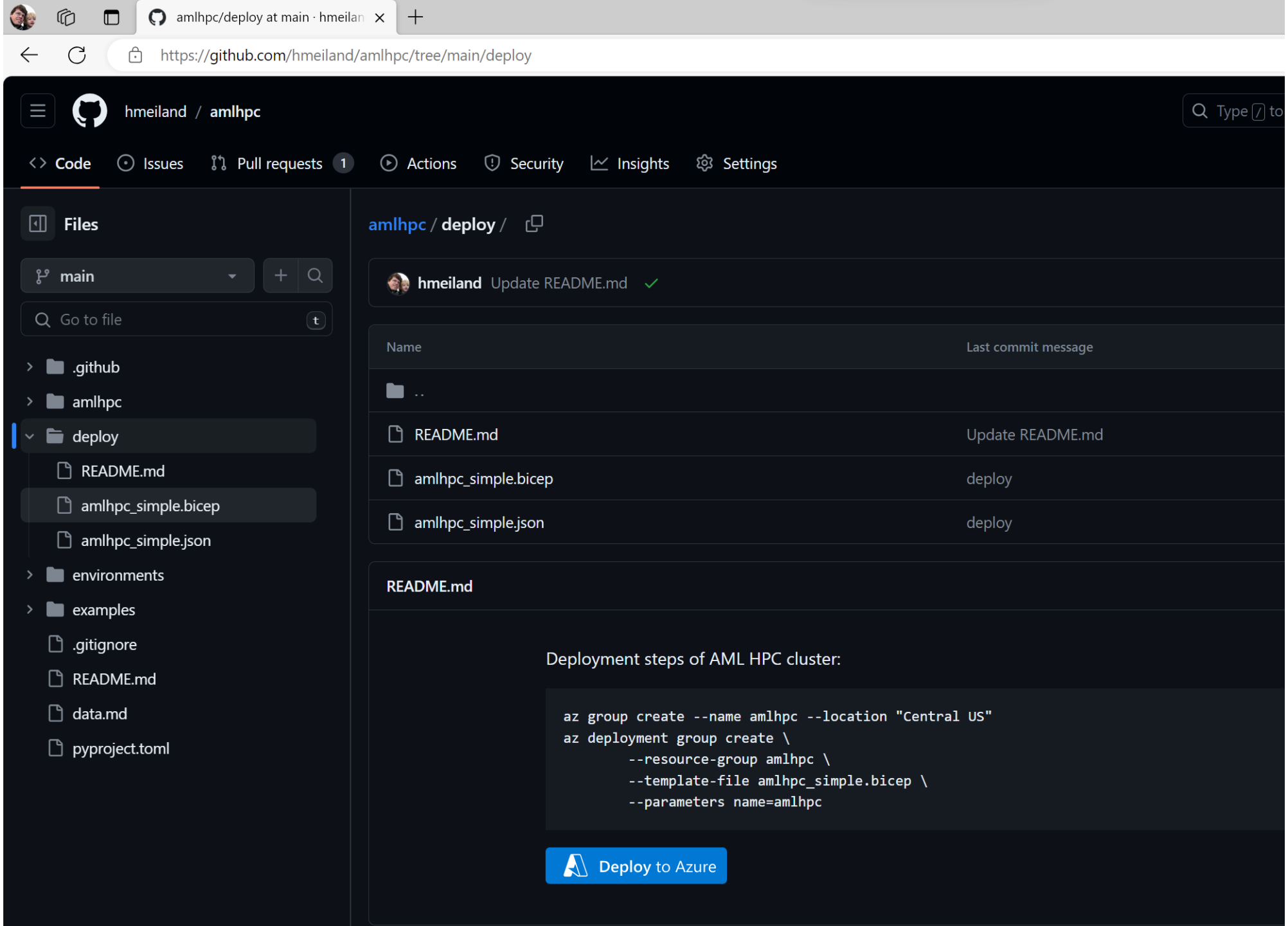
AML***HPC***
EESSI demo


amlhpc/deploy at main · hmeilan
https://github.com/hmeiland/amlhpc/tree/main/deploy
hmeiland / amlhpc
Type / to
Code
Issues
Pull requests 1
Actions
Security
Insights
Settings
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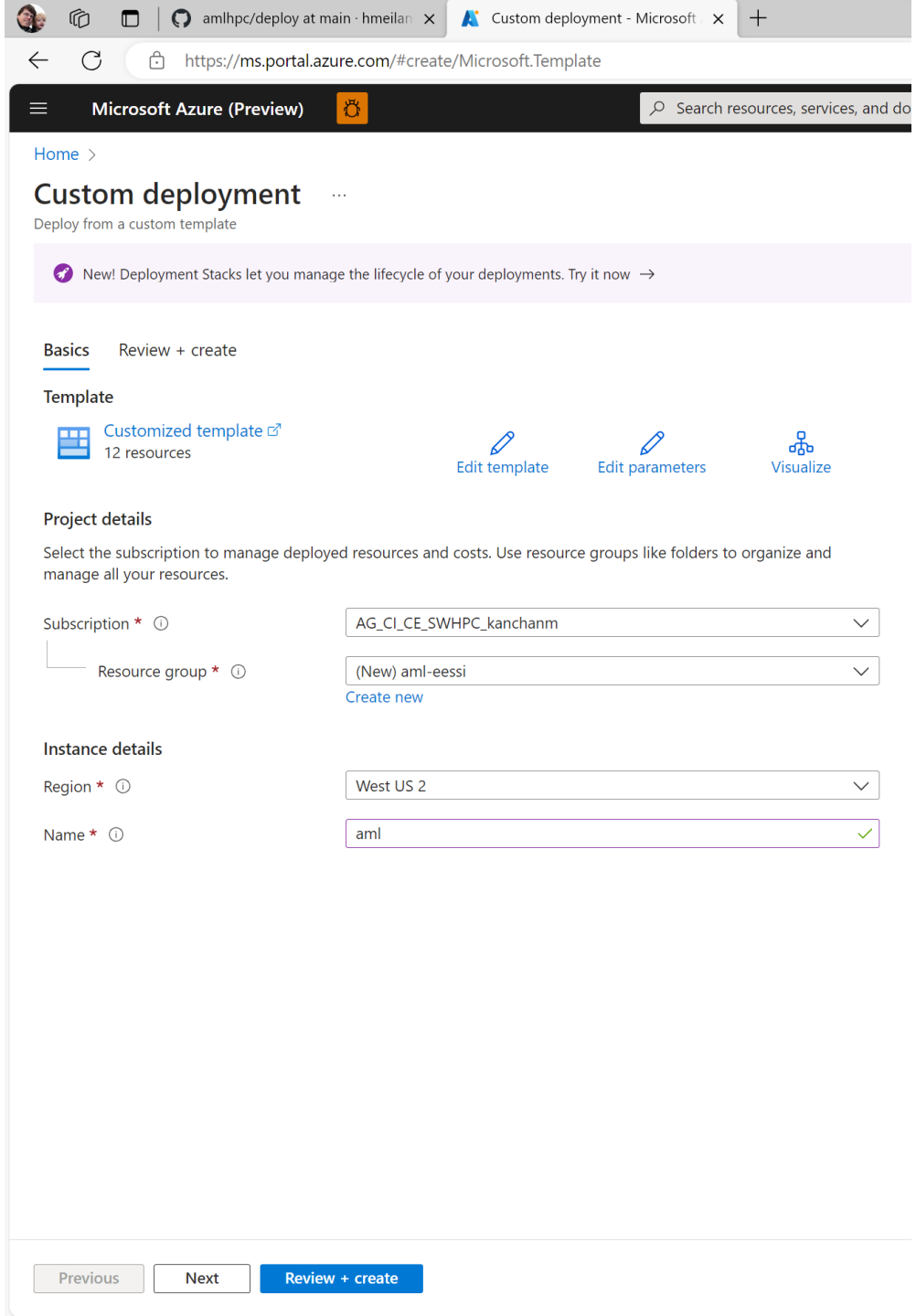
main
Go to file t
.github
amlhpc
deploy
README.md
amlhpc_simple.bicep
amlhpc_simple.json
environments
examples
.gitignore
README.md
data.md
pyproject.toml
amlhpc / deploy /
hmeiland Update README.md
Name
Last commit message
..
README.md
Update README.md
amlhpc_simple.bicep
deploy
amlhpc_simple.json
deploy
README.md
Deployment steps of AML HPC cluster:
az group create --name amlhpc --location "Central US"
az deployment group create \
--resource-group amlhpc \
--template-file amlhpc_simple.bicep \
--parameters name=amlhpc
Deploy to Azure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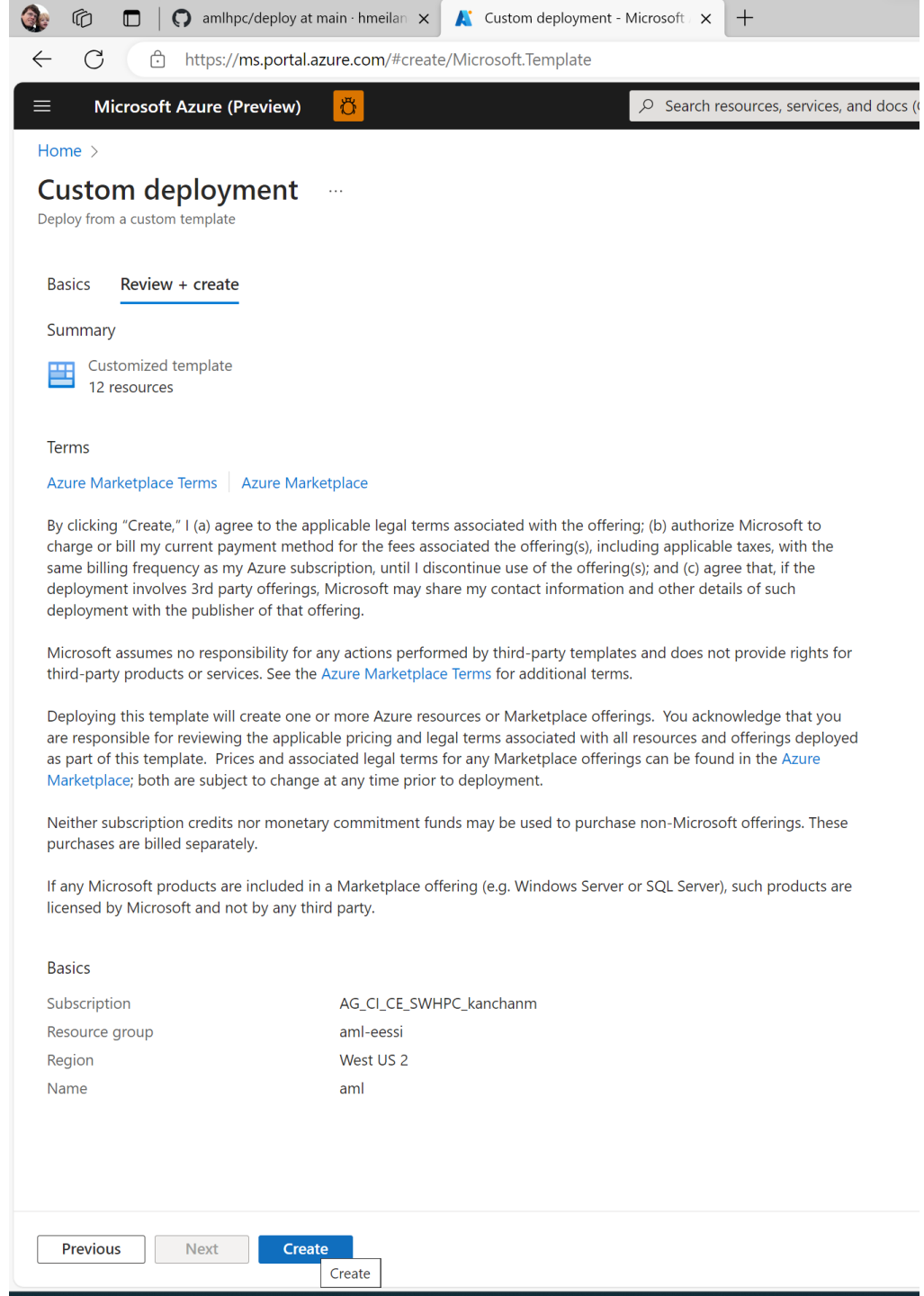
Custom deployment - Microsoft
https://ms.portal.azure.com/#create/Microsoft.Template
Microsoft Azure (Preview)
Search resources, services, and do
Home
Custom deployment
