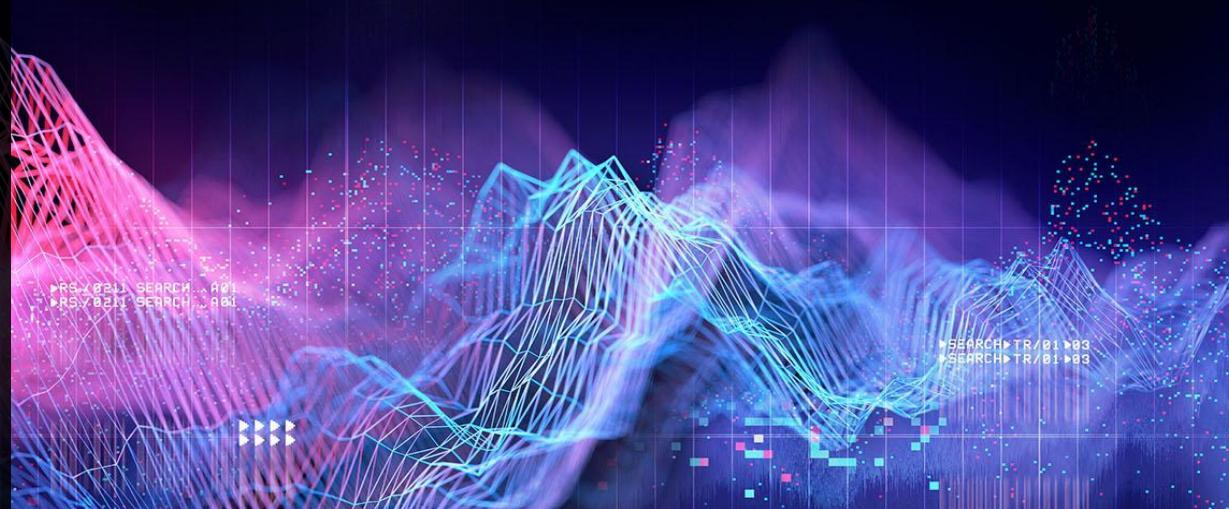




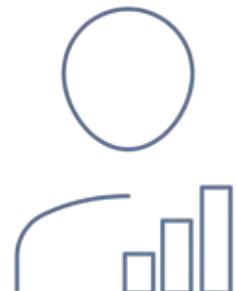
Advanced Data Science in Domino

Dr. Jennifer Davis
Rev3 May 4, 2022



Field Data Science Practice

- Assists at all phases of the project
 - Ideation
 - Research and development
 - Execution
- Expert data scientists and field engineers help you leverage Domino for success
 - Dedicated team of field data scientists and data engineers focus on your success
- We provide consultation services:
 - Best practices for data science on Domino
 - Developing Proof of Concepts and Minimum Viable Products
 - Execution of complex projects to solve business problems
 - Knowledge transfer upon project completion





Agenda

- Setting Up Your Project for Success
- Project Management Tools in Domino
- Environments in Domino
- On-Demand Distributed Compute
- Spark on-demand
- Ray on-demand
- Dask on-demand
- MPI on-demand
- Optimizing GPU usage



Advanced Course Objectives

- Upon completions of this course learners will be able to:
 - Explain Git integration with Domino
 - Discuss Domino Environments and Best Practices
 - Describe benefits and use cases for on-demand distributed computing on Domino
 - Discuss Spark, Ray, Dask and MPI integration with Domino
 - Demonstrate a 'calculate pi' example on distributed compute
 - Explain how GPUs provide performance and how to optimize GPU use in Domino

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 - Demonstrate a ‘calculate pi’ example on distributed compute
 - Explain a Deep Learning (Ray) and a Machine Learning (Dask) example
 - Explain how GPUs provide performance and how to optimize GPU use in Domino

Setting Up Your Project for Success

Setting Up Your Project for Success

- Project Management Tools in Domino
- Git in Domino
 - Code repositories (Git based projects)
- Environments in Domino
 - Naming Conventions
 - Reproducibility
 - More to come

Project Management Tools in Domino

Setting Up Your Project for Success

- All projects can have tags attached to them which make it easier to track projects by topic
- A clear description will let users know more about the project

The screenshot shows a project page for 'Ray_Quick_Start'. At the top, there's a back button and a link to 'Projects'. Below the title 'Ray_Quick_Start' and the date 'Updated January 10th 2022', there are two tabs: 'About' (which is underlined) and 'Manage'. In the 'Tags & Description' section, there's a 'Tags:' label followed by a list of tags: 'ReinforcementLearning' (with an 'X'), 'ray' (with an 'X'), 'quick-start' (with an 'X'), 'tune' (with an 'X'), 'rllib' (with an 'X'), 'computer vision' (with an 'X'), '+ 2 more' (with a '+' icon), and a blue edit icon. Below the tags is a 'Description:' label with the text: 'A tutorial and quick-start project on Using Ray for Deep Learning (examples in Deep Q-Learning and Computer Vision.)' followed by another blue edit icon.

Setting Up Your Project for Success

- To create a README file simply add one to your repository. The readme will automatically be populated to your project
- If you use a git-based project your README file will also show on your github/bitbucket project

Readme



Welcome to your very own Ray on Domino quick-start project!

Ray is an extensive distributed computing library of tools for parallel and distributed applications. Ray provides:

1. Simple primitives for building and running distributed applications.
2. Enables users to parallelize single machine code, with little to zero code changes.
3. Includes applications, libraries and tools for deep learning.

Ray has programming interfaces for Python, Java and C++ (Experimental).

This quick-start project has examples for running remote functions using Ray and some of its libraries. This includes performing basic reinforcement learning using RLLib, use of Tune for distributed data parallelism, and a fun example of trying to predict a stock market values of US and Bitcoin currency.

Before you get started, you might want to check out [our product tour video](#).

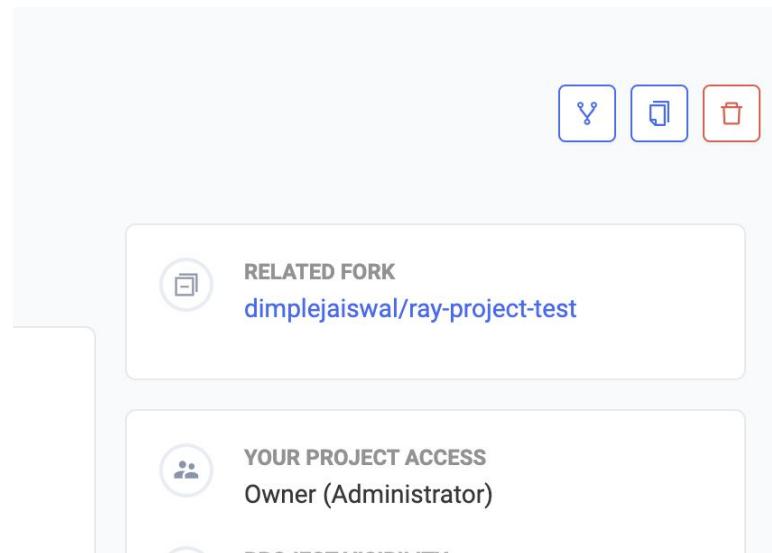
Starting a Ray Workspace

To start a Ray workspace you will need to design two environments. The first is an environment that will be used for the workspace. This environment should have Ray installed, preferably the latest version. One can build the workspace environment using the latest Domino Analytics Distribution as its base. The second environment – the workers environment should also have the identical version of Ray installed. An example of how to build the docker image for your environments is available upon request.

Then when starting a workspace you will go through the following steps

Forking Projects and QuickStarts

- Users can fork or clone projects they are interested in copying or learning from
- Users can use a particular project as “starter” project for other work they may want to do



Setting Up Project Goals, Tags and Assignments

- Setting goals for your project can help when forming collaborations
- Goals also let reviewers know clearly where in the development process the project is and next steps

Goal-1 Create Initial Notebooks Demonstrating use of Ray
Completed

Description Create three notebooks including one of basic use cases, one on using hyperparameter tuning, and one on tensortrade.
[See More](#)

Status Completed

Add a new comment

Goal-2 Write README file
Validation

Description Write a README file and describe the quick-start project.

Status Validation

Add a new comment

Goal-3 Finalize wording in README and Three Notebooks
Validation

Description @{{melanie_veale}} and @{{alireza_mounesisohi}} will provide feedback to @{{jddavis1000}} about how the notebooks are written and whether they are completely clear. @{{dimplejaiswal}} has provided feedback.
[See More](#)

Edited: Jan 13th, 2022

Using Goals, comments and tagging collaborators

- Once project goals are set, collaborators can be tagged for specific goals
- Comments can be made for each goal and each goal is tracked for stage. For example this goal is marked completed.

Ray_Quick_Start
Updated January 10th 2022

About Manage

Tags & Description

Tags: ReinforcementLearning ray quick-start tune rllib computer vision + 2 more +
Description: A tutorial and quick-start project on Using Ray for Deep Learning (examples in Deep Q-Learning and Computer Vision). [Edit](#)

Model APIs

Goal API	Description	Status
Goal-1	Create Initial Notebooks Demonstrating use of Ray	Completed
Goal-2	Create three notebooks including one of basic use cases, one on using hyperparameter tuning, and one on tensorstore.	In Progress

Add a new comment

Markdown and Mathjax are supported. You can also @mention people.

Commenting on Project Goals, Marking Completion

- Here's an example of a goal, its description, and how to mark the status
- This goal is in the validation stage, but there are other available stages

Markdown and Mathjax are supported. You can also @mention people.

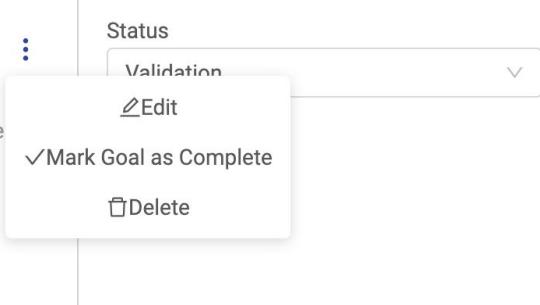
Goal-3 Finalize wording in README and Three Notebooks

Description @{{melanie_veale}} and @{{alireza_mounesisohi}} will provide feedback to @{{jddavis1000}} about how the notebooks are written and whether they are completely clear. @{{dimplejaiswal}} has provided feedback that there needs to be more explanation of some portions of the quick-start. Further details requested.

