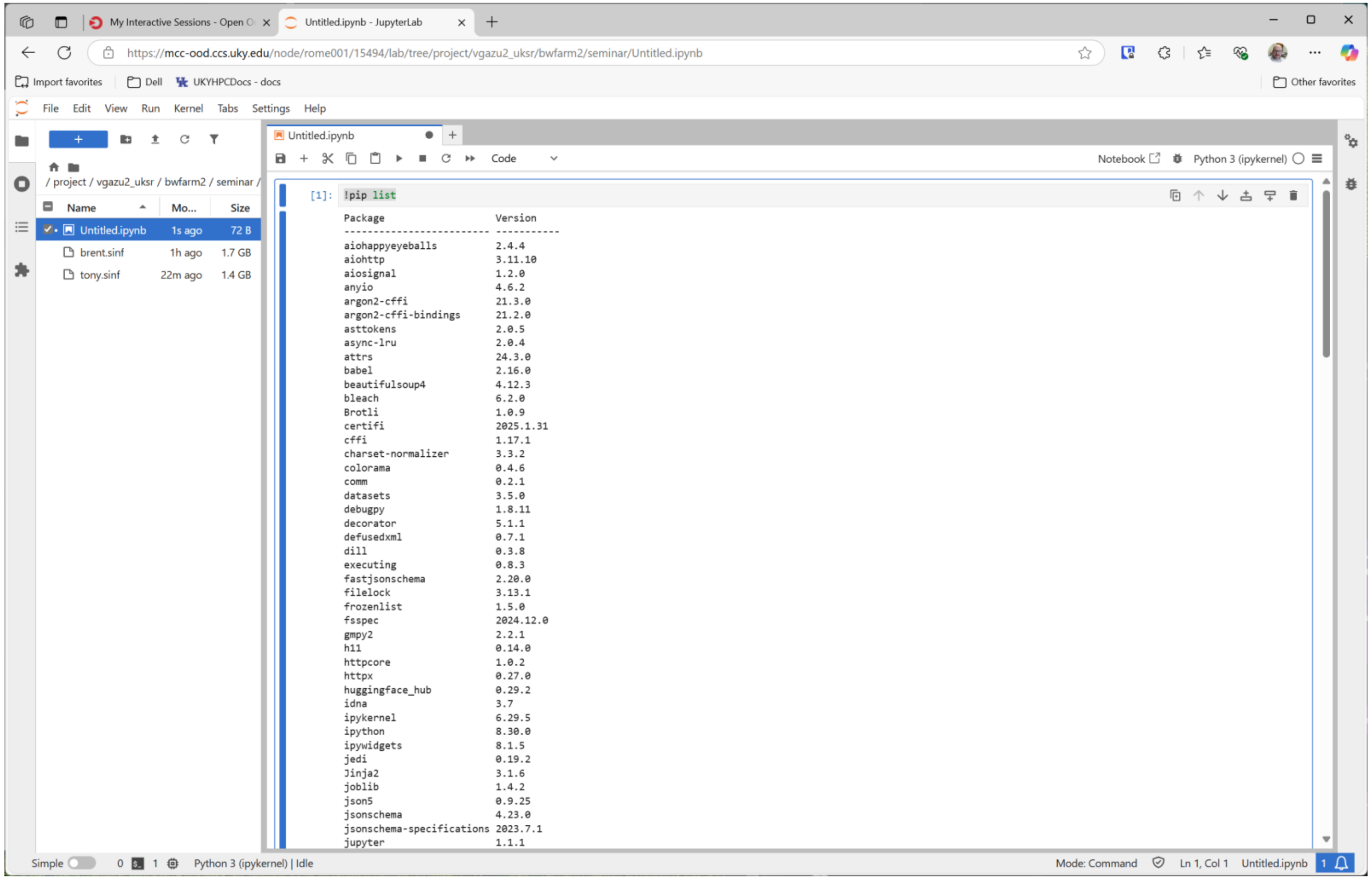
Host: rome001

Created at: 2025-04-02 15:01:19 EDT

Time Remaining: 3 hours and 59 minutes

Session ID: db0d2668-a5f7-4d10-9322-9d83dd547d59

Open OnDemand

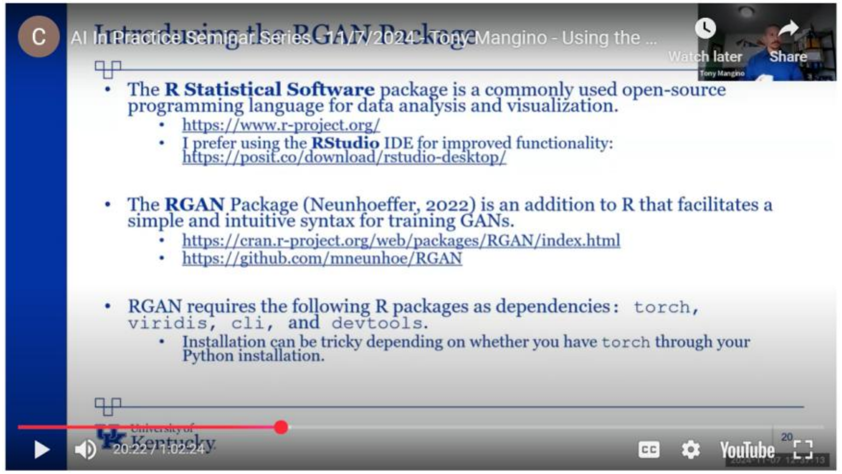


Name	Mo...	Size
Untitled.ipynb	1s ago	72 B
brent.sinf	1h ago	1.7 GB
tony.sinf	22m ago	1.4 GB

```
[1]: !pip list

Package                   Version
------------------------- ----------
aiohappyeyeballs          2.4.4
aiohttp                   3.11.10
aiosignal                 1.2.0
anyio                     4.6.2
argon2-cffi               21.3.0
argon2-cffi-bindings      21.2.0
asttokens                 2.0.5
async-lru                 2.0.4
attrs                     24.3.0
babel                     2.16.0
beautifulsoup4            4.12.3
bleach                    6.2.0
Brotli                    1.0.9
certifi                   2025.1.31
cffi                      1.17.1
charset-normalizer        3.3.2
colorama                  0.4.6
comm                      0.2.1
datasets                  3.5.0
debugpy                   1.8.11
decorator                 5.1.1
defusedxml                0.7.1
dill                      0.3.8
executing                 0.8.3
fastjsonschema            2.20.0
filelock                  3.13.1
frozenlist                1.5.0
fsspec                    2024.12.0
gmpy2                     2.2.1
h11                       0.14.0
httpcore                  1.0.2