Deploy from a custom template
New! Deployment Stacks let you manage the lifecycle of your deployments. Try it now
Basics
Review + create
Template
Customized template
12 resources
Edit template
Edit parameters
Visualize
Project details
Select the subscription to manage deployed resources and costs. Use resource groups like folders to organize and manage all your resources.
Subscription *
AG_CI_CE_SWHPC_kanchanm
Resource group *
(New) aml-eessi
Create new
Instance details
Region *
West US 2
Name *
aml
Previous
Next
Review + create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Custom deployment - Microsoft
https://ms.portal.azure.com/#create/Microsoft.Template
Microsoft Azure (Preview)
Search resources, services, and docs
Home
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Deploy from a custom template
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Review + create
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Basics
Subscription
AG_CI_CE_SWHPC_kanchanm
Resource group
aml-eessi
Region
West US 2
Name
aml
Previous
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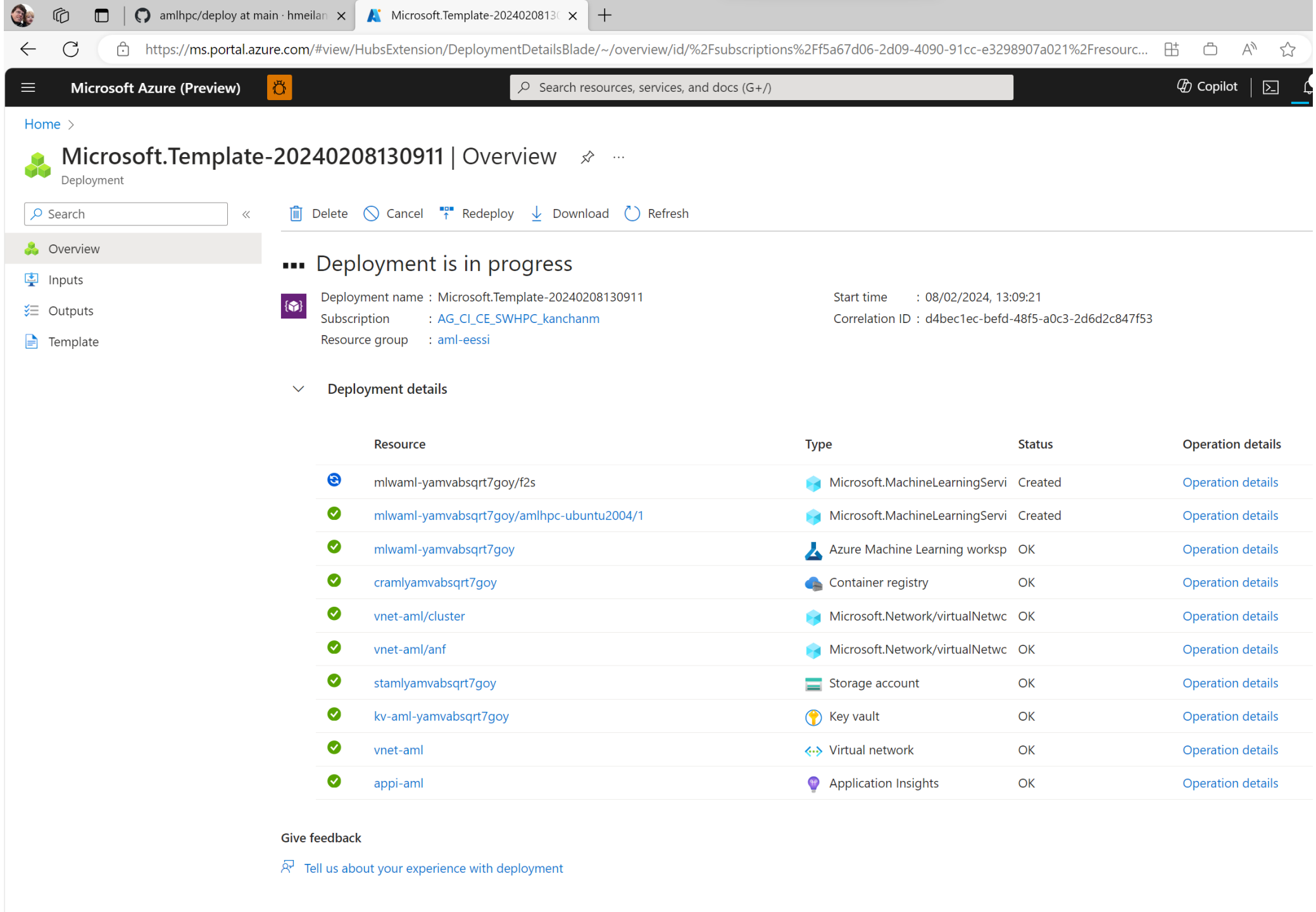
Create
Create