[See Less](#)

Edited: Jan 13th, 2022

Add a new comment



Users can search for project by keywords

- When using tagged and key words, one can search for projects by tag
- For example I added a project tag 'Ray'. Users can find my project when searching for 'Ray'

jddavis1000/Ray_Quick_Start

A tutorial and quick-start project on Using Ray for Deep Learning (examples in Deep Q-Learning and Computer Goal:

Create Initial Notebooks Demonstrating use of Ray

computer vision

deep learning

hyperparameter optimization

quick-start

ray

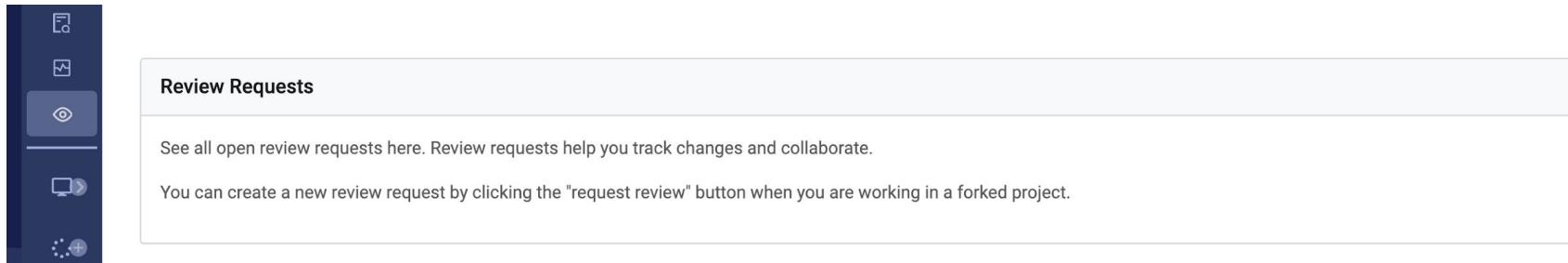
ReinforcementLearning

rllib

tune

Requesting Reviews

- When working in Domino Data Lab, one can ask collaborators in the project to review specific files related to a particular goal



The screenshot shows the Domino Data Lab interface. On the left is a vertical toolbar with icons for file operations (copy, paste, move, delete), a search bar, a user profile icon, a monitor icon, and a plus sign icon. The main area is titled "Review Requests". It contains the text: "See all open review requests here. Review requests help you track changes and collaborate." and "You can create a new review request by clicking the 'request review' button when you are working in a forked project."

Data Access and Sharing, Tagging within a Project

When sharing Data one can tag files and datasets to ask collaborators for review

Markdown and Mathjax are supported. You can also @mention people.

Goal-3 Finalize wording in README and Three Notebooks ⋮

Description @{{melanie_veale}} and @{{alireza_mounesisohi}} will provide feedback
[See More](#)

Edited: Jan 13th, 2022

Files: [Basic_Ray_Tutorial_with_Deep_Q_Learning \(4\).ipynb \(471a62e\)](#)
[Model_Creation_and_Training_DQN.ipynb \(471a62e\)](#)
[Simple Computer Vision MNIST using Distributed Data Parallel .ipynb \(471a62e\)](#)

Add a new comment ↗

Markdown and Mathjax are supported. You can also @mention people.

[View all 3 comments](#)

Linking files to a particular goal

- In this example a goal is associated with files
- This allows collaborators or reviewers to quickly know which code or files to review

The screenshot shows the Domino platform's project management interface. On the left, a sidebar menu lists various project sections: Overview, Activity, Reviews, RUN, Workspaces, Jobs, MATERIALS (Data, Files), PUBLISH (Scheduled Jobs, App, Model APIs, Launchers), and Settings. The 'Overview' section is currently selected.

The main content area displays the 'loan-prediction' project. At the top, there are 'About' and 'Manage' tabs, with 'Manage' being the active tab. Below this is a 'Tags & Description' section. It shows 'No tags' and a text input field for 'Description'. A note says 'No description provided.' with a link to edit it.

Under the 'Goals' section, there is one entry named 'Goal-1' with the description 'Data Wrangling'. There is a 'Status' dropdown set to 'Ideation'. Below the goal, a list of files is shown: start_job.py (d04aa38), model.py (d04aa38), running_job_test.py (d04aa38), requirements.txt (d04aa38), sync-test.ipynb (d04aa38), and spark.py (d04aa38). A comment from user '@jddavis1000' is displayed: 'can you take a look at these for me?' with a reply arrow icon. A note below says 'Markdown and MathJax are supported. You can also @mention people.'

At the bottom of the main content area, there is a 'View all 6 comments' link and a '+ Add New Goal' button.

On the right side, there is a sidebar with various project statistics: RELATED FORKS (5), YOUR PROJECT ACCESS (Owner (Administrator)), PROJECT VISIBILITY (Public), HARDWARE (Small), ENVIRONMENT (Domino Analytics Distribution 2020Q2), TOTAL RUNTIME (2 months), APPS (1), JOBS (425), WORKSPACES (0), and COMMENTS (5).

Example of notes in a particular goal

- This is a real team example of how comments were used for a particular goal in a group project
- Notice that comments can be used to tag people

The screenshot shows a Domino platform interface. At the top, there's a navigation bar with 'Status' and 'Ideatio'. Below it, a goal card for 'Goal-1' titled 'Data Wrangling' is displayed. The card includes sections for 'Add Description' and 'Files' (listing start_job.py, model.py, running_job_test.py, requirements.txt, sync-test.ipynb, and spark.py). A comment input field says 'Add a new comment' with a small icon. Below that, a note says 'Markdown and MathJax are supported. You can also @mention people.' and a 'Hide all 7 comments' link. Five comments from user 'larue_brown' are listed, each with a timestamp (January 14th 2022 @ 17:45 or 17:44) and edit/delete icons.

Goal-1 Data Wrangling

Add Description

Files:

- start_job.py (d04aa38)
- model.py (d04aa38)
- running_job_test.py (d04aa38)
- requirements.txt (d04aa38)
- sync-test.ipynb (d04aa38)
- spark.py (d04aa38)

Add a new comment

Markdown and MathJax are supported. You can also @mention people.

Hide all 7 comments

larue_brown
@jddavis1000 - can you take a look at these for me?
January 14th 2022 @ 17:45

larue_brown
Domino Project: loan-prediction File: sync-test.ipynb
Link: https://field.cs.domino.tech/u/larue_brown/loan-prediction/view/sync-test.ipynb
commitId=d04aa388590516e0d7f6b9f7249560e5f07bc2fa
January 14th 2022 @ 17:44

larue_brown
Domino Project: loan-prediction File: requirements.txt
Link: https://field.cs.domino.tech/u/larue_brown/loan-prediction/view/requirements.txt?
commitId=d04aa388590516e0d7f6b9f7249560e5f07bc2fa
January 14th 2022 @ 17:44

larue_brown
Domino Project: loan-prediction File: running_job_test.py
Link: https://field.cs.domino.tech/u/larue_brown/loan-prediction/view/running_job_test.py?
commitId=d04aa388590516e0d7f6b9f7249560e5f07bc2fa
January 14th 2022 @ 17:44

larue_brown
Domino Project: loan-prediction File: spark.py
Link: https://field.cs.domino.tech/u/larue_brown/loan-prediction/view/spark.py?
commitId=d04aa388590516e0d7f6b9f7249560e5f07bc2fa
January 14th 2022 @ 17:44

Summary of Project Tools

Tags for searchability

Project README file

Git Repository connectivity

Project management and versioning

- Assign project goals to individuals
- Make comments and tag individuals under project goals
- Set stage of project (e.g. completed, incomplete, validation, production)
- Link a file to a particular goal

Summary of Versioning and Project Set-up

Versioning

- Fork projects
- Ask for a review of work on a particular forked project
- Versioning of Datasets (can revert to former versions of data)

Project Set-up

- Set default environment
- Set default hardware tier
- Set permissions, e.g. contributor, owner, etc.

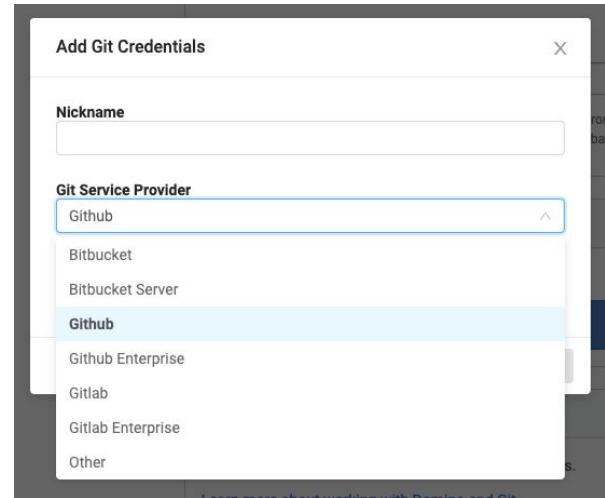
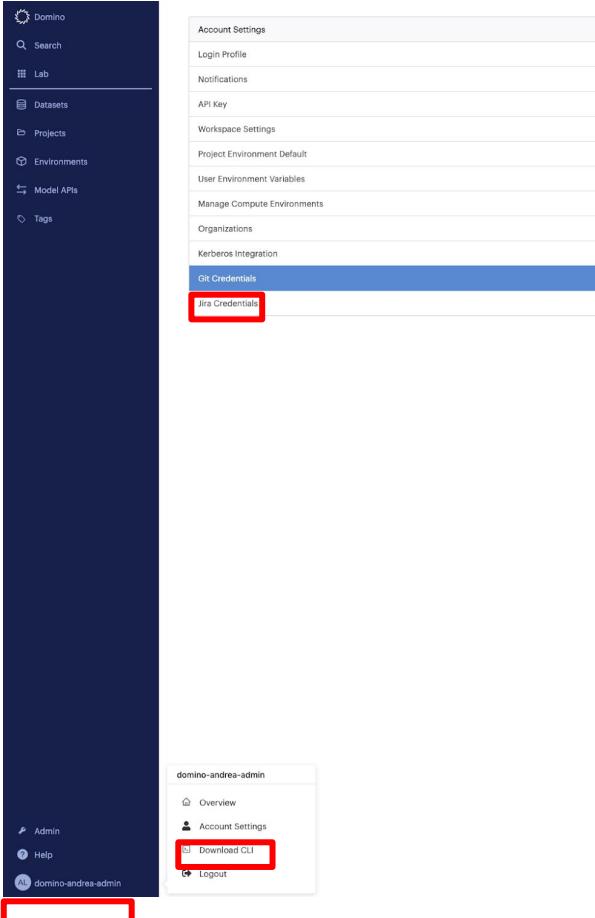
Git in Domino

Git Authentication

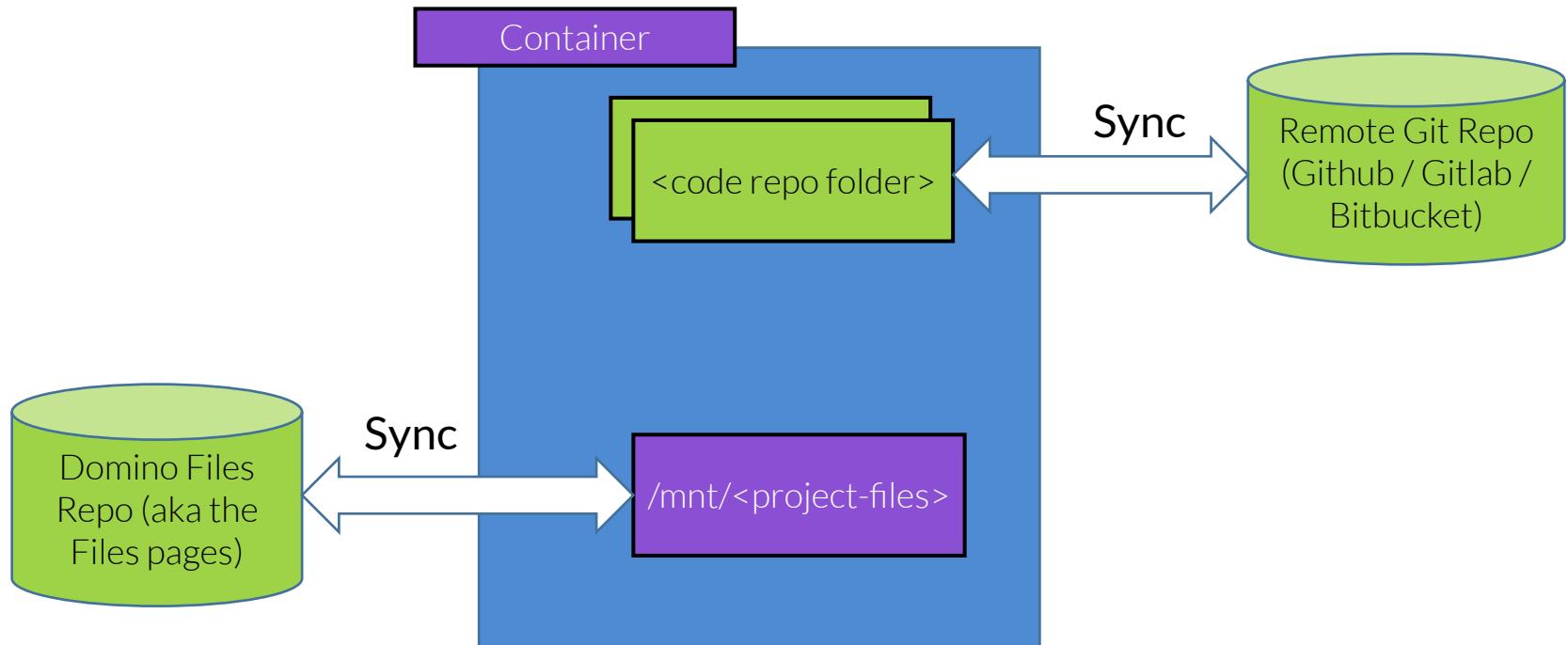
Add authentication
before creating project