httpx                     0.27.0
huggingface_hub           0.29.2
idna                      3.7
ipykernel                 6.29.5
ipython                   8.30.0
ipywidgets                8.1.5
jedi                      0.19.2
Jinja2                    3.1.6
joblib                    1.4.2
json5                     0.9.25
jsonschema                4.23.0
jsonschema-specifications 2023.7.1
jupyter                   1.1.1
```

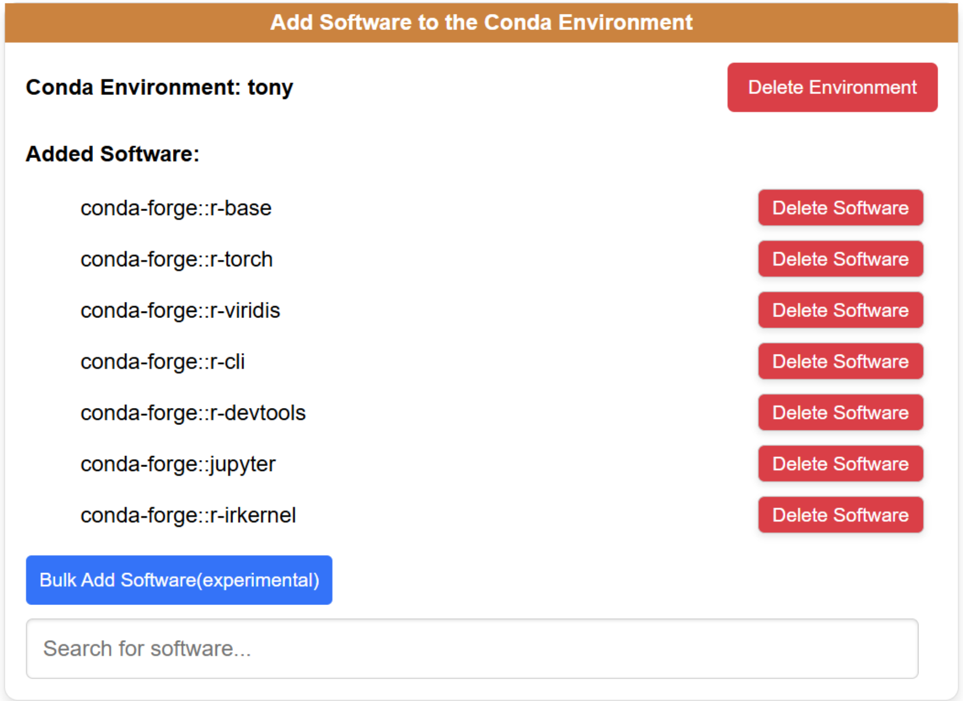
Containers for previous AI In Practice Seminars

- November 7, 2024
  - Tony Mangino, Biostatistics, UK
    - R with RGAN package
    - RGAN Dependencies
      - torch, virdis, cli, and devtools
    - We will interface with Jupyter Notebook



Introducing the RGAN Package

- The **R Statistical Software** package is a commonly used open-source programming language for data analysis and visualization.
  - https://www.r-project.org/
  - I prefer using the **RStudio** IDE for improved functionality: https://posit.co/download/rstudio-desktop/
- The **RGAN** Package (Neunhoeffer, 2022) is an addition to R that facilitates a simple and intuitive syntax for training GANs.
  - https://cran.r-project.org/web/packages/RGAN/index.html
  - https://github.com/mneunhoe/RGAN
- RGAN requires the following R packages as dependencies: `torch`, `viridis`, `cli`, and `devtools`.
  - Installation can be tricky depending on whether you have `torch` through your Python installation.