amlhpc/deploy at main · hmeilan
Microsoft.Template-20240208130
https://ms.portal.azure.com/#view/HubsExtension/DeploymentDetailsBlade/~/overview/id/%2Fsubscriptions%2Ff5a67d06-2d09-4090-91cc-e3298907a021%2Fresourc...
Microsoft Azure (Preview)
Search resources, services, and docs (G+/)
Copilot
Home
Microsoft.Template-20240208130911 | Overview
Deployment
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Overview
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Template
Delete
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Redeploy
Download
Refresh
Deployment is in progress
Deployment name : Microsoft.Template-20240208130911
Subscription : AG_CI_CE_SWHPC_kanchanm
Resource group : aml-eessi
Start time : 08/02/2024, 13:09:21
Correlation ID : d4bec1ec-befd-48f5-a0c3-2d6d2c847f53
Deployment details
Resource
Type
Status
Operation details
mlwaml-yamvabsqrt7goy/f2s
Microsoft.MachineLearningServi
Created
Operation details
mlwaml-yamvabsqrt7goy/amlhpc-ubuntu2004/1
Microsoft.MachineLearningServi
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Operation details
mlwaml-yamvabsqrt7goy
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Operation details
cramlyamvabsqrt7goy
Container registry
OK
Operation details
vnet-aml/cluster
Microsoft.Network/virtualNetwc
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Microsoft.Network/virtualNetwc
OK
Operation details
stamlyamvabsqrt7goy
Storage account
OK
Operation details
kv-aml-yamvabsqrt7goy
Key vault
OK
Operation details
vnet-aml
Virtual network
OK
Operation details
appi-aml
Application Insights
OK
Operation details
Give feedback
Tell us about your experience with deployment

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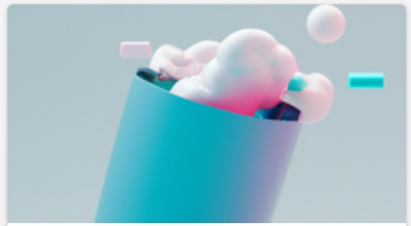
Linked Services PREVIEW

mlwaml

New | Customize view

Generative AI with Prompt flow

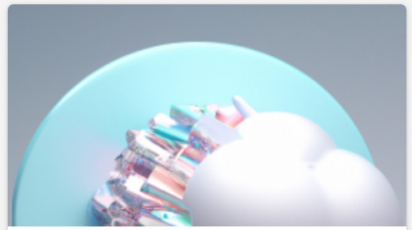
View prompt flow



Multi-Round Q&A on Your Data

Create a chatbot that uses LLM and data from your own indexed files to ground multi-round question and answering capabilities in enterprise chat scenarios.

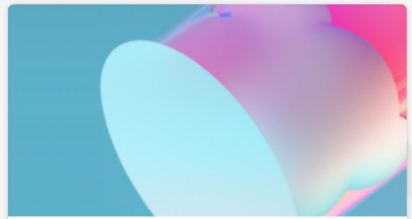
Start | Clone



Q&A on Your Data

Use LLM and data from your own indexed files to ground multi-round question and answering capabilities.

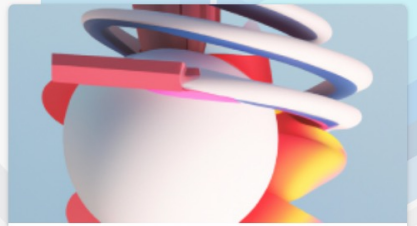
Start | Clone



Web Classification

Use LLM to classify URLs into multiple categories.

Start | Clone



Chat with Wikipedia

Create a chatbot that leverages Wikipedia data to ground the responses.

Start | Clone

Use GPT Funct

Learn how to use G extend the capabili external data sourc

Start

Generative AI models

View all

mistralai-Mistral-7B-v01	mistralai-Mixtral-8x7B-v01	tiiuae-falcon-40b	mistralai-Mistral-7B-Instru...	tiiuae-falc
Text generation	Text generation	Text generation	Chat completion	Text generation

Notebook samples

View all

Get started: Train and deploy a model

Train and deploy a sample image classification model.