This is done by clicking
on your user name →
Account Settings

Select *Git Service
Provider* and input
Personal Access Token
or Private SSH key



Integration with Git: Separation of Version Control Systems



Git Based Project Setup

Select Git for the *Code Repository*

Enter the repo link and select
your *Git Credentials*

You can also directly create a new
repo if using Github, Github
Enterprise, or Gitlab

Create New Project

Hosted By

Domino File System Git Service Provider (beta)

Git Service Provider

Github my-github

Git Credentials

Repository

Select a repo or directly paste a repo URL like <https://github.com/user/my-repo.git>

Owner/Organization

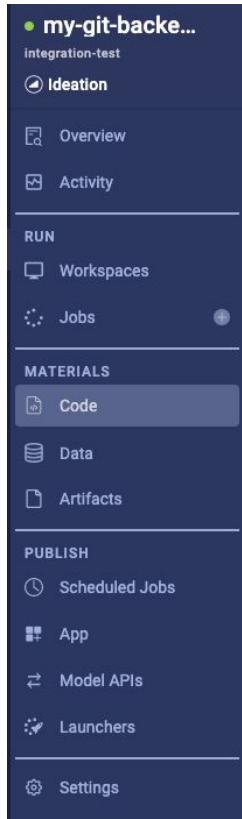
Repository Visibility

Private Public

[Back](#) [Create](#)



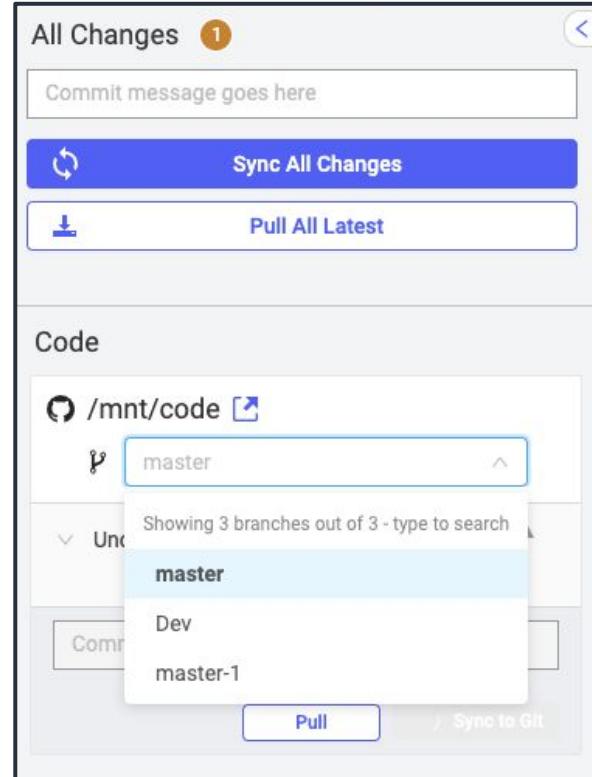
Git Based Projects Overview



- Code is separated from data and artifacts
- The *Artifacts* page can store any file type and contains commits for any changes made to the project
- Branching and merging of the project is handled through Git
- See docs [here](#) for more info

Git Integration

- You can change branches and resolve conflicts directly in Domino
- Branch updates and status will be reflected in your Workspaces
- See details in [Domino 101](#)



Import Git Repos

Any number of git repos can be imported into a standard Domino project or a git-based project

The screenshot shows the Domino interface with a sidebar on the left containing navigation links: Overview, Activity, Reviews, RUN, Workspaces, Jobs, MATERIALS, Data, and Files. The 'Files' link is highlighted with a red box. The main content area has tabs at the top: Local, Other Projects, and GIT Repositories, with 'GIT Repositories' also highlighted with a red box. Below the tabs, there's a section titled 'Import from external Git repositories' with the sub-instruction 'This project can import files from external Git repositories hosted by services like GitHub.' followed by a link 'Learn more about repositories.' A 'Not importing any repositories.' message is displayed. On the right side, there's a blue button labeled 'Add a New Repository' with a red box around it.

Environments in Domino

Environments

- An environment is a Domino abstraction on top of a [Docker](#) image, that provides additional flexibility and versioning
- When Domino starts your run, it creates a Docker container based on the environment associated with your project - Each run takes place in an isolated Docker container
- See [docs](#) for detailed instructions and info on advanced options

⊕ Compute environment What's this ?

Domino Analytics Distribution Py3.6 R3.6 Manage Environment

Global

- Domino Analytics Distribution py3.6 R3.5 - shap & lime
- Domino Analytics Distribution Py3.6 R3.6**
- HyperOpt Domino Analytics Distribution Py3.6 R3.6
- Image_Drift_Keras_TF
- OpenAI Gym with Python 3.6
- Tensorflow 2.0 Py3.6 R3.5

test

- testenv

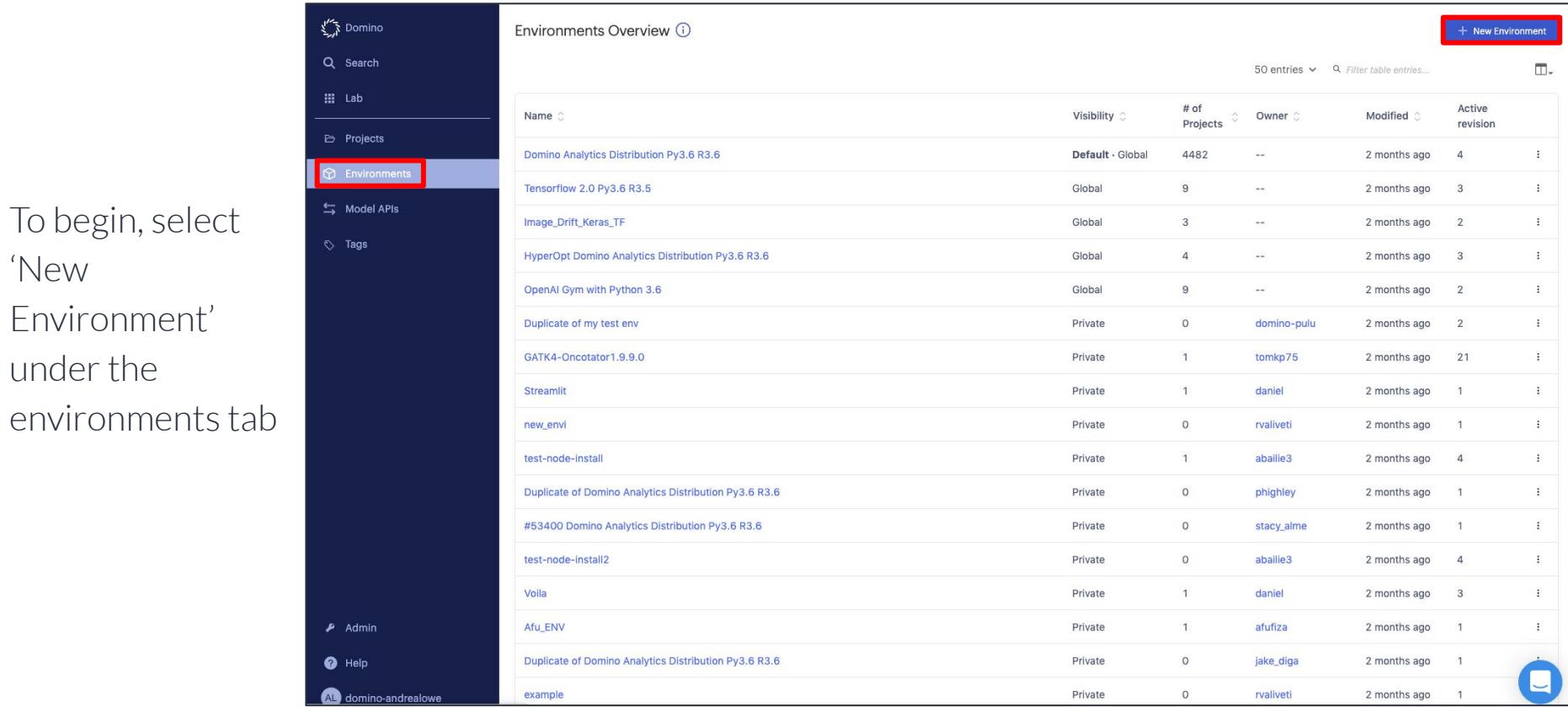
Private

By default, environments are passed verbatim, without any escaping.

ntime. Name conflicts with value of a variable, just set it

Environments

To begin, select
'New
Environment'
under the
environments tab



Environments Overview ⓘ

50 entries ⓘ Filter table entries...

Name	Visibility	# of Projects	Owner	Modified	Active revision
Domino Analytics Distribution Py3.6 R3.6	Default - Global	4482	--	2 months ago	4
Tensorflow 2.0 Py3.6 R3.5	Global	9	--	2 months ago	3
Image_Drift_Keras_TF	Global	3	--	2 months ago	2
HyperOpt Domino Analytics Distribution Py3.6 R3.6	Global	4	--	2 months ago	3
OpenAI Gym with Python 3.6	Global	9	--	2 months ago	2
Duplicate of my test env	Private	0	domino-pulu	2 months ago	2
GATK4-Oncotator1.9.9.0	Private	1	tomkp75	2 months ago	21
Streamlit	Private	1	daniel	2 months ago	1
new_envi	Private	0	rvaliveti	2 months ago	1
test-node-install	Private	1	aballie3	2 months ago	4
Duplicate of Domino Analytics Distribution Py3.6 R3.6	Private	0	phighley	2 months ago	1
#53400 Domino Analytics Distribution Py3.6 R3.6	Private	0	stacy_alme	2 months ago	1
test-node-install2	Private	0	aballie3	2 months ago	4
Volta	Private	1	daniel	2 months ago	3
Afu_ENV	Private	1	afufiza	2 months ago	1
Duplicate of Domino Analytics Distribution Py3.6 R3.6	Private	0	jake_diga	2 months ago	1
example	Private	0	rvaliveti	2 months ago	1

Environments

Base image

Contains many of the common packages for data scientists

See docs [here](#) for more info

The screenshot shows the Domino platform's interface for creating a new environment. On the left is a dark sidebar with navigation links: Search, Lab, Projects, Environments (which is highlighted), Model APIs, and Tags. At the bottom of the sidebar are Admin, Help, and a user profile icon for domino-andrealowe. The main area is titled 'New Environment'. It has fields for 'Name' (empty) and 'Base Image' (set to 'Domino Analytics Distribution Py3.6 R3.6'). There are three radio button options under 'Visibility': 'Private' (selected, set to 'domino-andrealowe'), 'Available to an Organization' (set to 'Bombora'), and 'Globally Accessible'. A large text area for 'Description (Optional)' is empty. At the bottom are 'Cancel' and '+ Create Environment' buttons.