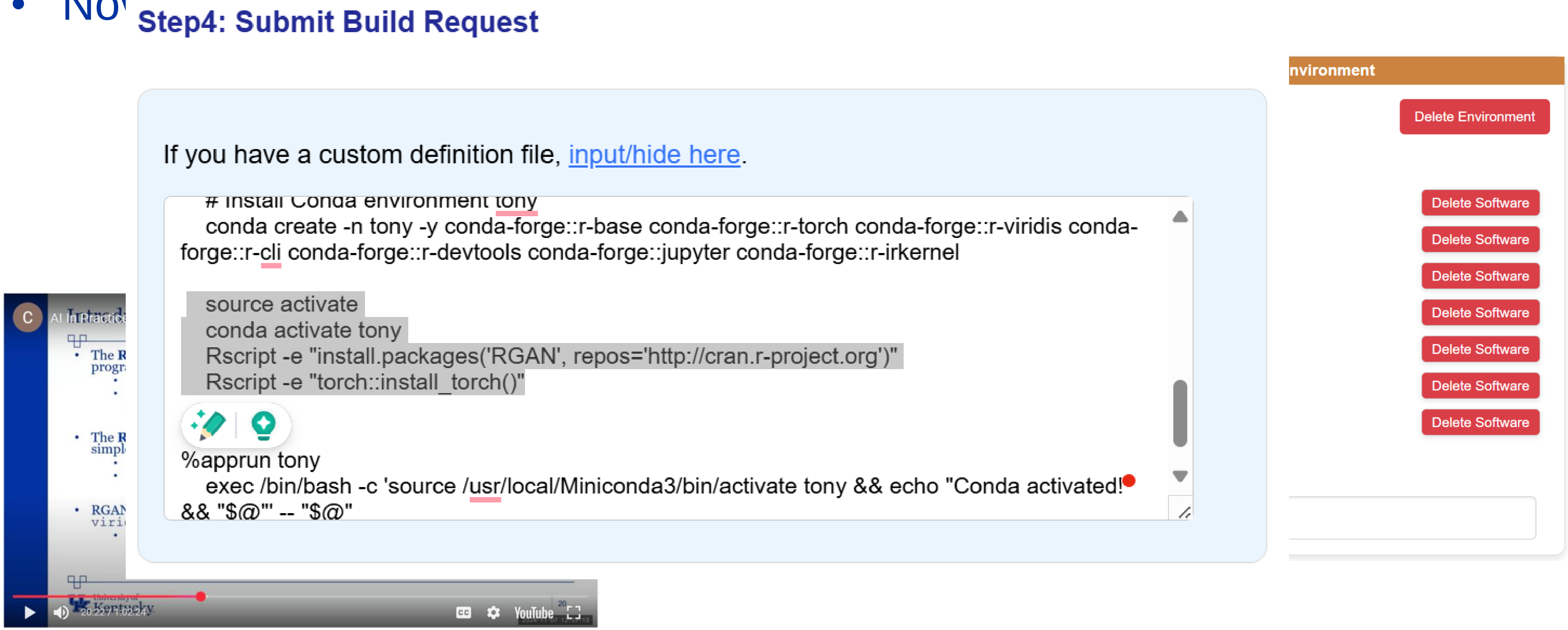
Conda Environment: tony

Added Software:

conda-forge::r-base
conda-forge::r-torch
conda-forge::r-viridis
conda-forge::r-cli
conda-forge::r-devtools
conda-forge::jupyter
conda-forge::r-irkernel