Start | 25 minutes

Index and search your own data with GPT

Bring your own data to look up using GPT with LangChain

Start | 20 minutes

Distributed GPU training

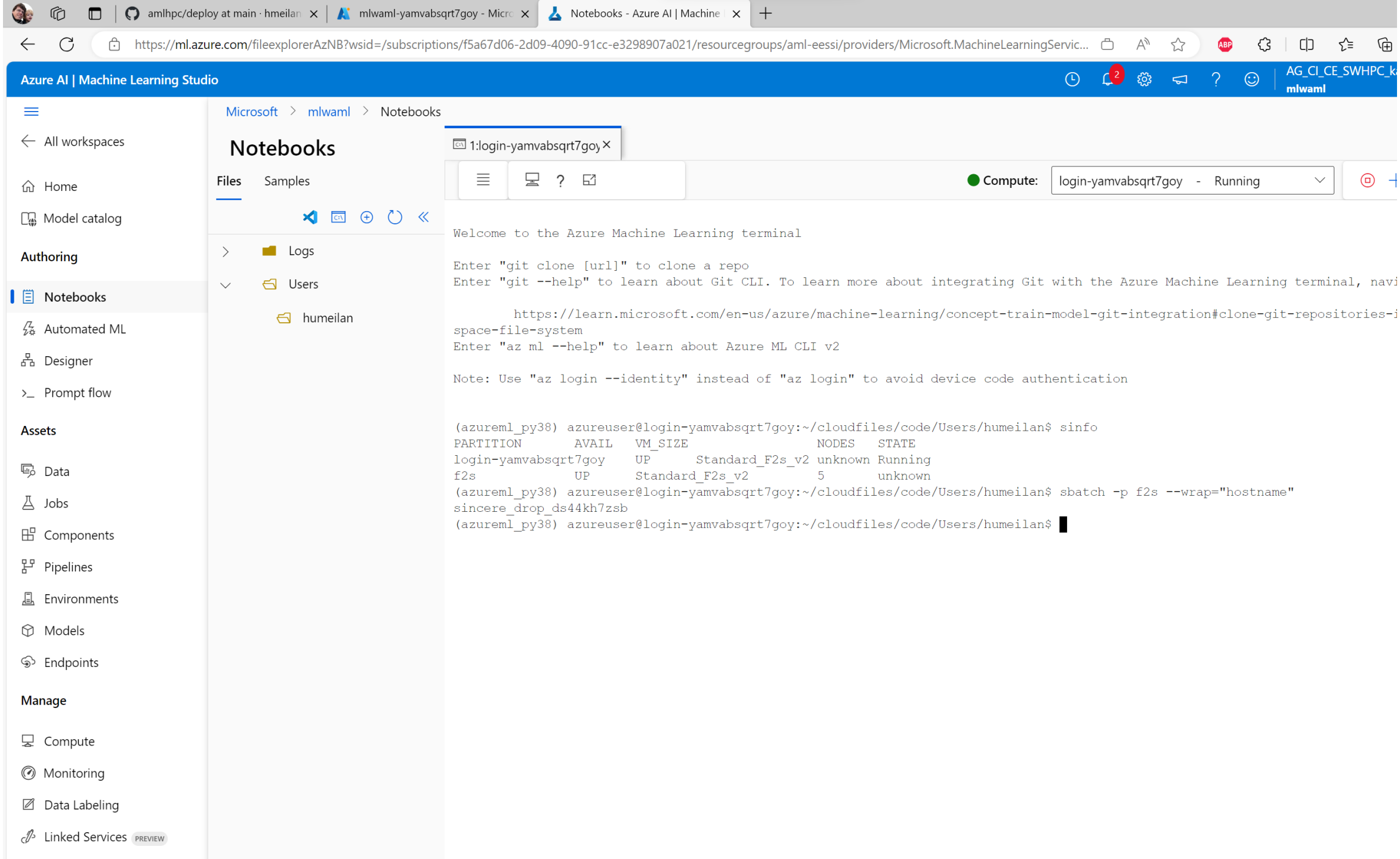
Run a sample multi-GPU image classification experiment.

Start | 30 minutes

Automate with Pipelines

Create a production pipeline for a credit default prediction sample.