Environments in Domino

You can now use a custom image, such as NVIDIA [NGC containers](#), and have Domino make it automatically compatible with Workspaces and Jobs

Changes can still be made to the Dockerfile instructions

New Environment

Name
NGC Tensorflow Image

Description
Optional

Base Environment / Image

Start from an existing Environment
Inherit a base image, Dockerfile instructions & scripts from a Domino environment

Start from a custom base image
Use a custom Docker or container image URI from a registry like NGC

FROM nvcr.io/nvidia/tensorflow:21.11-tf2-py3

Automatically make compatible with Domino
You can review and update this configuration later

Supported Clusters

none Spark Ray Dask

Visibility

Private i
integration-test

Globally Accessible i

Cancel Customize before building Create Environment

Environments

Edit Dockerfile
instructions to add
packages

Buttons to add
template code are
available for simple
R and Python
additions

The screenshot shows the Domino web interface with a dark blue sidebar on the left and a white main content area. The sidebar includes links for Domino, Search, Lab, Projects, Environments (which is highlighted in purple), Model APIs, Tags, Admin, Help, and a user profile for domino-andrealowe. The main content area has a title "Edit the definition of Intro-to-Domino-Environment" and a sub-section "Docker Settings". Under "Docker Settings", there is a "Base Image" section with a dropdown menu containing "Domino Analytics Distribution Py3.6 R3.6". Below it are three radio button options: "Default image", "Select the default base image specified in your deployment.", and "Custom image", followed by a text input field for specifying a custom Dockerfile URI. A "Dockerfile Instructions" section contains a code editor with the following Python command:

```
1 RUN pip install "pystan==2.17.1.0" "plotly<4.0.0" "holidays==0.9.12" "fbprophet==0.5" papermill requests dash
```

. Below the code editor, a note says "Your Dockerfile layer. Do not use the FROM instruction here. It will be generated from the Docker image field." and "Click to add an R Package" or "Python Package". A link "For more help, read about managing environments" is also present. The bottom section is titled "Pluggable Workspace Tools" with a "Properties for Workspaces" link and a code editor area.

Environments

Select 'Build' at the bottom of the page after adding instructions

The screenshot shows the Domino web interface with the following details:

- Left Sidebar:** Includes links for Domino, Search, Lab, Projects, Environments (which is selected and highlighted in blue), Model APIs, and Tags.
- Top Navigation:** Shows the user's name (AL domino-andrealowe) and Admin status.
- Environment Configuration:** A large central area for configuring an environment, divided into sections:
 - Post Run Script:** A code editor for a script to execute after a run.
 - Environment variables:** A table for defining environment variables with columns for Variable Name and Value. A note states: "For every environment variable you define here, you must also declare it in the Dockerfile Instructions with an ARG statement."
 - Advanced:** A dropdown menu currently set to "Summary".
 - Summary:** Fields for Revision Summary and a brief description of changes.
 - Cancel:** A button to cancel the changes.
 - Build:** A green button at the bottom right of the summary section, which is highlighted with a red box.
 - Force docker image rebuild:** A checkbox next to the Build button.

Example Docker file Instructions

quay.io/domino/base:Ubuntu18_DAD_Py3.8_R4.0-20210503_CUDA11

Supported Clusters

- None
- Domino managed Spark [①](#)
- Domino managed Ray [①](#)
- Domino managed Dask [①](#)

Dockerfile Instructions

```
1  ### Change Ray version as needed.
2  USER root
3
4  ENV RAY_VERSION=1.9.0
5
6  ### If you want install Ray RLLib or "all", which includes it, you must
7  ### install "cmake" first.
8  RUN apt-get update && apt-get install -y apt-transport-https
9  RUN apt-get install -y cmake
10 RUN apt-get install -y rsync
11
12 #python libraries
13 RUN pip install GPyUtil
14 RUN pip install torch torchvision tensortrade
15
16 ### Change this depending on which Ray extras you want to install:
17 ### All options are ray, ray[tune], ray[rllib], ray[serve]
18 ### If you want everything you can just use ray[all].
19 ### See note above the "cmake" is required for ray[rllib] or ray[all].
20 RUN pip install ray[all]==$RAY_VERSION
21 RUN pip install pytorch-lightning git+https://github.com/ray-project/ray_lightning#ray_lightning
22 RUN pip install aioredis==1.3.8
23 RUN pip install torch torchvision
24
25 ### Add any additional packages that you may need which are not included
26 ### in the base image you are using for the compute environment. You would
27 ### want the versions of these to match the versions of these packages on
28 ### the base Ray cluster image.
29 ### For example, for Torch you may include
30 ### RUN pip install torch==1.8.0 torchvision==0.9.0
31
32 USER 1001
```

Environments Best Practices

- Docker optimizes its build process by keeping track of commands it has run and caching the results
- This means that if it sees the same set of commands as a previous build, it will assume it can use the cached version
- A single new command will invalidate the caching of all subsequent commands

Environments Best Practices

- There is a limit to the number of layers (that is, commands) a docker image can have. Currently, this limit is 127
- Keep in mind that the image upon which you are building may have already used many layers
- One way to work around this limit is to combine several commands into one via
 & &

Environments Best Practices

- If you are installing multiple python packages via pip, it's almost always best to use a single pip install command
- This ensures that dependencies and package versions are properly resolved.
- If you install via separate commands, you may end up inadvertently overriding a package with the wrong version, due a dependency specified by a later installation

Naming Conventions

- Name of the environment should be informative and include:
 - Version or Python and R
 - Name or abbreviation of Department
 - Key information on how the Environment will be used

[Back](#)

**FDS_Best_Prac_Survival_RWD_Py3.8_R4.1 -
Revision #1 ↴**

Information about Associated Projects

- Any projects that use the environment should have their default environment set to that specific environment
- The projects should show up in the ‘projects’ tab
- Before making any changes to the environment, stakeholders whose projects use the environment should be consulted
- If the environment is specific to an organization, a ‘gate-keeper’ should be responsible for updating or changing the environment

Overview	Revisions	Projects	Data Sets	Models	20 entries	Filter table entries...	Print
Project Path	Running	Runs	Results	jddavis1000/JnJ_Technical_Efficiencies_Working_Group	--	15 hours ago	

List Key Tools / Features

- At the top of the environment, the version of Ubuntu, key tools and features should be listed so that they are easily available for people considering use of the environment

Overview Revisions Projects Data Sets Models

Description

Ubuntu 18
R4.1
Python 3.8
Pandas
Sklearn
Matplotlib
Numpy
Psycopg2
Shap
Xgboost
Lifelines
Scipy
DSE Libraries

(Edit description)
Visibility
Globally Accessible (Edit Visibility)

Docker Settings

Base Environment



Install Packages in one line of code when possible

- Keep Docker file code clean and remove anything that is unnecessary (such as commented out code or instructions)

Dockerfile Instructions

```
1 RUN pip install pandas sklearn matplotlib numpy psycopg2 shap xgboost lifelines scipy
```

Your Dockerfile layers.

[Edit Dockerfile](#)

Pluggable Workspace Tools

Consider creating 'Starter' Files for Best Coding Practices

- A starter file can be created using a Run Setup Script
- The file should include instructions on how to use it
- The file should demonstrate best practices or how to import key libraries
- Files can be written in Python, R or both

Run Setup Scripts

Bash scripts to execute at the specified step in the lifecycle of your execution. These scripts are executed at runtime, so they are not run as root. They are not cached.

Pre Run Script

```
1 cat <<EOF >starter.py
2
3 """
4     This file is a best practices starter file. To use the file in your project please rename it to your ch
5
6 import pandas
7 import sklearn
8 import pandas.io.sql as sqlio
9 import psycopg2
10 import numpy
11 import seaborn
12 import matplotlib
13 import functions
14 from functools import reduce
15 import sklearn
16 from sklearn.model_selection import train_test_split
17 from sklearn.compose import ColumnTransformer
18 from sklearn.preprocessing import OrdinalEncoder
19 from sklearn.preprocessing import StandardScaler
20 from sklearn.model_selection import RandomizedSearchCV
21 from sklearn.model_selection import GridSearchCV
22 import sksurv
23 from sksurv.ensemble import RandomSurvivalForest
24 from sksurv.linear_model import CoxPHSurvivalAnalysis, CoxnetSurvivalAnalysis
25 from sksurv.metrics import concordance_index_censored
26 from sksurv.ensemble import GradientBoostingSurvivalAnalysis
27 import warnings
28 import shap
29 import xgboost
30 import lifelines
31 from lifelines.fitters.coxph_fitter import CoxPHFitter
32 from lifelines.statistics import proportional_hazard_test
33 import scipy
34 from scipy.stats import reciprocal
35 EOF
```

Script to execute after your project post-setup script

Where the Starter File Appears

- This can be set up in the pre-run script, but the suggestion is to use the /mnt/ directory as its easy for users to find
- The file will appear each time a new workspace is started, so users should rename any starter file they are working on before closing the workspace.

The screenshot shows the Jupyter Notebook interface with the 'Files' tab selected. The top navigation bar includes 'Files', 'Running', and 'Clusters'. On the left, there's a sidebar with a 'jupyter' icon. The main area displays a file list with the following details:

	Name	Last Modified	File size
<input type="checkbox"/>	0		
<input type="checkbox"/>	/ mnt		
	..	seconds ago	
<input type="checkbox"/>	results	19 days ago	
<input type="checkbox"/>	starter.py	2 hours ago	1.16 kB
<input type="checkbox"/>	working_file_2.py	19 days ago	960 B

Actions at the top right include 'Upload', 'New', and a refresh icon. A message at the bottom says 'Select items to perform actions on them.'

What the Starter File Looks Like

jupyter starter.py 2 hours ago

File Edit View Language Python

```
1 """
2     This file is a best practices starter file. To use the file in your project please rename it to your choice of names. A new
3     starter file will appear when you open your workspace next time."""
4
5 import pandas
6 import sklearn
7 import pandas.io.sql as sqlio
8 import psycopg2
9 import numpy
10 import seaborn
11 import matplotlib
12 import functions
13 from functools import reduce
14 import sklearn
15 from sklearn.model_selection import train_test_split
16 from sklearn.compose import ColumnTransformer
17 from sklearn.preprocessing import OrdinalEncoder
18 from sklearn.preprocessing import StandardScaler
19 from sklearn.model_selection import RandomizedSearchCV
20 from sklearn.model_selection import GridSearchCV
21 import sksurv
22 from sksurv.ensemble import RandomSurvivalForest
23 from sksurv.linear_model import CoxPHSurvivalAnalysis, CoxnetSurvivalAnalysis
24 from sksurv.metrics import concordance_index_censored
25 from sksurv.ensemble import GradientBoostingSurvivalAnalysis
26 import warnings
27 import shap
28 import xgboost
29 import lifelines
30 from lifelines.fitters.coxph_fitter import CoxPHFitter
31 from lifelines.statistics import proportional_hazard_test
32 import scipy
33 from scipy.stats import reciprocal
```



Spinning Up Your Workspace

On-Demand Distributed Computing

What is Parallel Computing?