Containers for previous AI In Practice Seminars

- November 7, 2024

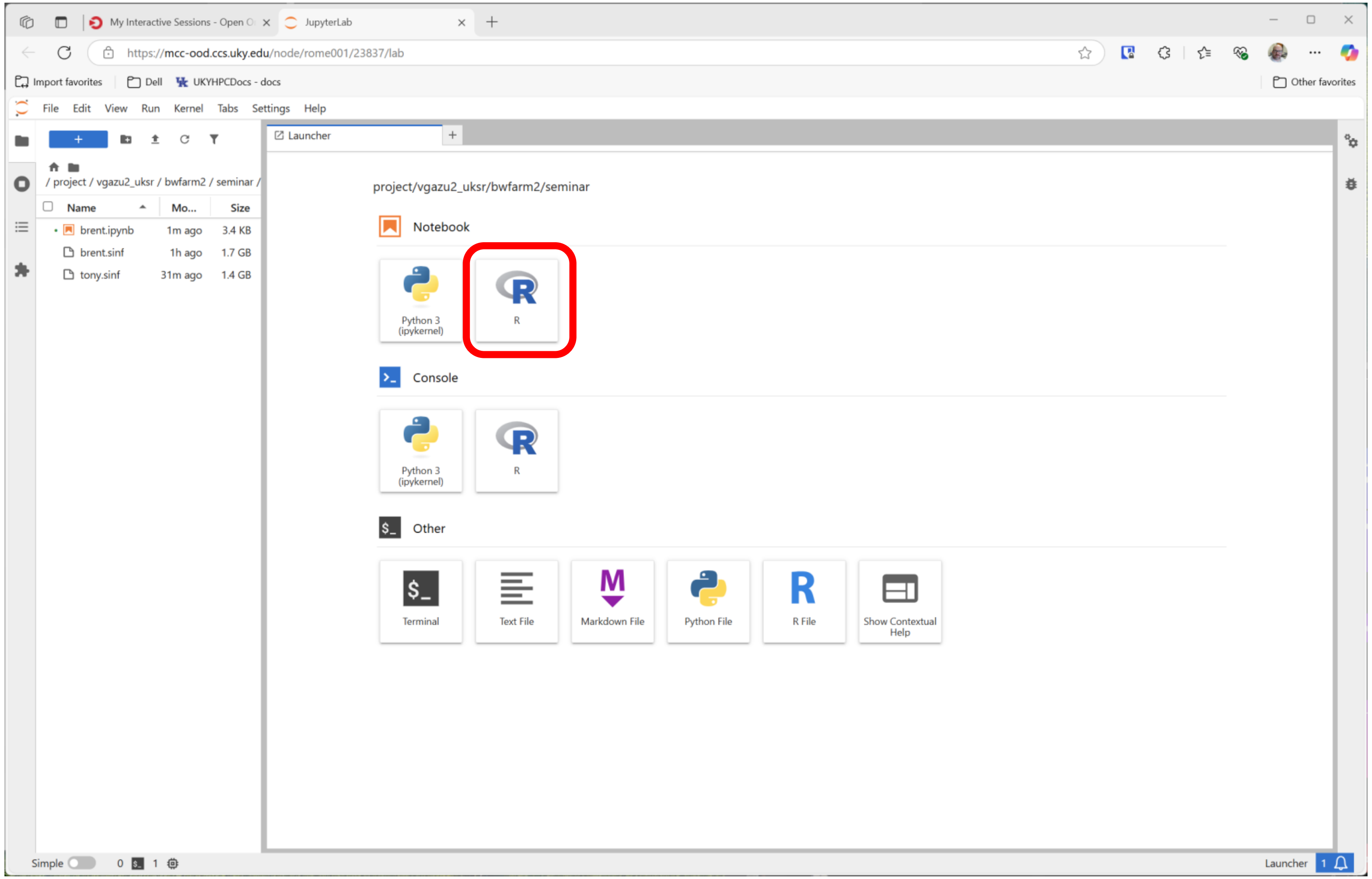


Step4: Submit Build Request

If you have a custom definition file, input/hide here.

```
   # Install Conda environment tony
   conda create -n tony -y conda-forge::r-base conda-forge::r-torch conda-forge::r-viridis conda-forge::r-cli conda-forge::r-devtools conda-forge::jupyter conda-forge::r-irkernel

   source activate
   conda activate tony
   Rscript -e "install.packages('RGAN', repos='http://cran.r-project.org')"
   Rscript -e "torch::install_torch()"

%apprun tony
   exec /bin/bash -c 'source /usr/local/Miniconda3/bin/activate tony && echo "Conda activated!"
&& "$@"' -- "$@"
```

Open OnDemand



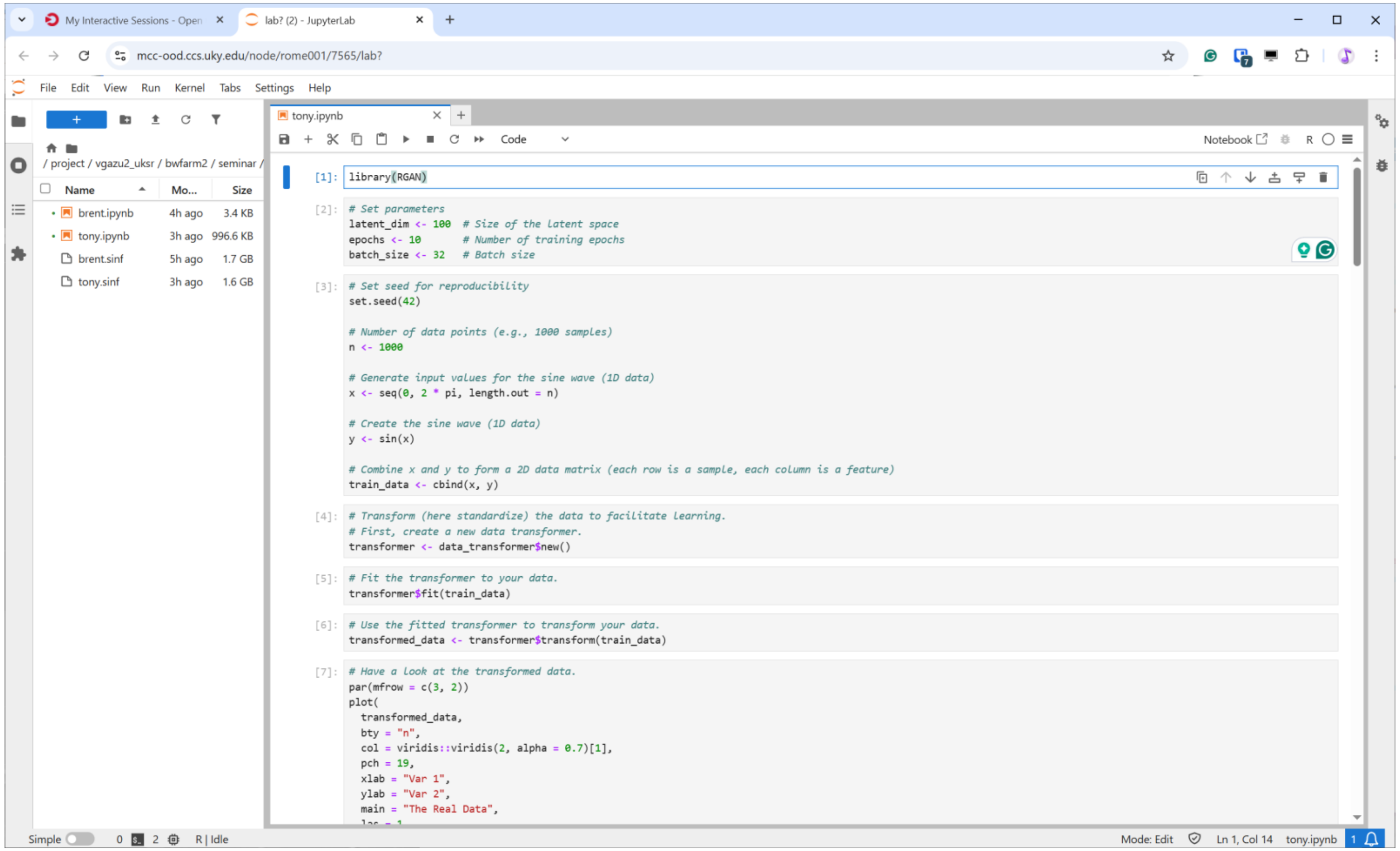
https://mcc-ood.ccs.uky.edu/node/rome001/23837/lab