Start | 35 minutes


amlhpc/deploy at main · hmeilan
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Notebooks - Azure AI | Machine
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Monitoring
Data Labeling
Linked Services PREVIEW
Microsoft > mlwaml > Notebooks
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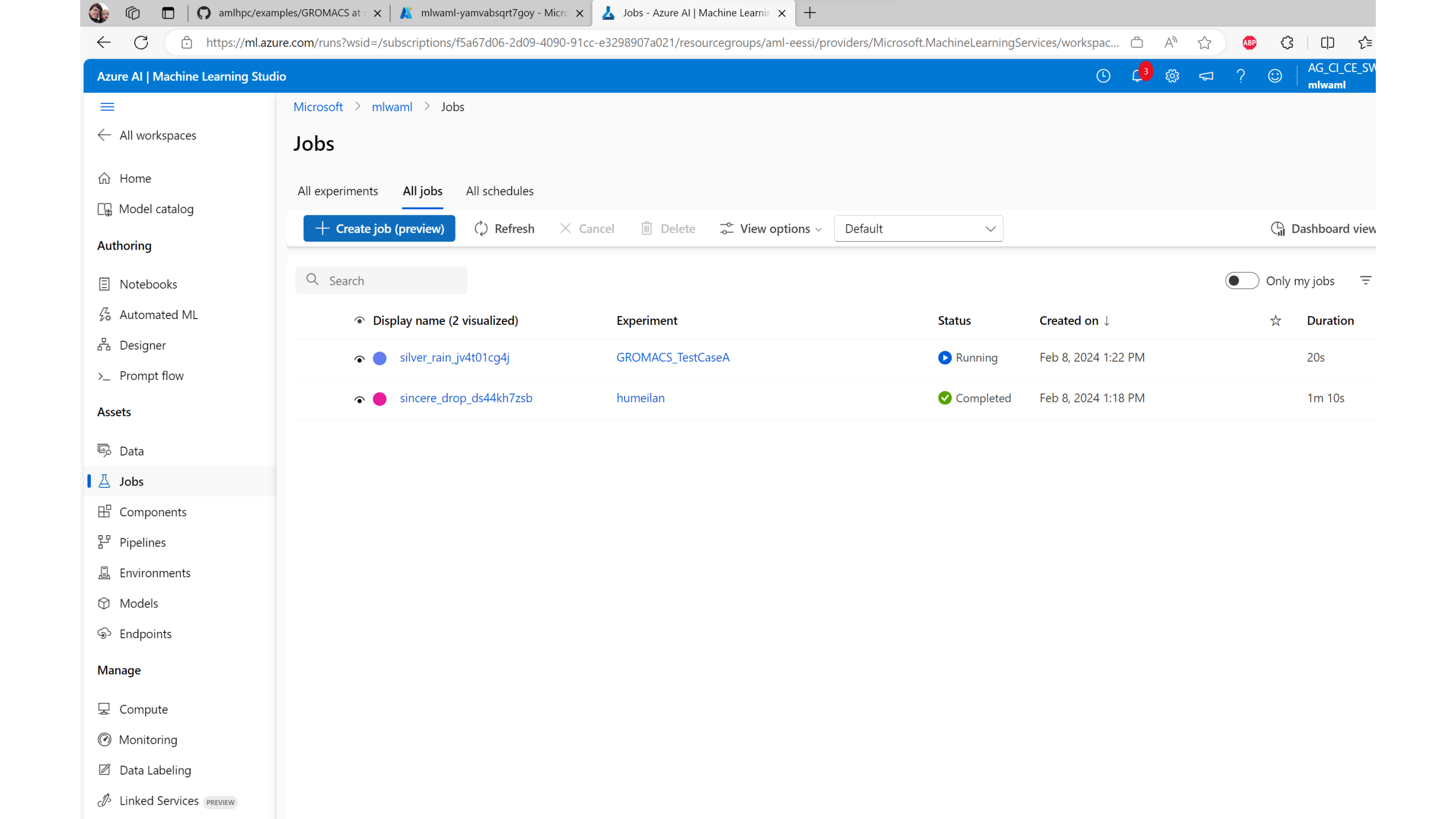
Files
Samples
Logs
Users
humeilan
1:login-yamvabsqrt7goy
Compute:
login-yamvabsqrt7goy - Running
Welcome to the Azure Machine Learning terminal
Enter "git clone [url]" to clone a repo
Enter "git --help" to learn about Git CLI. To learn more about integrating Git with the Azure Machine Learning terminal, navi
https://learn.microsoft.com/en-us/azure/machine-learning/concept-train-model-git-integration#clone-git-repositories-i
space-file-system
Enter "az ml --help" to learn about Azure ML CLI v2
Note: Use "az login --identity" instead of "az login" to avoid device code authentication
(azureml_py38) azureuser@login-yamvabsqrt7goy:~/cloudfiles/code/Users/humeilan$ sinfo
PARTITION AVAIL VM_SIZE NODES STATE
login-yamvabsqrt7goy UP Standard_F2s_v2 unknown Running
f2s UP Standard_F2s_v2 5 unknown
(azureml_py38) azureuser@login-yamvabsqrt7goy:~/cloudfiles/code/Users/humeilan$ sbatch -p f2s --wrap="hostname"
sincere_drop_ds44kh7zsb
(azureml_py38) azureuser@login-yamvabsqrt7goy:~/cloudfiles/code/Users/humeilan$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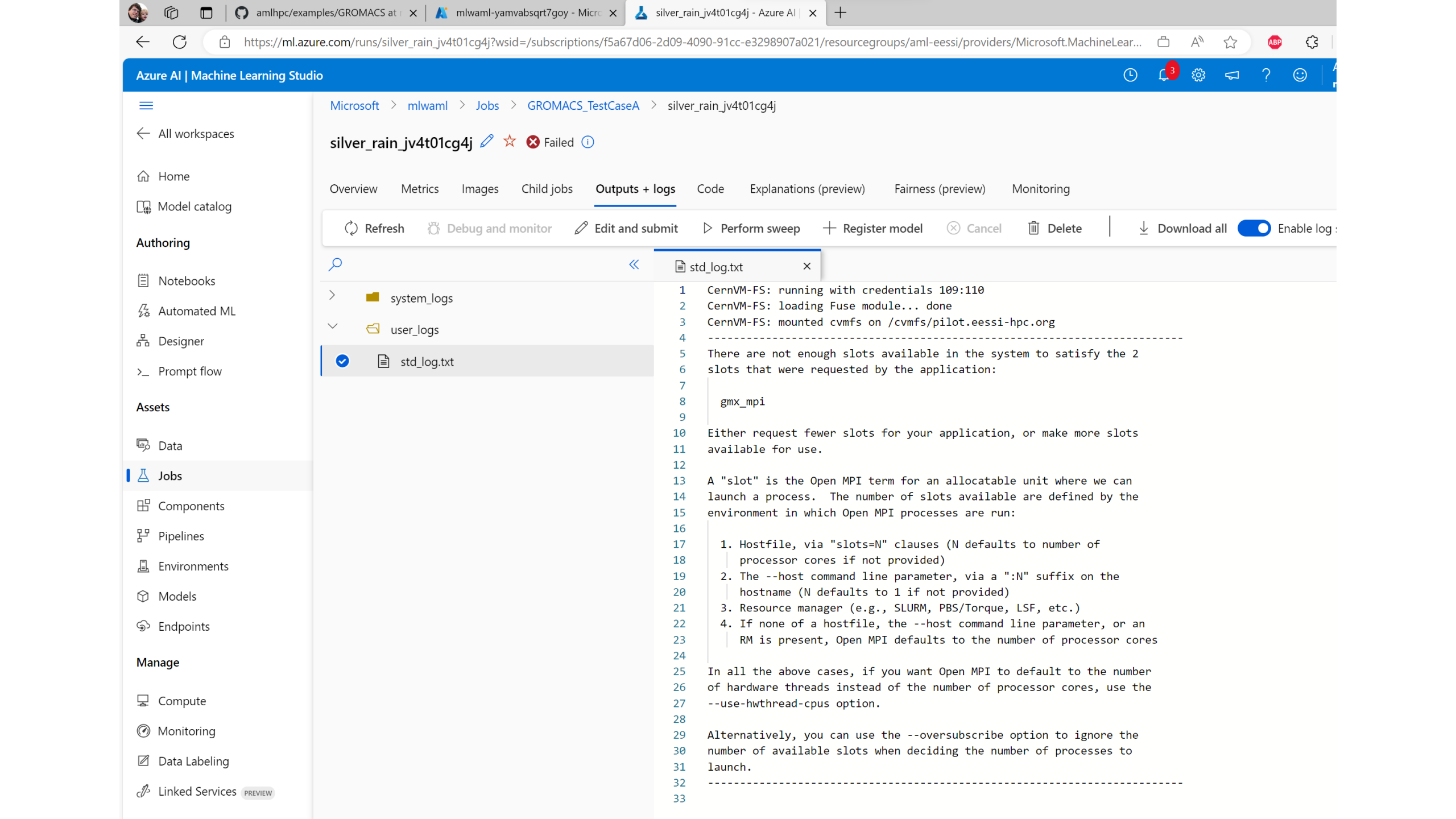
All jobs
All schedules
Create job (preview)
Refresh
Cancel
Delete
View options
Default
Dashboard view
Search
Only my jobs
Display name (2 visualized)
Experiment
Status
Created on
Duration
silver_rain_jv4t01cg4j
GROMACS_TestCaseA
Running
Feb 8, 2024 1:22 PM
20s
sincere_drop_ds44kh7zsb
humeilan
Completed
Feb 8, 2024 1:18 PM
1m 10s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silver_rain_jv4t01cg4j - Azure AI
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silver_rain_jv4t01cg4j
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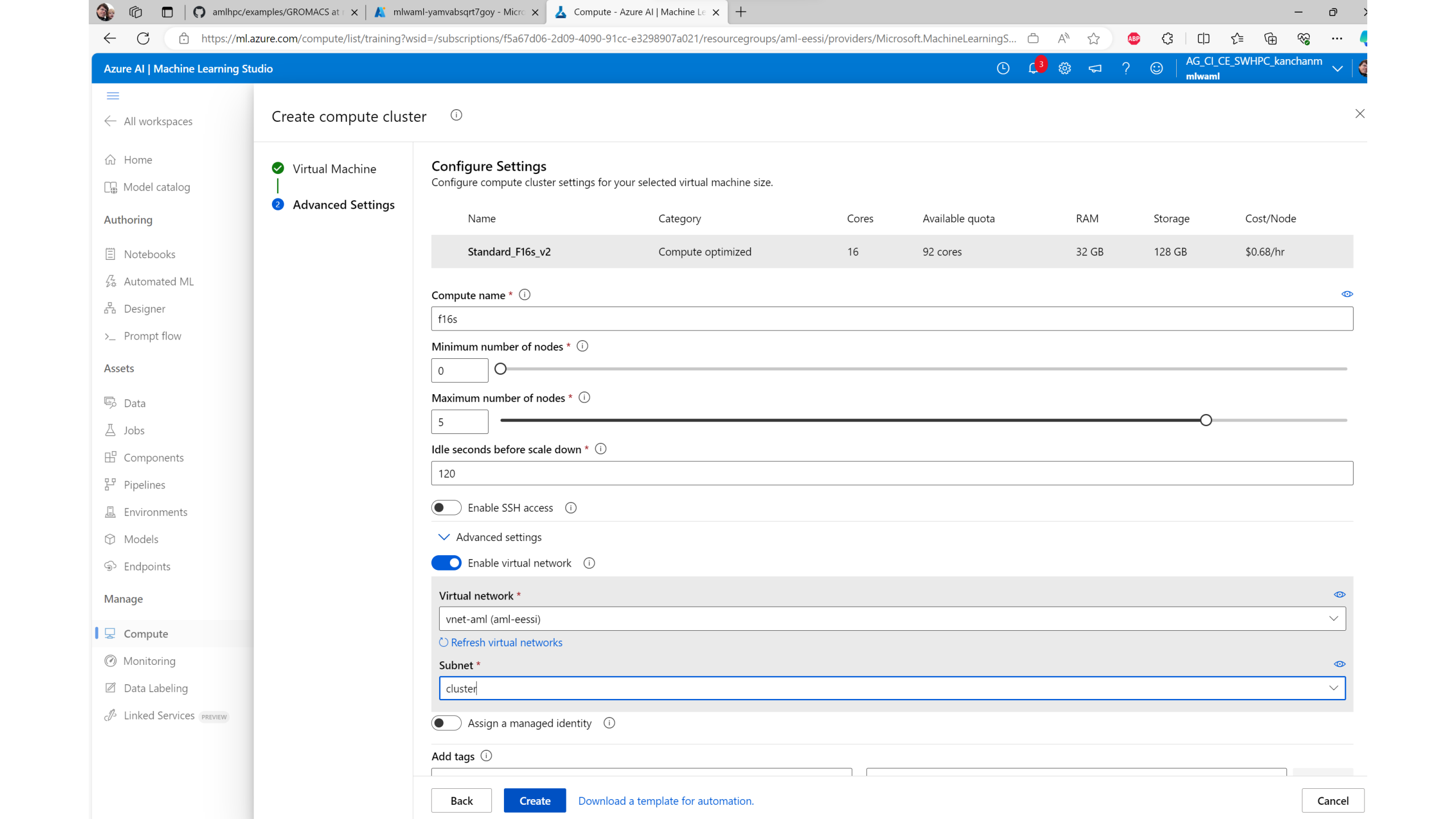
Enable log
system_logs
user_logs
std_log.txt
std_log.txt
CernVM-FS: running with credentials 109:110
CernVM-FS: loading Fuse module... done
CernVM-FS: mounted cvmfs on /cvmfs/pilot.eessi-hpc.org
There are not enough slots available in the system to satisfy the 2