- Type of computing in which many calculations or processes are carried out simultaneously on several nodes and threads within a CPU or GPU
- Limits
 - Available Parallelism
 - Load Balancing
 - Managing communication between processes
- Pros
 - Faster speeds for data processing and computations
 - Enabling Big Data and Machine Learning

What is Distributed Computing?

- When multiple computers, CPUs or GPUs are used, tasks can be distributed among the cluster components unevenly and in parallel
- First rule: Don't distribute your workload on clusters unless you see a need to
- Most deep learning and big data machine learning will be more performant on a distributed system
- Reinforcement learning is computationally intense, so distributed computing is helpful

Cluster Environments on Domino

When using on-demand Clusters in Domino you will have two separate environments:

1. One for the workspace/job
 - o See dockerfile instructions for [Spark](#), [Ray](#), [Dask](#) and MPI
2. One for the cluster workers/executors
 - o Developed with a different base image - see docs for [Spark](#), [Ray](#), [Dask](#) and MPI

Cluster Settings

- Select the Attach Cluster option
- Set the number of Workers/Executors, and hardware tiers for each
- Dedicated local storage will be mounted to /tmp and de-provisioned when the cluster is shut down

Launch New Workspace

Environment & Hardware
Domino Analytics and Small...

Data
demo-DFS-project

Compute Cluster (optional)

Attach Compute Cluster

none Spark Ray

Number of Workers 1 Max: 78

Worker Hardware Tier

Small (Kubernetes)
1 core · 1 GiB RAM · \$0.0011/min < 1 MIN

Head Hardware Tier

Small (Kubernetes)
1 core · 1 GiB RAM · \$0.0011/min < 1 MIN

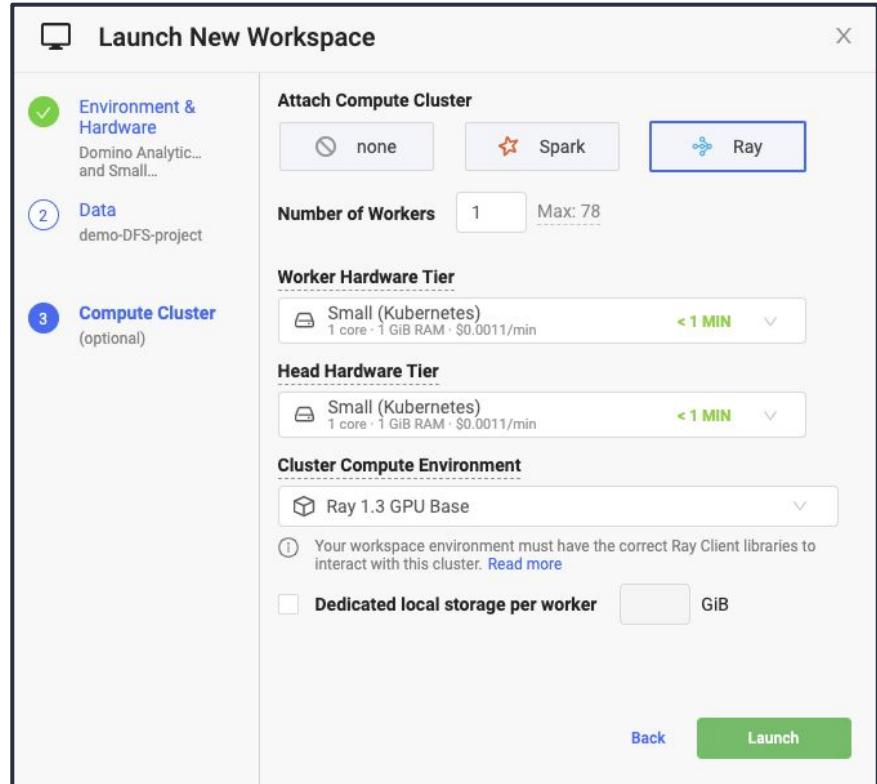
Cluster Compute Environment

Ray 1.3 GPU Base

Your workspace environment must have the correct Ray Client libraries to interact with this cluster. [Read more](#)

Dedicated local storage per worker GiB

Back Launch



Distributed Compute: Batch Jobs

- Set up the cluster when running a Job from the quick-action, files page, or Job dashboard
- The Spark or Ray UI is available for running Jobs from the details tab

The screenshot shows a job details page with the following information:

- Logs**, **Results**, **Details** (selected), **Comments**, **Resource Usage**
- Command**: [pi.py 2](#)
- Started on:** Apr 26th, 2020 @ 08:57:34 PM
- Input files**, **Output files**, **Results**
- Hardware:** Small (with a question mark icon)
- Environment:** Domino Analytics Distribution Py3.6 R3.6 - Revision #1
- Spark Cluster Settings** (status: Ready)
- NUM EXECUTORS**: 2
- EXECUTOR LOCAL STORAGE**: 30 GiB
- EXECUTOR HARDWARE**: small-k8s
- MASTER HARDWARE**: small-k8s
- COMPUTE ENVIRONMENT**: Spark base | **Spark**
- Spark Web UI** (link highlighted with a red box)

On-Demand Spark

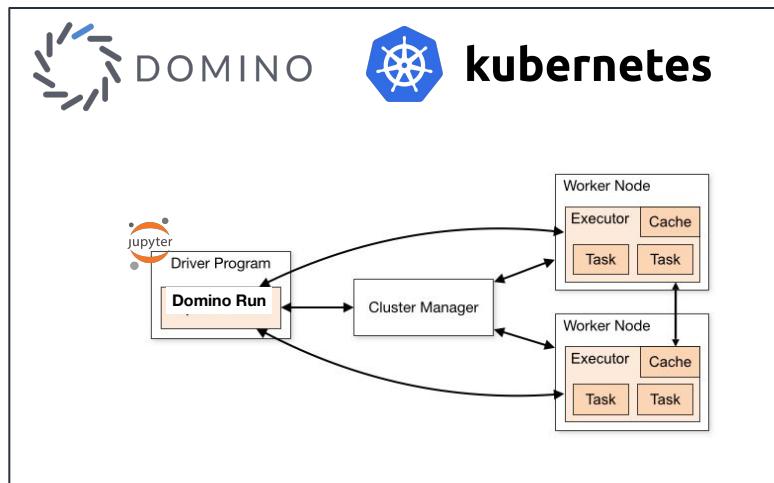
Agenda

- Setting up a Distributed Compute workspace for Spark
- Review of what Spark can do
- Spark Use Cases
- Calculating Pi – examples of non-parallel, parallel and distributed with Ray

Distributed Compute in Domino

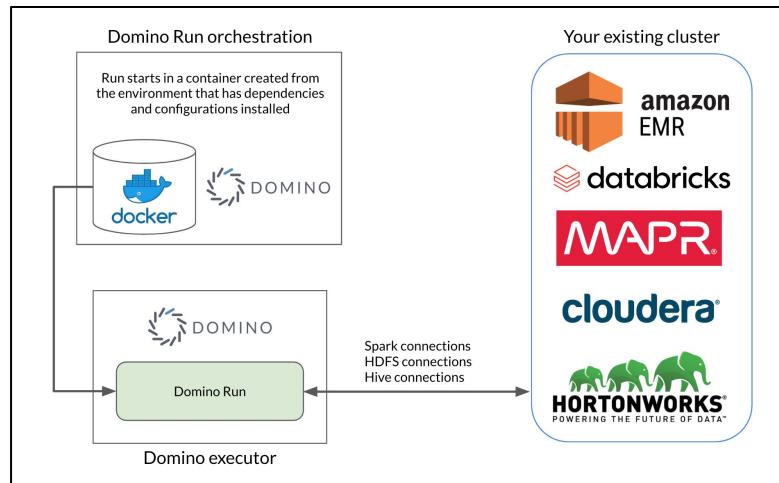
On-Demand Clusters

Natively orchestrated directly on Domino controlled infrastructure



External Clusters

Leverage existing long-lived Spark deployments in the enterprise



Spark on Demand in Domino: Use Cases

Distributed Machine Learning

Parallelize compute heavy workloads such as distributed training or hyper-parameter tuning

Take advantage of powerful machine learning algorithms from Spark MLlib

Interactive Exploratory Analysis

Efficiently load large data sets in distributed manner

Explore and understand the data using a familiar interface with Spark SQL

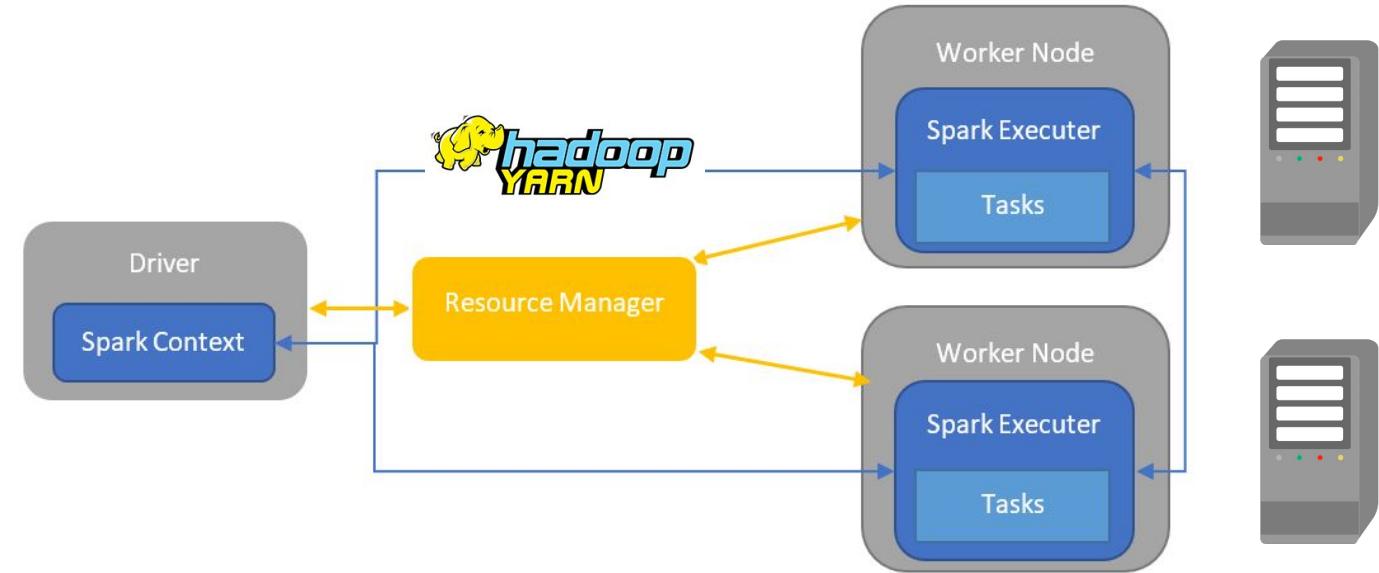
For experienced Spark practitioners

Featurization and Transformation

Sample, aggregate, and re-label large data sets

Optimal performance may require a practitioner who is skilled in tuning Spark

Spark Overview



On-Demand Distributed Computing Overview

- Available only to the current execution
- Use with data residing outside the cluster - i.e. in Domino datasets or an S3 buckets
- Web UIs for the associated cluster are available in the same workspace
- Learn more in [Domino 201](#)
- Clusters can be auto-scaled

Launch New Workspace

Environment & Hardware
Domino Standard and Small

Data
prediction_data

Compute Cluster (optional)

Attach Compute Cluster

none Spark Ray Dask

Cluster Size Limit: 23 executors
Min executors Max executors

1 Auto-scale executors

Executor Hardware Tier

Small 1 core · 4 GiB RAM < 1 MIN

Master Hardware Tier

Small 1 core · 4 GiB RAM < 1 MIN

Cluster Compute Environment

5.0 Spark Cluster Environment

ⓘ Your workspace environment must have the correct Spark Client libraries to interact with this cluster. [Read more](#)

Dedicated local storage per executor GiB

[Back](#) [Launch](#)

Accessing the Distributed Cluster UI

Available as a dedicated tab within your workspace

Screenshot of the Domino Data Lab interface showing the Spark Web UI tab highlighted.