/ project / vgazu2_uksr / bwfarm2 / seminar /

Name	Mo...	Size
brent.ipynb	1m ago	3.4 KB
brent.sinf	1h ago	1.7 GB
tony.sinf	31m ago	1.4 GB

project/vgazu2_uksr/bwfarm2/seminar

Open OnDemand

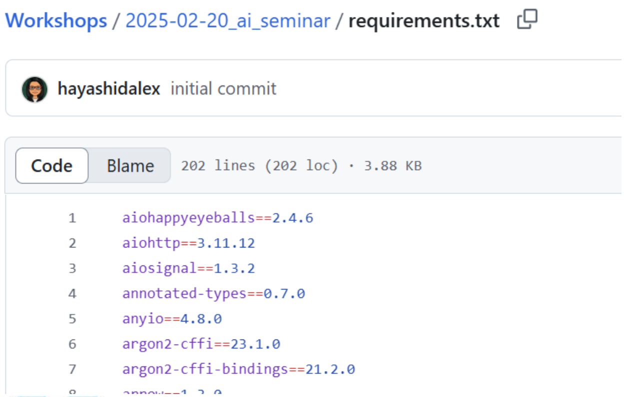


Name	Mo...	Size
brent.ipynb	4h ago	3.4 KB
tony.ipynb	3h ago	996.6 KB
brent.sinf	5h ago	1.7 GB
tony.sinf	3h ago	1.6 GB

```
[1]: library(RGAN)

[2]: # Set parameters
     latent_dim <- 100  # Size of the latent space
     epochs <- 10       # Number of training epochs
     batch_size <- 32   # Batch size

[3]: # Set seed for reproducibility
     set.seed(42)

     # Number of data points (e.g., 1000 samples)
     n <- 1000

     # Generate input values for the sine wave (1D data)
     x <- seq(0, 2 * pi, length.out = n)

     # Create the sine wave (1D data)
     y <- sin(x)

     # Combine x and y to form a 2D data matrix (each row is a sample, each column is a feature)
     train_data <- cbind(x, y)

[4]: # Transform (here standardize) the data to facilitate learning.
     # First, create a new data transformer.
     transformer <- data_transformer$new()

[5]: # Fit the transformer to your data.
     transformer$fit(train_data)

[6]: # Use the fitted transformer to transform your data.
     transformed_data <- transformer$transform(train_data)

[7]: # Have a look at the transformed data.
     par(mfrow = c(3, 2))
     plot(
       transformed_data,
       bty = "n",
       col = viridis::viridis(2, alpha = 0.7)[1],
       pch = 19,
       xlab = "Var 1",
       ylab = "Var 2",
       main = "The Real Data",
       las = 1
```

Containers for previous AI In Practice Seminars

- February 20, 2025
  - Mami Hayashida (ITS) and Vikram Gazula (CCS), UK
    - Conda Environment with ollama installed
    - Python Packages:
      - ollama langchain_core langchain_ollama langchain_chroma langchain langchain_huggingface langchain_community typing typing_extensions langgraph Ipython
    - Has a requirements.txt file!

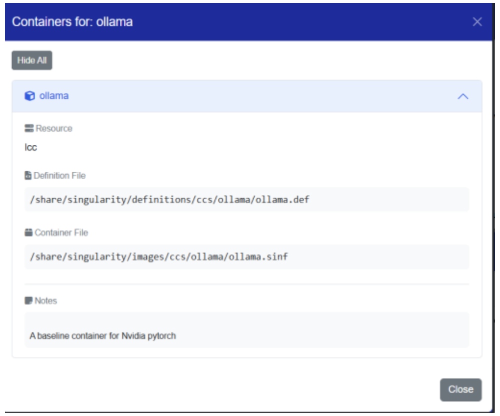


Workshops / 2025-02-20_ai_seminar / requirements.txt

hayashidalex initial commit

202 lines (202 loc) · 3.88 KB

```
aiohappyeyeballs==2.4.6
aiohttp==3.11.12
aiosignal==1.3.2
annotated-types==0.7.0
anyio==4.8.0
argon2-cffi==23.1.0
argon2-cffi-bindings==21.2.0
```



Containers for: ollama

Resource: lcc

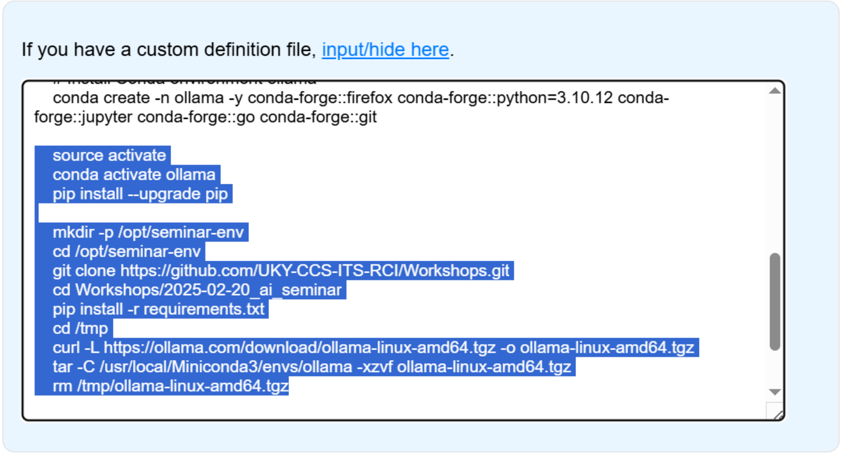
Definition File: `/share/singularity/definitions/ccs/ollama/ollama.def`