slots that were requested by the application:
gmx_mpi
Either request fewer slots for your application, or make more slots
available for use.
A "slot" is the Open MPI term for an allocatable unit where we can
launch a process. The number of slots available are defined by the
environment in which Open MPI processes are run:
1. Hostfile, via "slots=N" clauses (N defaults to number of
processor cores if not provided)
2. The --host command line parameter, via a ":N" suffix on the
hostname (N defaults to 1 if not provided)
3. Resource manager (e.g., SLURM, PBS/Torque, LSF, etc.)
4. If none of a hostfile, the --host command line parameter, or an
RM is present, Open MPI defaults to the number of processor cores
In all the above cases, if you want Open MPI to default to the number
of hardware threads instead of the number of processor cores, use the
--use-hwthread-cpus option.
Alternatively, you can use the --oversubscribe option to ignore the
number of available slots when deciding the number of processes to
launch.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Configure Settings
Configure compute cluster settings for your selected virtual machine size.
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Storage
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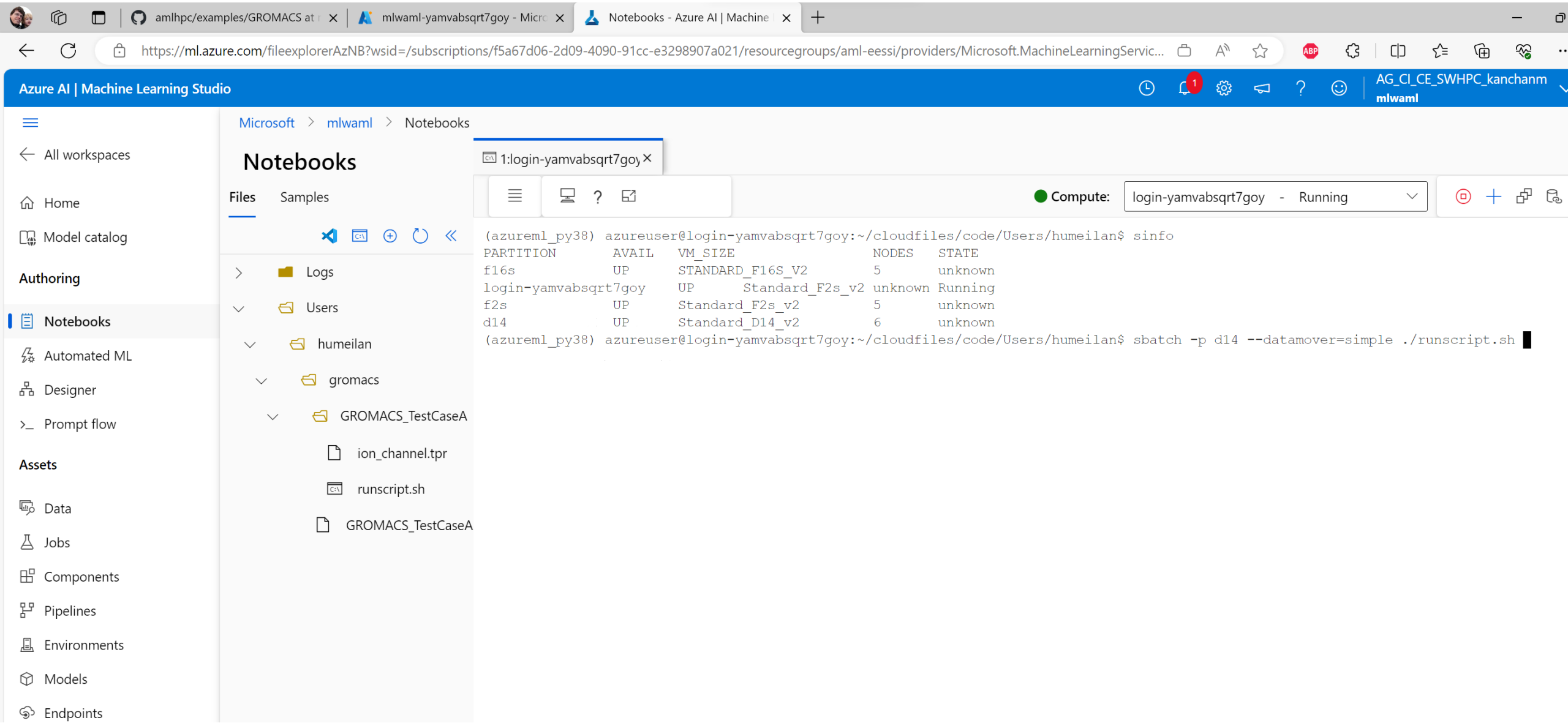
Standard_F16s_v2
Compute optimized
16
92 cores
32 GB
128 GB
$0.68/hr
Compute name *
f16s
Minimum number of nodes *
0
Maximum number of nodes *
5
Idle seconds before scale down *
120
Enable SSH access
Advanced settings
Enable virtual network
Virtual network *
vnet-aml (aml-eessi)
Refresh virtual networks
Subnet *
cluster
Assign a managed identity
Add tags
Back
Create
Download a template for automation.
Cancel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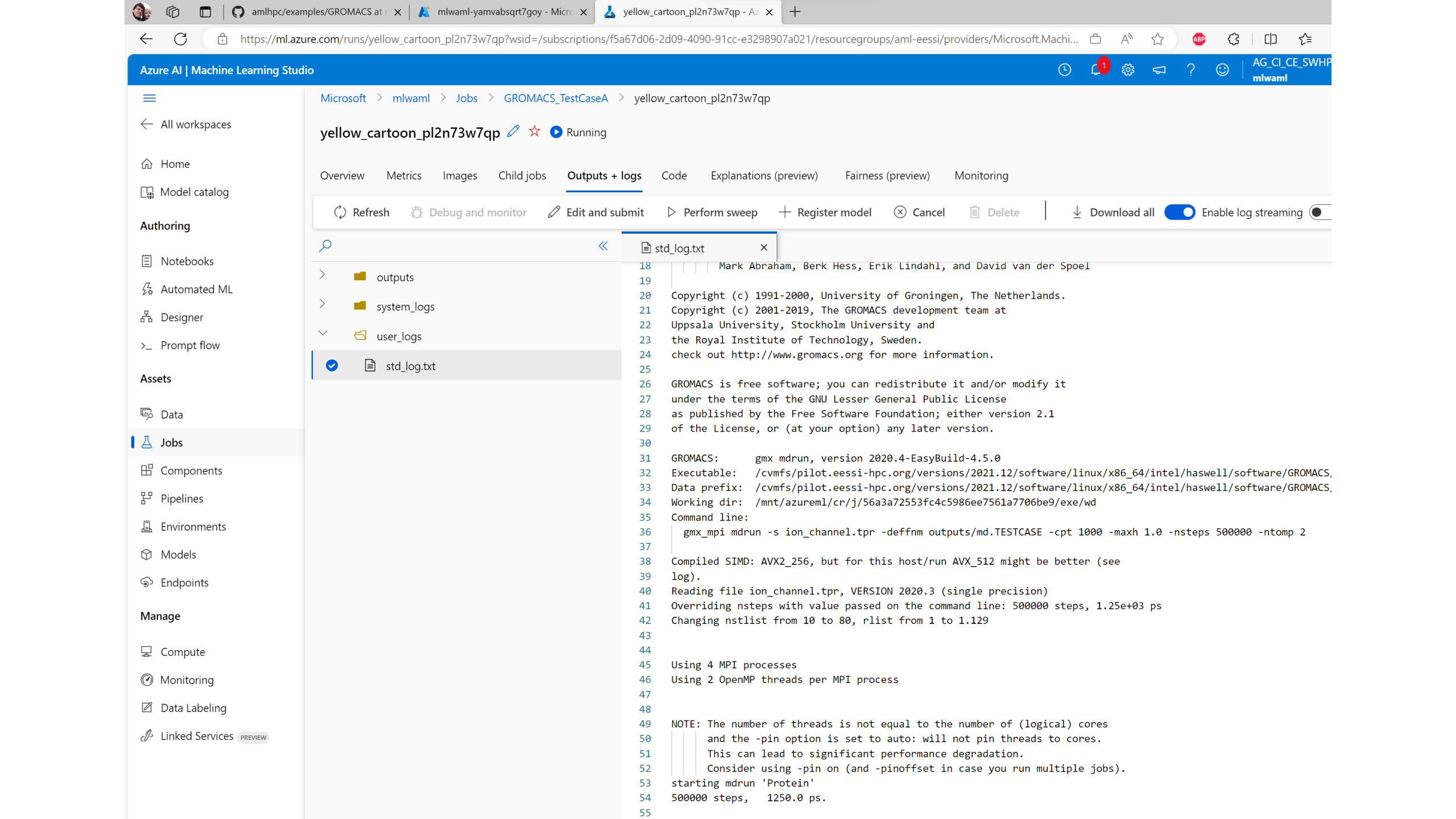
ion_channel.tpr
runscript.sh
GROMACS_TestCaseA
1:login-yamvabsqrt7goy
Compute:
login-yamvabsqrt7goy - Running
(azureml_py38) azureuser@login-yamvabsqrt7goy:~/cloudfiles/code/Users/humeilan$ sinfo
PARTITION AVAIL VM_SIZE NODES STATE
f16s UP STANDARD_F16S_V2 5 unknown
login-yamvabsqrt7goy UP Standard_F2s_v2 unknown Running
f2s UP Standard_F2s_v2 5 unknown
d14 UP Standard_D14_v2 6 unknown
(azureml_py38) azureuser@login-yamvabsqrt7goy:~/cloudfiles/code/Users/humeilan$ sbatch -p d14 --datamover=simple ./runscript.sh