Apache Spark 2.4.6

Spark Master at spark://spark-5f05747f6ec09a5660dcd538-master-0.spark-5f05747f6ec09a5660dcd538-headless.aws-staging-compute.svc.cluster.local:7077

URL: spark://spark-5f05747f6ec09a5660dcd538-master-0.spark-5f05747f6ec09a5660dcd538-headless.aws-staging-compute.svc.cluster.local:7077

Alive Workers: 3

Cores in use: 6 Total, 6 Used

Memory in use: 7.1 GB Total, 6.0 GB Used

Applications: 1 Running, 0 Completed

Drivers: 0 Running, 0 Completed

Status: ALIVE

Workers (3)

Worker Id	Address	State	Cores	Memory
worker-20200708072351-100.96.214.12-33084	100.96.214.12:33084	ALIVE	2 (2 Used)	2.4 GB (2.0 GB Used)
worker-20200708072351-100.96.242.37-34939	100.96.242.37:34939	ALIVE	2 (2 Used)	2.4 GB (2.0 GB Used)
worker-20200708072401-100.96.33.89-46588	100.96.33.89:46588	ALIVE	2 (2 Used)	2.4 GB (2.0 GB Used)

Running Applications (1)

Application ID	Name	Cores	Memory per Executor	Submitted Time	User	State	Duration
app-20200708072815-0000	(kill) Spark Test	6	2.0 GB	2020/07/08 07:28:15	ubuntu	RUNNING	8 s

Completed Applications (0)

Application ID	Name	Cores	Memory per Executor	Submitted Time	User	State	Duration
----------------	------	-------	---------------------	----------------	------	-------	----------

Tools and APIs for Spark

- Python API, PySpark
 - Easily use Python to code Spark applications
 - Syntax is a bit different than regular Python
 - Syntax is functional rather than object oriented
- R API, SparklyR
 - Syntax is the same as R code
 - Many R libraries are available natively
 - Many machine learning libraries are easily available
 - Hyper parameter tuning is available



Demo: 'Hello World' Example, Calculate Pi

On-Demand Ray

Agenda

- Setting up a Distributed Compute workspace for Ray
- Review of what Ray can do
- Ray Use Cases
- What Process Identifiers are and how to use them
- Calculating Pi – examples of non-parallel, parallel and distributed with Ray

Learning Goals

- Starting up your Workspace
- Understanding what Ray can do
- Understanding when Ray is appropriate to use
- Understanding the difference between regular calculations and distributed with Ray
- Know what a Process Identifier is and how to use it

Ray Overview

[Ray.io](#) provides a set of core low-level primitives ([Ray Core](#)) as well as pre-packaged libraries that take advantage of these primitives to enable solving powerful machine learning problems.

The following libraries come packaged with Ray:

- Tune: Scalable Hyperparameter Tuning
- Ray Train (formerly RaySGD): Distributed Training Wrappers
- RLlib: Scalable Reinforcement Learning
- Ray Serve: Scalable and Programmable Serving
- Ray Lightning - Distributed Pytorch Lightning

Ray on Demand in Domino: Use Cases

Distributed Multi-Node Training

Take existing PyTorch and Tensorflow models and scale them across multiple machines to dramatically reduce training times

Ray is suitable for both distributed CPU and GPU training

Hyperparameter Optimization

Launch a distributed hyperparameter sweep with just a few lines of code.

Take advantage of a large number of advanced parameter search algorithms.

Reinforcement Learning

Take advantage of a number of built-in reinforcement learning algorithms, along with a general framework for developing your own.

Steps to setting up your workspace

- Name your workspace
 - Use a name you will remember that indicates whether it is distributed or not and the type of tool used (i.e. in this case Ray)
- Choose your workspace environment
- Ensure your datasets are available
- Choose your scheduler and compute hardware tier
- Choose the number of workers

Distributed Compute |

Setting up your workspace

- With only a handful of specified parameters, such as the number of workers and the capacity of each worker, Domino will set up the cluster and seamlessly manage its lifecycle.
- Administrators retain control since the cluster configuration is based on the established Domino concepts of Hardware Tiers and Compute Environments.

Update Workspace

Attach Compute Cluster

Environment & Hardware and Small

Data CatsAndDogs

3 Compute Cluster (optional)

Number of Workers 8 Quota Max: 40

Worker Hardware Tier
Small 1 core · 4 GiB RAM < 1 MIN

Scheduler Hardware Tier
Small 1 core · 4 GiB RAM < 1 MIN

Cluster Compute Environment
Dask Worker

Your workspace environment must have the correct Dask Client libraries to interact with this cluster. [Read more](#)

Dedicated local storage per worker 50 GiB

[Back](#) [Save & Restart](#)

Accessing the Ray Cluster

Domino sets up key environment variables

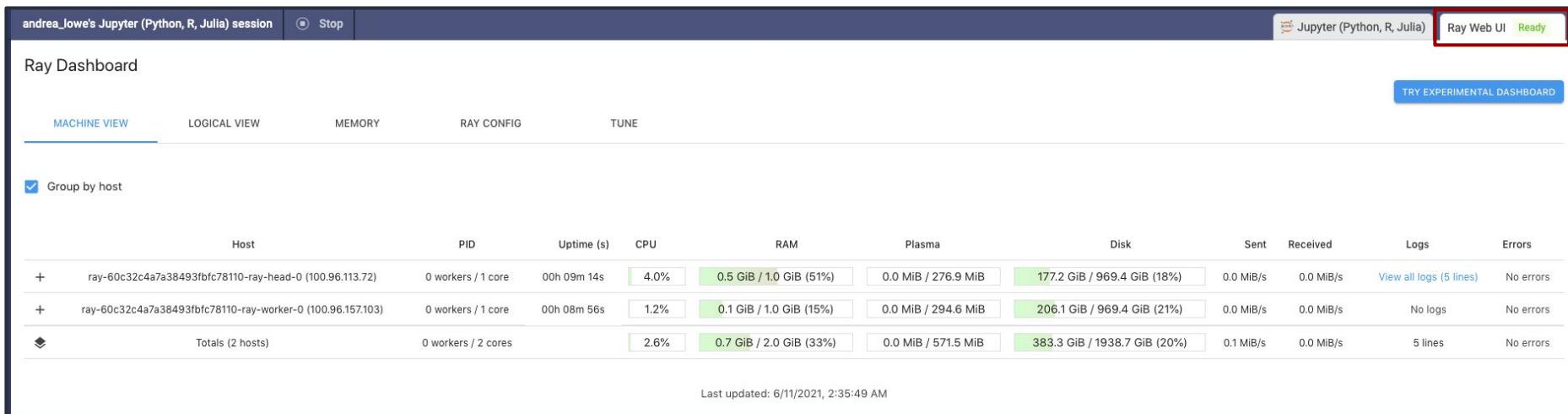
Use Ray Client instead of ray.init()

```
import ray
import ray.util
import os

if ray.is_initialized() == False:
    service_host = os.environ["RAY_HEAD_SERVICE_HOST"]
    service_port = os.environ["RAY_HEAD_SERVICE_PORT"]
    ray.util.connect(f"{service_host}:{service_port}")
```

Accessing Ray UI

The Ray dashboard is available as a dedicated tab within your workspace



The screenshot shows a Jupyter notebook interface with several tabs at the top: "andrea_lowe's Jupyter (Python, R, Julia) session", "Stop", "Jupyter (Python, R, Julia)", and "Ray Web UI Ready". The "Ray Web UI" tab is highlighted with a red box. Below the tabs, the content area is titled "Ray Dashboard". It features a navigation bar with tabs: "MACHINE VIEW" (which is active and highlighted in blue), "LOGICAL VIEW", "MEMORY", "RAY CONFIG", and "TUNE". There is also a "TRY EXPERIMENTAL DASHBOARD" button. Under the "MACHINE VIEW" tab, there is a checkbox labeled "Group by host" which is checked. The main table displays two hosts and their resource usage:

Host	PID	Uptime (s)	CPU	RAM	Plasma	Disk	Sent	Received	Logs	Errors
+ ray-60c32c4a7a38493fbfc78110-ray-head-0 (100.96.113.72)	0 workers / 1 core	00h 09m 14s	4.0%	0.5 GiB / 1.0 GiB (51%)	0.0 MiB / 276.9 MiB	177.2 GiB / 969.4 GiB (18%)	0.0 MiB/s	0.0 MiB/s	View all logs (5 lines)	No errors
+ ray-60c32c4a7a38493fbfc78110-ray-worker-0 (100.96.157.103)	0 workers / 1 core	00h 08m 56s	1.2%	0.1 GiB / 1.0 GiB (15%)	0.0 MiB / 294.6 MiB	206.1 GiB / 969.4 GiB (21%)	0.0 MiB/s	0.0 MiB/s	No logs	No errors
◆ Totals (2 hosts)	0 workers / 2 cores		2.6%	0.7 GiB / 2.0 GiB (33%)	0.0 MiB / 571.5 MiB	383.3 GiB / 1938.7 GiB (20%)	0.1 MiB/s	0.0 MiB/s	5 lines	No errors

At the bottom of the dashboard, it says "Last updated: 6/11/2021, 2:35:49 AM".



Demo: Workspace Set-up

Ray Remote Functions

- Parallelism or distribution of regular python functions
- The decorator `@ray.remote` is used to tell ray to set up the function as a series of objects, and the `ray.get` function will tell ray to execute the process and return the object.
- The `ray.put` function will put an object into memory for ray to use later to execute ray functions upon
- Must be written correctly or ray will not work

Turning a Regular Function into a Ray / Distributed Function

A few more examples below show how to appropriately use Ray to speed up calculations.

```
In [12]: def return_multiple():
    time.sleep(5)
    return 1, 2, 3

    st = time.time()
    a, b, c = return_multiple()
    end = time.time()
    print(a,b,c)
    print('The wall-clock time is ', str(end-st))
```

```
1 2 3
The wall-clock time is  5.00536847114563
```

```
In [13]: @ray.remote(num_returns=3)
def return_multiple():
    time.sleep(5)
    return 1, 2, 3

    st = time.time()
    a, b, c = return_multiple.remote()
    end = time.time()
    print(ray.get(a), ray.get(b), ray.get(c))
    print('The wall-clock time is ', str(end-st))
```

```
1 2 3
The wall-clock time is  0.0034894943237304688
```

How Ray Works: Process Identifier (PID)

- Each Ray session has a unique name
 - By default the name is `session_{timestamp}_{pid}` and `pid` belongs to the start-up process as it's the process that calls `ray.init()`
 - The process identifier can be used to trouble-shoot or trace errors during runs (i.e., is the error emanating from a head node or worker nodes).
- Ray can be run in parallel where all processes are run on a single node
- Ray can be run in a distributed fashion where some processes are on a head node and some are on a worker node