Container File: `/share/singularity/images/ccs/ollama/ollama.sinf`

Notes: A baseline container for Nvidia pytorch

From SDS

Step4: Submit Build Request



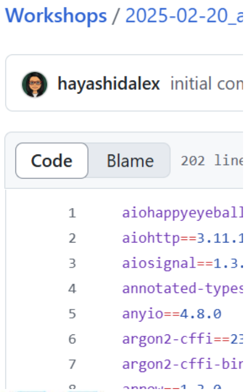
If you have a custom definition file, input/hide here.

```
    conda create -n ollama -y conda-forge::firefox conda-forge::python=3.10.12 conda-
forge::jupyter conda-forge::go conda-forge::git

    source activate
    conda activate ollama
    pip install --upgrade pip

    mkdir -p /opt/seminar-env
    cd /opt/seminar-env
    git clone https://github.com/UKY-CCS-ITS-RCI/Workshops.git
    cd Workshops/2025-02-20_ai_seminar
    pip install -r requirements.txt
    cd /tmp
    curl -L https://ollama.com/download/ollama-linux-amd64.tgz -o ollama-linux-amd64.tgz
    tar -C /usr/local/Miniconda3/envs/ollama -xzvf ollama-linux-amd64.tgz
    rm /tmp/ollama-linux-amd64.tgz
```