amlhpc/examples/GROMACS at
mlwaml-yamvabsqrt7goy - Micr
yellow_cartoon_pl2n73w7qp - Az
https://ml.azure.com/runs/yellow_cartoon_pl2n73w7qp?wsid=/subscriptions/f5a67d06-2d09-4090-91cc-e3298907a021/resourcegroups/aml-eessi/providers/Microsoft.Machi...
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outputs
system_logs
user_logs
std_log.txt
std_log.txt
Mark Abraham, Berk Hess, Erik Lindahl, and David van der Spoel
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Uppsala University, Stockholm University and
the Royal Institute of Technology, Sweden.
check out http://www.gromacs.org for more information.
GROMACS is free software; you can redistribute it and/or modify it
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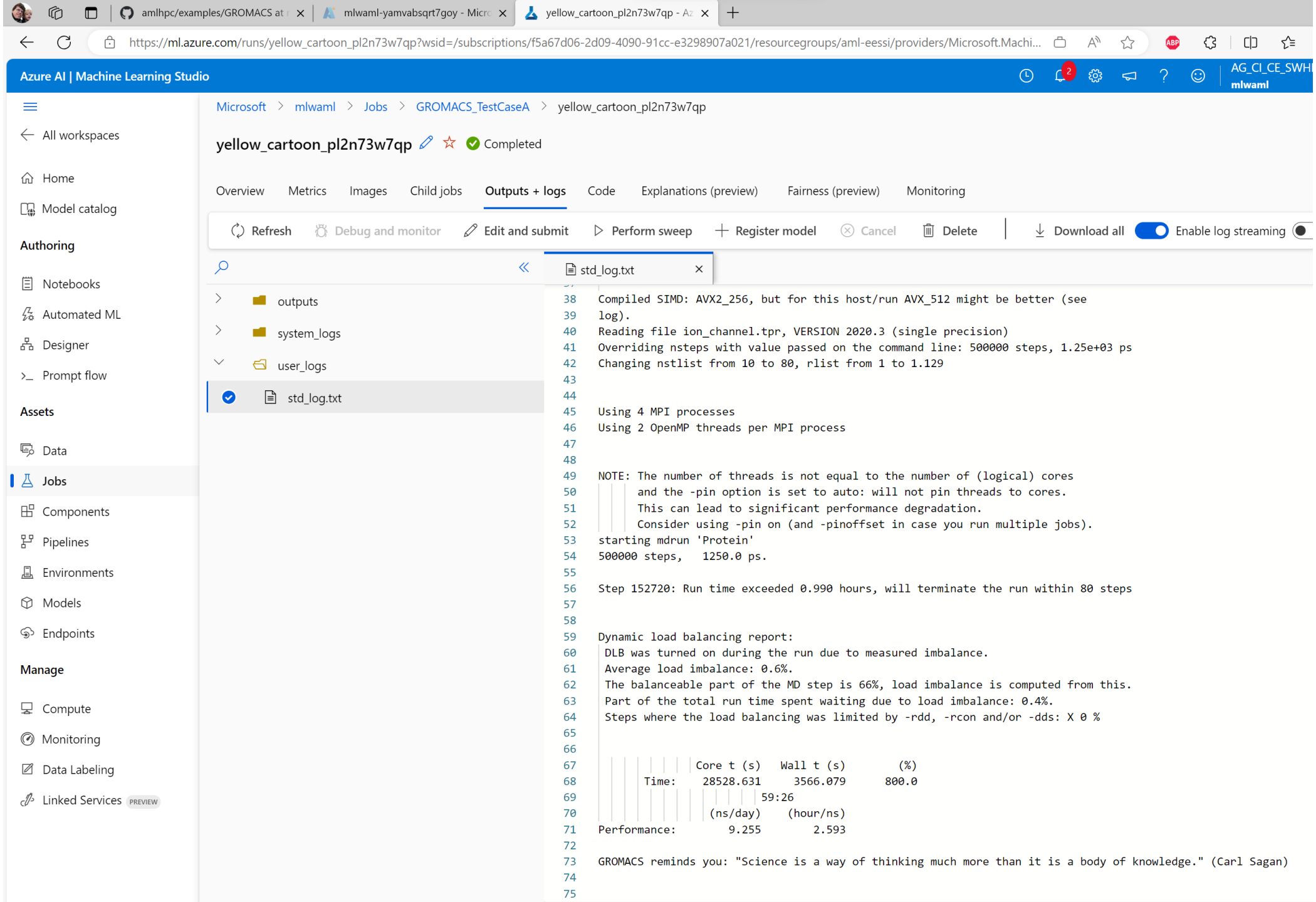
GROMACS: gmx mdrun, version 2020.4-EasyBuild-4.5.0
Executable: /cvmfs/pilot.eessi-hpc.org/versions/2021.12/software/linux/x86_64/intel/haswell/software/GROMACS,
Data prefix: /cvmfs/pilot.eessi-hpc.org/versions/2021.12/software/linux/x86_64/intel/haswell/software/GROMACS,
Working dir: /mnt/azureml/cr/j/56a3a72553fc4c5986ee7561a7706be9/exe/wd
Command line:
gmx_mpi mdrun -s ion_channel.tpr -deffnm outputs/md.TESTCASE -cpt 1000 -maxh 1.0 -nsteps 500000 -ntomp 2
Compiled SIMD: AVX2_256, but for this host/run AVX_512 might be better (see
log).
Reading file ion_channel.tpr, VERSION 2020.3 (single precision)
Overriding nsteps with value passed on the command line: 500000 steps, 1.25e+03 ps
Changing nstlist from 10 to 80, rlist from 1 to 1.129
Using 4 MPI processes
Using 2 OpenMP threads per MPI process
NOTE: The number of threads is not equal to the number of (logical) cores
and the -pin option is set to auto: will not pin threads to cores.
This can lead to significant performance degradation.
Consider using -pin on (and -pinoffset in case you run multiple jobs).
starting mdrun 'Protein'
500000 steps, 1250.0 ps.