Example Code: Function without Ray

computing. Let's take a closer look below.

```
In [4]: import time
import os
import ray

y = 1
object_ref = y

def add(x, a=1):
    if x == 'add':
        answer = a + 1
    else:
        answer = a
    time.sleep(5)
    print(answer)

number_add = add('add')
number_none = add('hello')

object_ids = []
st = time.time()
for x in range(2):
    x = x
    y_id = add('add')
    object_ids.append(y_id) # the object ids will print out

## getting the results to pass to another function
objects = object_ids
end = time.time()
print("Time taken: ", str(end-st))

2
1
2
2
Time taken: 10.007688760757446
```

Example Code: Function with Ray

and see the difference

```
In [5]: import ray
import time

y = 1
object_ref = ray.put(y)

@ray.remote
def add(x, a=1):
    if x == 'add':
        answer = a + 1
    else:
        answer = a
    time.sleep(5)
    print(answer)

number_add = ray.get(add.remote('add'))
number_none = ray.get(add.remote('hello'))

object_ids = []
st = time.time()
for x in range(2):
    x = x
    y_id = add.remote('add')
    object_ids.append(y_id) # the object ids will print out

## getting the results to pass to another function
objects = ray.get(object_ids)
end = time.time()
print(str(end-st))

#notice that the process ids (pid) have the same number (223) except for the head node which has the number 221

(add pid=1056) 2
(add pid=1056) 1
(add pid=1056) 2
5.0638556480407715
(add pid=1054) 2
```

- Process IDs for this code included
- 1056 (three IDs)
- 1054 (one id)
- Each set of calculations was assigned a PID



Demo – Create a Remote Function, and Process Identifiers

Break

Calculating Pi with and without Ray

- Demonstrates use of large numbers / data with:
 - No parallelism or distribution of calculations
 - Parallelism using Python's multiprocessing library
 - Distributed and Parallelized code using Ray
- Pay special attention to the speed of the calculations
 - No parallelism or distribution of calculations is slowest
 - Parallelism helps
 - Distributed parallelism is the most efficient



Demo: Calculating Pi with Large Numbers using Distributed Compute with Ray

Recap of What We've Learned

- How to start a workspace
- How to turn a basic function into a Ray distributed Function
- Understanding how Ray works with Process Identifiers
- Calculating pi using Ray to demonstrate Ray's speed with big data

Recap Use Cases Ray

- Deep learning
- Computer vision
- Natural Language processing
- Transfer Learning
- Natural Language Generation
- Converting Tensorflow to distributed compute
- Converting Pytorch to distributed compute
- Hyper-parameter optimization

Dask in Domino

Agenda

- Differences between parallel and distributed computing
- Setting up a Distributed Compute workspace for Dask
- Review of what Dask can do
- Dask Use Cases
- Calculating Pi – "Hello World" Example
- Dask Pandas-Like Library
- Dask Machine Learning Library
- Recap

Learning Goals

- Starting up your Workspace
- Understanding what Dask can do
- Understanding when Dask is appropriate to use
- Understanding the difference between regular calculations and distributed with Dask
- Understand how to rewrite code to run on Dask

Dask Overview

- Dask provides a set of libraries with familiar syntax that are easy to use and distributes calculations or data operations over several workers (CPUs or GPUs).
- The following libraries that can be used with Dask (but aren't limited to):
 - Pandas-like library (built-in to Dask)
 - Scikit-learn-like library (Dask Machine Learning)
 - Xgboost integration with Dask
 - Ability to take a regular python function and convert it to a Dask (distributed) Function

Dask Distributed Compute | Benefits

Self-serve access

Bring up Dask clusters on-demand directly on the underlying Domino infrastructure with just a few clicks.

Parallelize workloads

Speed up training jobs by scaling beyond a single large machine.
Use multiple CPUs, GPUs, or large memory pools.

Use with popular libraries

Tight integration with NumPy, Pandas, Scikit-Learn and other popular data science packages to minimize existing code rewrite.

Dask on Demand in Domino: Use Cases

Working with Large Datasets

Great for scaling up Python data analysis or transformation where processing requires more resources than can be provided by a single machine.

Performed with minimal modification and without having to switch over to a different ecosystem like Spark.

Distributed Training

Dask provides a simple way to parallelize existing scikit-learn models.
For larger memory-bound workloads, there are Dask specific ML libraries (e.g. Parallel Meta-estimators, Incremental Hyperparameter Optimizers)

Custom Distributed Computations

The low-level Dask scheduling APIs can be used to build custom algorithms that can benefit from parallelism.

You control the business logic while Dask handles task dependencies, network communication, workload resilience, diagnostics, etc.



Demo: Creating Distributed Functions in Dask

Steps to setting up a workspace

- Name your workspace
 - Use a name you will remember that indicates whether it is distributed or not and the type of tool used (i.e. in this case Dask)
- Choose your workspace environment
- Ensure your datasets are available
- Choose your scheduler and compute hardware tier
- Choose the number of workers

Distributed Compute |

Setting up your workspace

- With only a handful of specified parameters, such as the number of workers and the capacity of each worker, Domino will set up the cluster and seamlessly manage its lifecycle.
- Administrators retain control since the cluster configuration is based on the established Domino concepts of Hardware Tiers and Compute Environments.

Update Workspace

Attach Compute Cluster

Environment & Hardware and Small

Data CatsAndDogs

3 Compute Cluster (optional)

Number of Workers 8 Quota Max: 40

Worker Hardware Tier
Small 1 core · 4 GiB RAM < 1 MIN

Scheduler Hardware Tier
Small 1 core · 4 GiB RAM < 1 MIN

Cluster Compute Environment
Dask Worker

Your workspace environment must have the correct Dask Client libraries to interact with this cluster. [Read more](#)

Dedicated local storage per worker 50 GiB

[Back](#) [Save & Restart](#)

Dask Distributed Functions

- Parallelism or distribution of regular python functions
- The decorator `@dask.delayed` is used to tell Dask to set up the function as a series of objects, and the addition of `.compute` function will tell Dask to execute the process and return the object.
- Must be written correctly or Dask will not work
- Let's look at a code snippet and see how it works

Turning a Regular Function into a Dask / Distributed Function

```
In [46]:
```

```
%%time

import dask

@dask.delayed
def inc(x):
    return x + 1

@dask.delayed
def add(x, y):
    return x + y

a = inc(1)      # no work has happened yet
b = inc(2)      # no work has happened yet
c = add(a, b)  # no work has happened yet
c = c.compute() # work starts and finishes
print(c)
```

```
5
```

```
CPU times: user 10.5 ms, sys: 0 ns, total: 10.5 ms
Wall time: 18.6 ms
```

Dask Distribution: Client Set-up

```
In [25]: from dask.distributed import Client
import os

service_host = os.environ["DASK_SCHEDULER_SERVICE_HOST"]
service_port = os.environ["DASK_SCHEDULER_SERVICE_PORT"]
client = Client(f"{service_host}:{service_port}")

# look at the client and scheduler

client

# you should now be connected to the cluster
# Dashboard link from the client object is clickable but will not route in Domino
# Use the embedded Dask Web UI tab instead
```

Out[25]:



Client

Client-72a8af49-793c-11ec-8160-da15e17a09f3

Connection method: Direct

Dashboard: <http://dask-61e8143c3d51792f465e7f27-dask-scheduler.fieldc272254-compute.svc.cluster.local:8787/status>

Scheduler Info

Submitting Jobs to the Client

- Two ways to do this:
 - Dask Delayed function creates a future that is executed with the .compute() is called
 - Client.submit function can take a regular function and submit it to the client to distribute to workers
- Both methods are equivalent except that Dask delayed creates a future function (stored in memory) that is not executed on until the .compute() is called
- Submitting to the client directly can be useful when one does not want to store functions in memory
 - To submit directly the syntax client.submit(function, term) is used

Using Dask Delayed: Example

```
WALL TIME: 11.2 s
```

```
In [8]: %%time
```

```
from dask import delayed

pi = delayed(pi)(10**7)
pi.compute()
```

```
CPU times: user 11.6 ms, sys: 64 µs, total: 11.7 ms
Wall time: 11.2 s
```

```
Out[8]: 3.1415925535897915
```

Using Dask's Client: Example

```
In [6]: import time
## compute pi without Dask - WIP - doesn't seem to be available

def pi(N):
    time.sleep(10)

    # Initialize denominator
    k = 1

    # Initialize sum
    s = 0

    for i in range(N):

        # even index elements are positive
        if i % 2 == 0:
            s += 4/k
        else:
            s -= 4/k

        # denominator is odd
        k += 2
    return s
```

```
In [7]: %%time

pi_client = client.submit(pi, 10**7)
pi_client = pi_client.result()
print(pi_client)

3.1415925535897915
CPU times: user 7.33 ms, sys: 3.67 ms, total: 11 ms
Wall time: 11.3 s
```



Demo: Calculating Pi with Large Numbers using Distributed Compute with Dask

Calculating Pi

- Demonstrates use of large numbers / data with:
 - No parallelism or distribution of calculations
 - Parallelism using Python's multiprocessing library
 - Distributed and Parallelized code using Dask
- Pay special attention to the speed of the calculations

Example Code: Calculate Pi without Dask

In [9]:

```
import time

def pi_single_term(i):
    time.sleep(0.01)
    # denominator is odd
    k = 2*i + 1
    # even index elements are positive
    if i % 2 == 0:
        x = 4/k
    # odd index elements are negative
    else:
        x = - 4/k
    return x
```

In [10]:

```
%%time
## compute pi without Dask
s = []
for i in range(10**3):
    s.append(pi_single_term(i))
sum(s)
```

```
CPU times: user 13.5 ms, sys: 3.4 ms, total: 16.9 ms
Wall time: 10.1 s
```

Pi is calculated using inference and a single term without distribution of the calculation

Example Code: Calculate Pi Dask Delayed

```
In [11]: %%time
## compute pi with Dask using Delayed

s = []
for i in range(10**3):
    s.append(dask.delayed(pi_single_term)(i))
dask.delayed(sum)(s).compute()

CPU times: user 77.9 ms, sys: 19 ms, total: 96.9 ms
Wall time: 984 ms

Out[11]: 3.140592653839794
```

Pi is calculated using inference and a single term with distribution of the calculation using Dask Delayed

Example Code: Calculate Pi Dask Client

```
In [12]: %%time
## compute pi with Dask using Client

s=[]
for i in range(10**3):
    s.append(client.submit(pi_single_term, i))
client.submit(sum, s).result()

CPU times: user 167 ms, sys: 10.1 ms, total: 177 ms
Wall time: 896 ms

Out[12]: 3.140592653839794
```

Pi is calculated using inference and a single term distribution of the calculation using Dask client



Demo: Using Pandas with Dask

Pandas versus Dask Dataframe

- Pandas dataframes are stored on a single CPU or GPU and not distributed across workers
- Dask Dataframes can be distributed across workers
- Syntax between the two is almost identical
- Easy to do data munging with very large data using Dask Dataframes

Reading a csv and getting results using Pandas

```
In [19]: import pandas as pd

df = pd.read_csv("/domino/datasets/local/polioData/polioData.csv")

def get_counts(df):
    by_state = df.groupby("state")
    incidence = by_state["incidence_ratio"]
    return incidence.value_counts()

result = get_counts(df)
result.sort_values(ascending=False, inplace=True)

print(result)

state  incidence_ratio
DE      0.00          1072
WY      0.00          1043
UT      0.00           949
MT      0.00           940
ID      0.00           940
...
KY      1.14            1
       1.13            1
       1.06            1
       1.05            1
WY      8.93            1
Name: incidence_ratio, Length: 6939, dtype: int64
```