Containers for previous AI In Practice Seminars

- Febr
  -

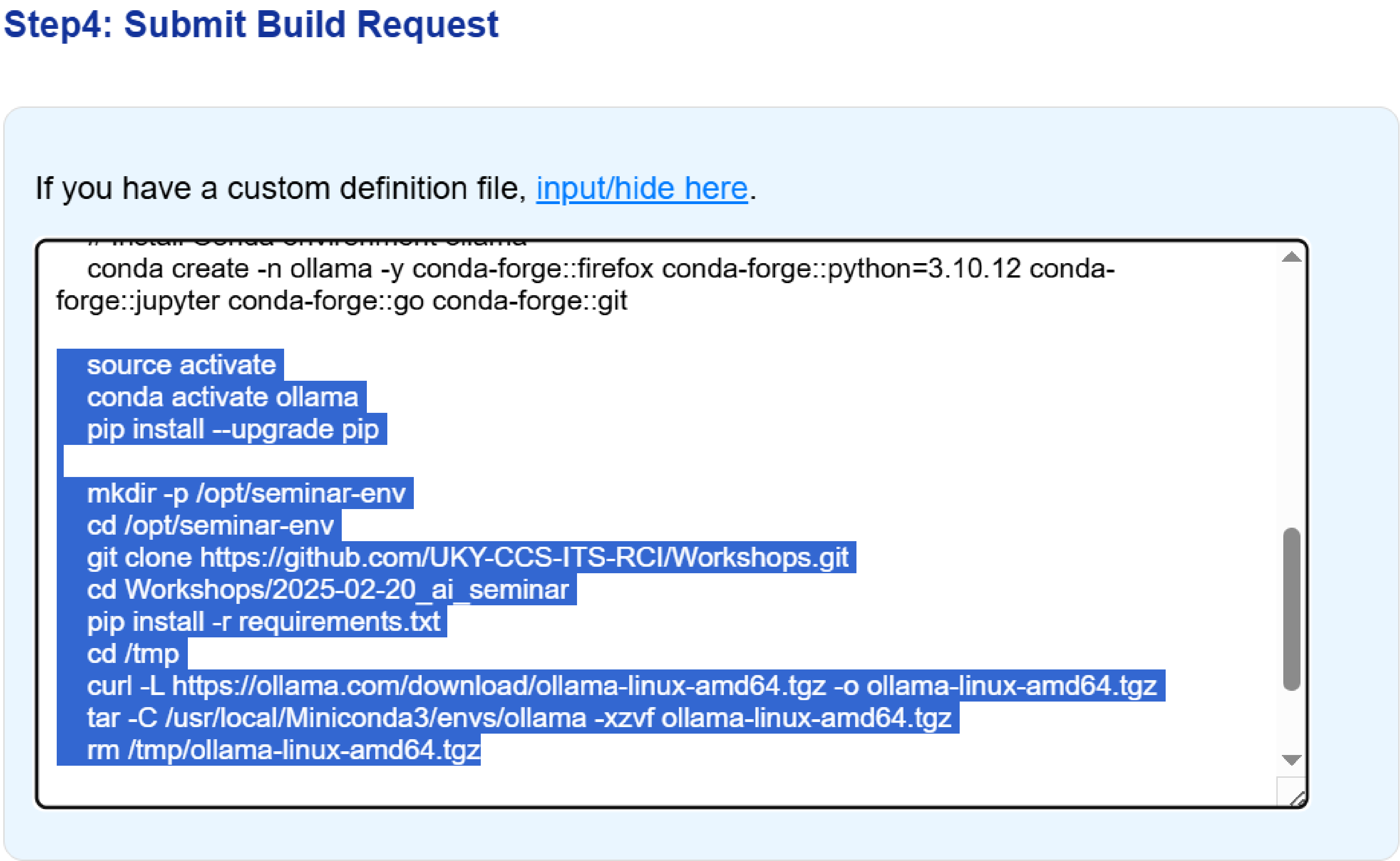
langchain_huggingface



Workshops / 2025-02-20_a

hayashidalex initial con

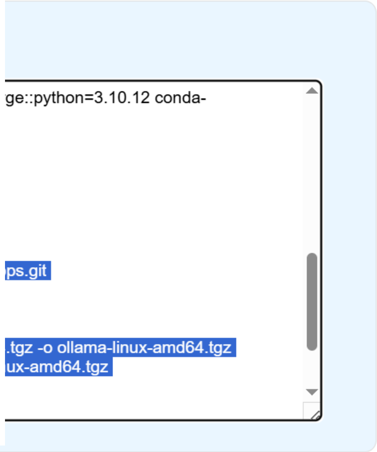
```
aiohappyeyeball
aiohttp==3.11.1
aiosignal==1.3.
annotated-types
anyio==4.8.0
argon2-cffi==23
argon2-cffi-bir
```



Step4: Submit Build Request

If you have a custom definition file, input/hide here.

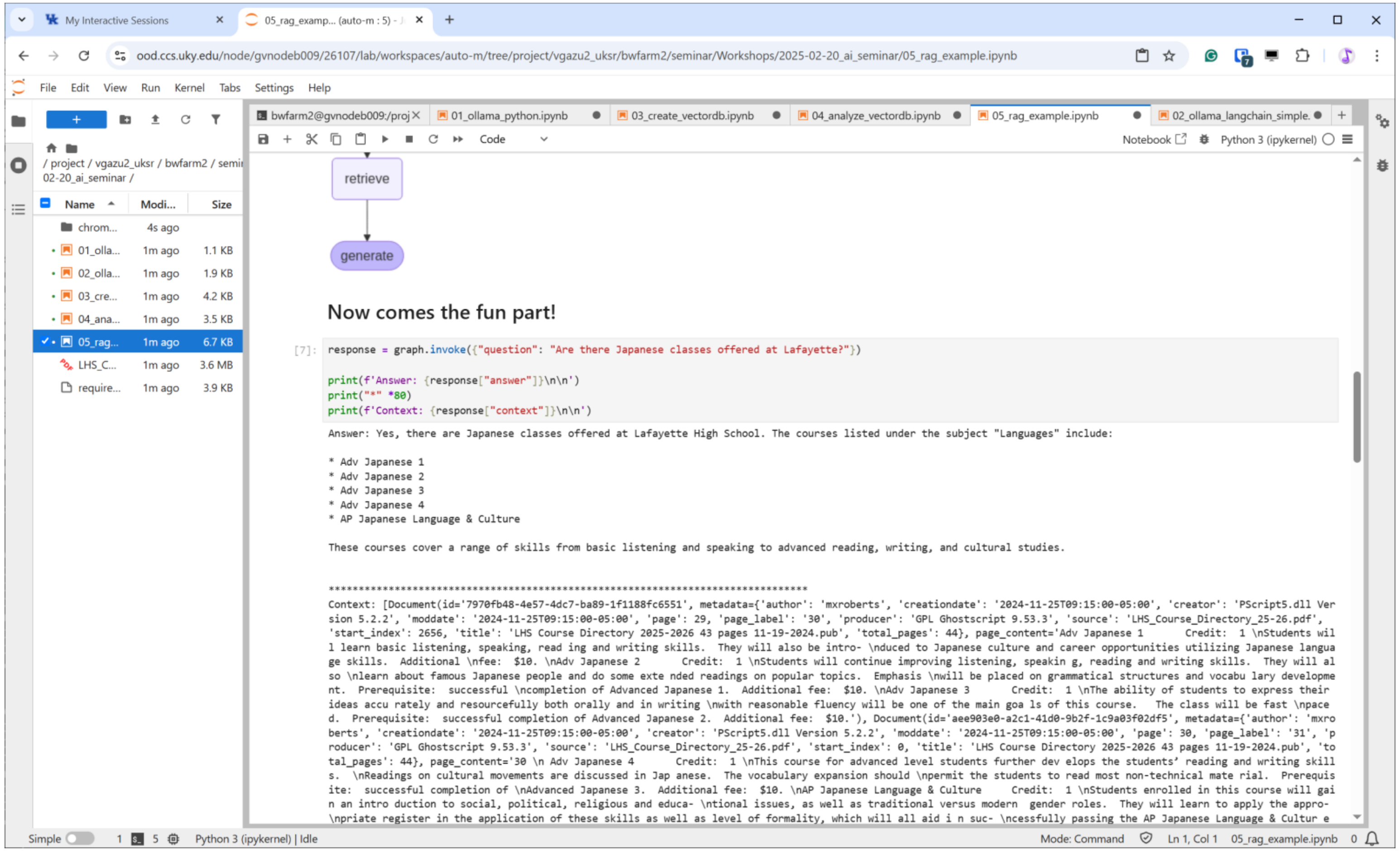
```
   conda create -n ollama -y conda-forge::firefox conda-forge::python=3.10.12 conda-
forge::jupyter conda-forge::go conda-forge::git

   source activate
   conda activate ollama
   pip install --upgrade pip

   mkdir -p /opt/seminar-env
   cd /opt/seminar-env
   git clone https://github.com/UKY-CCS-ITS-RCI/Workshops.git
   cd Workshops/2025-02-20_ai_seminar
   pip install -r requirements.txt
   cd /tmp
   curl -L https://ollama.com/download/ollama-linux-amd64.tgz -o ollama-linux-amd64.tgz
   tar -C /usr/local/Miniconda3/envs/ollama -xzvf ollama-linux-amd64.tgz
   rm /tmp/ollama-linux-amd64.tgz
```



```
ge::python=3.10.12 conda-

ps.git

.tgz -o ollama-linux-amd64.tgz
ux-amd64.tgz
```