amlhpc/examples/GROMACS at
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std_log.txt
38 Compiled SIMD: AVX2_256, but for this host/run AVX_512 might be better (see
39 log).
40 Reading file ion_channel.tpr, VERSION 2020.3 (single precision)
41 Overriding nsteps with value passed on the command line: 500000 steps, 1.25e+03 ps
42 Changing nstlist from 10 to 80, rlist from 1 to 1.129
43
44
45 Using 4 MPI processes
46 Using 2 OpenMP threads per MPI process
47
48
49 NOTE: The number of threads is not equal to the number of (logical) cores
50 and the -pin option is set to auto: will not pin threads to cores.
51 This can lead to significant performance degradation.
52 Consider using -pin on (and -pinoffset in case you run multiple jobs).
53 starting mdrun 'Protein'
54 500000 steps, 1250.0 ps.
55
56 Step 152720: Run time exceeded 0.990 hours, will terminate the run within 80 steps
57
58
59 Dynamic load balancing report:
60 DLB was turned on during the run due to measured imbalance.
61 Average load imbalance: 0.6%.
62 The balanceable part of the MD step is 66%, load imbalance is computed from this.
63 Part of the total run time spent waiting due to load imbalance: 0.4%.
64 Steps where the load balancing was limited by -rdd, -rcon and/or -dds: X 0 %
65
66
67 Core t (s) Wall t (s) (%)
68 Time: 28528.631 3566.079 800.0
69 59:26
70 (ns/day) (hour/ns)
71 Performance: 9.255 2.593
72
73 GROMACS reminds you: "Science is a way of thinking much more than it is a body of knowledge." (Carl Sagan)
74
75