From SDS

Open OnDemand



Name	Modi...	Size
chrom...	4s ago	
01_olla...	1m ago	1.1 KB
02_olla...	1m ago	1.9 KB
03_cre...	1m ago	4.2 KB
04_ana...	1m ago	3.5 KB
05_rag...	1m ago	6.7 KB
LHS_C...	1m ago	3.6 MB
require...	1m ago	3.9 KB

Now comes the fun part!

```python
[7]: response = graph.invoke({"question": "Are there Japanese classes offered at Lafayette?"})

print(f'Answer: {response["answer"]}\n\n')
print("*" *80)
print(f'Context: {response["context"]}\n\n')
```

```
Answer: Yes, there are Japanese classes offered at Lafayette High School. The courses listed under the subject "Languages" include:

* Adv Japanese 1
* Adv Japanese 2
* Adv Japanese 3
* Adv Japanese 4
* AP Japanese Language & Culture

These courses cover a range of skills from basic listening and speaking to advanced reading, writing, and cultural studies.


********************************************************************************
Context: [Document(id='7970fb48-4e57-4dc7-ba89-1f1188fc6551', metadata={'author': 'mxroberts', 'creationdate': '2024-11-25T09:15:00-05:00', 'creator': 'PScript5.dll Ver
sion 5.2.2', 'moddate': '2024-11-25T09:15:00-05:00', 'page': 29, 'page_label': '30', 'producer': 'GPL Ghostscript 9.53.3', 'source': 'LHS_Course_Directory_25-26.pdf',
'start_index': 2656, 'title': 'LHS Course Directory 2025-2026 43 pages 11-19-2024.pub', 'total_pages': 44}, page_content='Adv Japanese 1      Credit:  1 \nStudents wil
l learn basic listening, speaking, read ing and writing skills.  They will also be intro- \nduced to Japanese culture and career opportunities utilizing Japanese langua
ge skills.  Additional \nfee:  $10. \nAdv Japanese 2      Credit:  1 \nStudents will continue improving listening, speakin g, reading and writing skills.  They will al
so \nlearn about famous Japanese people and do some exte nded readings on popular topics.  Emphasis \nwill be placed on grammatical structures and vocabu lary developme
nt.  Prerequisite:  successful \ncompletion of Advanced Japanese 1.  Additional fee:  $10. \nAdv Japanese 3      Credit:  1 \nThe ability of students to express their
ideas accu rately and resourcefully both orally and in writing \nwith reasonable fluency will be one of the main goa ls of this course.   The class will be fast \npace
d.  Prerequisite:  successful completion of Advanced Japanese 2.  Additional fee:  $10.'), Document(id='aee903e0-a2c1-41d0-9b2f-1c9a03f02df5', metadata={'author': 'mxro
berts', 'creationdate': '2024-11-25T09:15:00-05:00', 'creator': 'PScript5.dll Version 5.2.2', 'moddate': '2024-11-25T09:15:00-05:00', 'page': 30, 'page_label': '31', 'p
roducer': 'GPL Ghostscript 9.53.3', 'source': 'LHS_Course_Directory_25-26.pdf', 'start_index': 0, 'title': 'LHS Course Directory 2025-2026 43 pages 11-19-2024.pub', 'to
tal_pages': 44}, page_content='30 \n Adv Japanese 4      Credit:  1 \nThis course for advanced level students further dev elops the students’ reading and writing skill
s.  \nReadings on cultural movements are discussed in Jap anese.  The vocabulary expansion should \npermit the students to read most non-technical mate rial.  Prerequis
ite:  successful completion of \nAdvanced Japanese 3.  Additional fee:  $10. \nAP Japanese Language & Culture     Credit:  1 \nStudents enrolled in this course will gai
n an intro duction to social, political, religious and educa- \ntional issues, as well as traditional versus modern  gender roles.  They will learn to apply the appro-
\npriate register in the application of these skills as well as level of formality, which will all aid i n suc- \ncessfully passing the AP Japanese Language & Cultur e
```

University of Kentucky

Conclusions

- ***Navigating HPC software can be challenging.*** The Software Discovery Service helps researchers quickly find the tools they need.
- ***Containerization enhances reproducibility and collaboration.*** Isolated environments ensure consistency across systems.
- ***The Singularity Container Composer simplifies container creation***, making it accessible to all users.

- All containers/notebooks demo'd are available on MCC/LCC:
  `/share/examples/MCC/AI-In-Practice-Seminars`
  `/share/examples/LCC/AI-In-Practice-Seminars`

Thanks

- Sandesh Lamichhane and the UK ACCESS-CI students for their work on the “Software Discovery Service” tool.

- Pinyi Shi for his work on the “Singularity Container Composer”.

- Mami Hayashida and Vikram Gazula for the RAG notebooks.

Questions?