Reading a csv and getting results using Dask Dataframes

```
In [20]: import dask.dataframe as dd

dd = dd.read_csv("/domino/datasets/local/polioData/polioData.csv")

def get_counts(df):
    by_state = df.groupby("state")
    incidence = by_state[ "incidence_ratio" ]
    return incidence.value_counts()

result = get_counts(dd)
result = result.compute(num_workers=4)
result.sort_values(ascending=False, inplace=True)

print(result)
```

```
state  incidence_ratio
DE      0.00          1072
WY      0.00          1043
UT      0.00           949
ID      0.00           940
MT      0.00           940
...
KY      1.19            1
      1.18            1
      1.14            1
      1.13            1
WY      8.93            1
Name: incidence_ratio, Length: 6939, dtype: int64
```

Recap of What We've Learned

- How to start a workspace
- How to turn a basic function into a Dask delayed Function
- Understanding how the Dask Client works
- Calculating pi using Dask to demonstrate Dask's speed with big data
- Pandas-like Library in Dask (`dask_distributed`)



Demo Using Dask – A Simple K-Means Clustering Example

Dask and Scikit-Learn Integration

- Dask has a machine learning library that closely mimics Sci-kit learn Libraries
- Scikit-learn can also be used natively with Dask using the @delayed futures
- Let's look at two ways to create a k-means function
 - Without Dask, just using Sci-kit Learn

K-means Clustering using Scikit Learn

Using Scikit Learn heavily on back we see a training time as noted below.

```
In [14]: # import libraries

from sklearn import cluster
import time
from sklearn import datasets
import matplotlib.pyplot as plt
%matplotlib inline
```

```
In [15]: X, y = datasets.make_blobs(n_samples=10**8, random_state=0,
                                 centers=3)
```

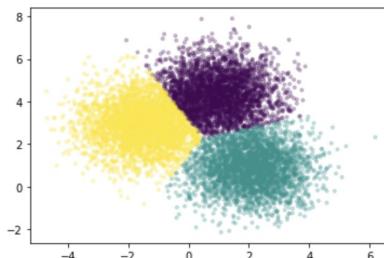
```
In [19]: %%time

km = cluster.KMeans(n_clusters=3)
km.fit(X)

CPU times: user 6min 34s, sys: 44.9 s, total: 7min 19s
Wall time: 3min 38s
```

```
Out[19]: KMeans(n_clusters=3)
```

```
In [20]: fig, ax = plt.subplots()
ax.scatter(X[:10000, 0], X[:10000, 1], marker='.', c=km.labels_[:10000],
           cmap='viridis', alpha=0.25);
```



K-means Clustering using Dask: Create Data and Dataframe

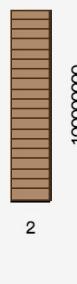
```
In [26]: ## import dask ml libraries
```

```
import dask_ml.datasets
import dask_ml.cluster
import time
import matplotlib.pyplot as plt
%matplotlib inline
```

```
In [27]: X, y = dask_ml.datasets.make_blobs(n_samples=10**8,
                                         chunks=1000000,
                                         random_state=0,
                                         centers=3)
X = X.persist()
X
```

```
Out[27]:
```

	Array	Chunk	
Bytes	1.49 GiB	15.26 MiB	
Shape	(100000000, 2)	(1000000, 2)	
Count	100 Tasks	100 Chunks	
Type	float64	numpy.ndarray	2



K-means Clustering Using Dask: Perform and Visualize

In [31]:

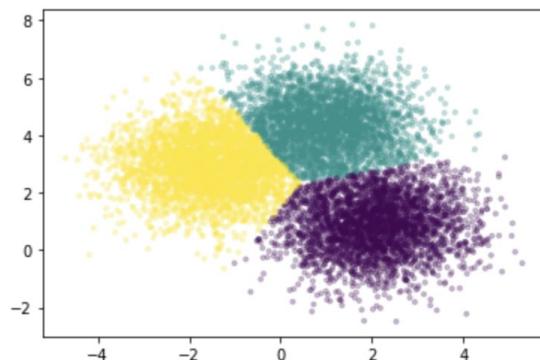
```
%%time  
  
km = dask_ml.cluster.KMeans(init='k-means||', n_clusters=3, init_max_iter=2, oversampling_factor=10)  
km.fit(X)
```

CPU times: user 1.81 s, sys: 23.7 ms, total: 1.83 s
Wall time: 33.6 s

Out[31]: KMeans(init_max_iter=2, n_clusters=3, oversampling_factor=10)

In [24]:

```
fig, ax = plt.subplots()  
ax.scatter(X[:10000, 0], X[:10000, 1], marker='.', c=km.labels_[:10000],  
          cmap='viridis', alpha=0.25);
```



Recap of What We've Learned

- How to start a workspace
- How to turn a basic function into a Dask delayed Function
- Understanding how the Dask Client works
- Calculating pi using Dask to demonstrate Dask's speed with big data
- Pandas-like Library in Dask (dask_distributed)
- An example of a distributed K-mean Clustering

Recap Use Cases Dask

- Large-scale Machine Learning
- Data munging with Pandas-like functions
- Visualizations
- Xgboost libraries

Dask and Ray Quick-Starts

- Quick-Start Projects are available in Domino Data Lab's open repository
- Dask and Ray quick starts are available
- Dask quick start here: [Dask Quick-Start](#)
- Ray quick start here: [Ray Quickstart](#)

☰ README.md

Welcome to Dask tutorial session in Domino!

- The purpose of this quick start project is to go through some fundamental Dask parallel computing capabilities on the Domino platform.
- This Quick Start Project will be useful for data scientists who plan to leverage Dask in their projects.
- Before starting this Dask Quick Start project, it is recommended to have Domino 101 and Domino 201 completed.
- This README.md file describes how to set up the environment and get started with Dask. Please take the following steps:

Step 0: Setup the environments for workspace base and compute cluster

Before launching a Dask cluster in Domino, you will need to have two Compute Environments set up:

- "Dask Workspace Environment" (please refer to appendix A for more information).
- "Dask Base Cluster Environment" (please refer to appendix B for more information).

You may want to check with your Domino admin to see if suitable Dask environments are already available before creating your own, or ask them to follow the instructions in appendix A and B to create "Global" environments so that any users can make use of them.

Step 1: Create the project and download the files

This project consists of this README file and three tutorial notebooks, hosted at <https://github.com/dominodatalab/domino-quickstart-dask>. Follow these steps to create your Dask quick-start project in Domino:

1. Create a new Project named "Dask-QuickStart" (or whatever name you like), hosted by Domino File System.
2. Download the files from this repo, then upload them to the Files section of your project.
 - 1-Calculate-Pi.ipynb
 - 2-Dask-DataFrame.ipynb



On-demand Open MPI Clusters

What is MPI?

MPI, or message passing interface, is a communication library widely used in high-performance computing

- It is one underlying communication mechanism for many higher-level machine learning frameworks (e.g. PyTorch, Tensorflow, Keras, MXNet etc)
- Frequently used in conjunction with Horovod but also applicable for broader use cases
- Python API exist called mpi4py

Domino On-demand MPI Use Cases

Domino on-demand MPI clusters are suitable for the following workloads:

- Distributed Multi-GPU Training: Open MPI is ideal for distributed multi-GPU training for Tensorflow, PyTorch, Keras, or MXNet models.
- High Performance Computing MPI clusters are generally faster than other distributed computing systems and highly customizable.
- Domino offers an easy interface for use of MPI (not HPC)

MPI Cluster Setup

MPI Environment Setup

When using on-demand MPI in Domino you will have two separate environments:

1. A Base environment for the workspace/job
2. The Open MPI cluster environment

The environments must have the same version of Open MPI installed, located in the same directory

MPI Environment Setup

We recommended using an NVIDIA [NGC container image](#) with MPI support for both environments

Use the option to make it [automatically compatible](#) for the Workspace/Job environment

New Environment

Name
MPI Environment

Description
Optional

Base Environment / Image

Start from an existing Environment
Inherit a base image, Dockerfile instructions & scripts from a Domino environment

Start from a custom base image
Use a custom Docker or container image URI from a registry like NGC

FROM nvcr.io/nvidia/tensorflow:22.03-tf1-py3

Automatically make compatible with Domino
You can review and update this configuration later

Supported Clusters

none Spark Ray Dask MPI

Visibility

Private (i)

Globally Accessible (i)

Cancel Customize before building Create Environment

MPI Environment Setup

We recommended using an NVIDIA [NGC container image](#) with MPI support for both environments

Select MPI for the cluster environment

 New Environment

Name
MPI Cluster Environment

Description
Optional

Base Environment / Image

Start from an existing Environment
Inherit a base image, Dockerfile instructions & scripts from a Domino environment

Start from a custom base image
Use a custom Docker or container image URI from a registry like NGC

FROM nvcr.io/nvidia/tensorflow:22.03-tf1-py3

Supported Clusters

 none  Spark  Ray  Dask  MPI

Visibility

Private ⓘ

Globally Accessible ⓘ

Cancel Customize before building Create Environment

MPI Cluster Environment Setup

For simple, CPU-only workloads, we vendor matching images:

Workspace/Job:

quay.io/domino/mpi-environment:ubuntu18-py3.8-r4.1-mpi4.1.2-domino5.1.1

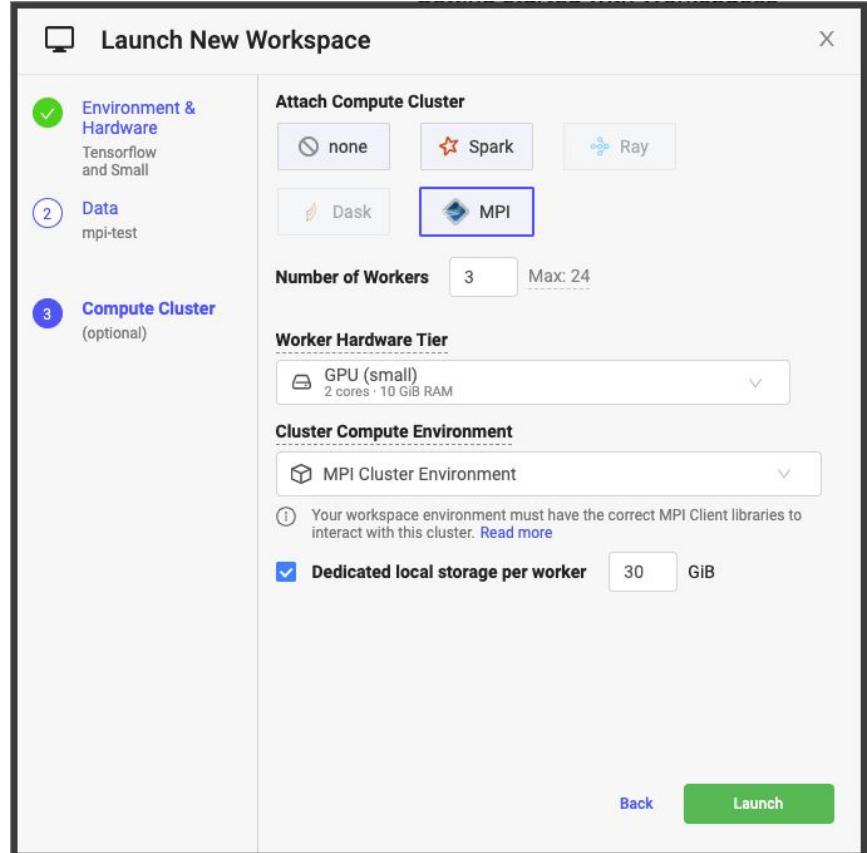
Cluster:

quay.io/domino/mpi:Mpi4.1.2-Py3.8.12

Working with MPI Clusters

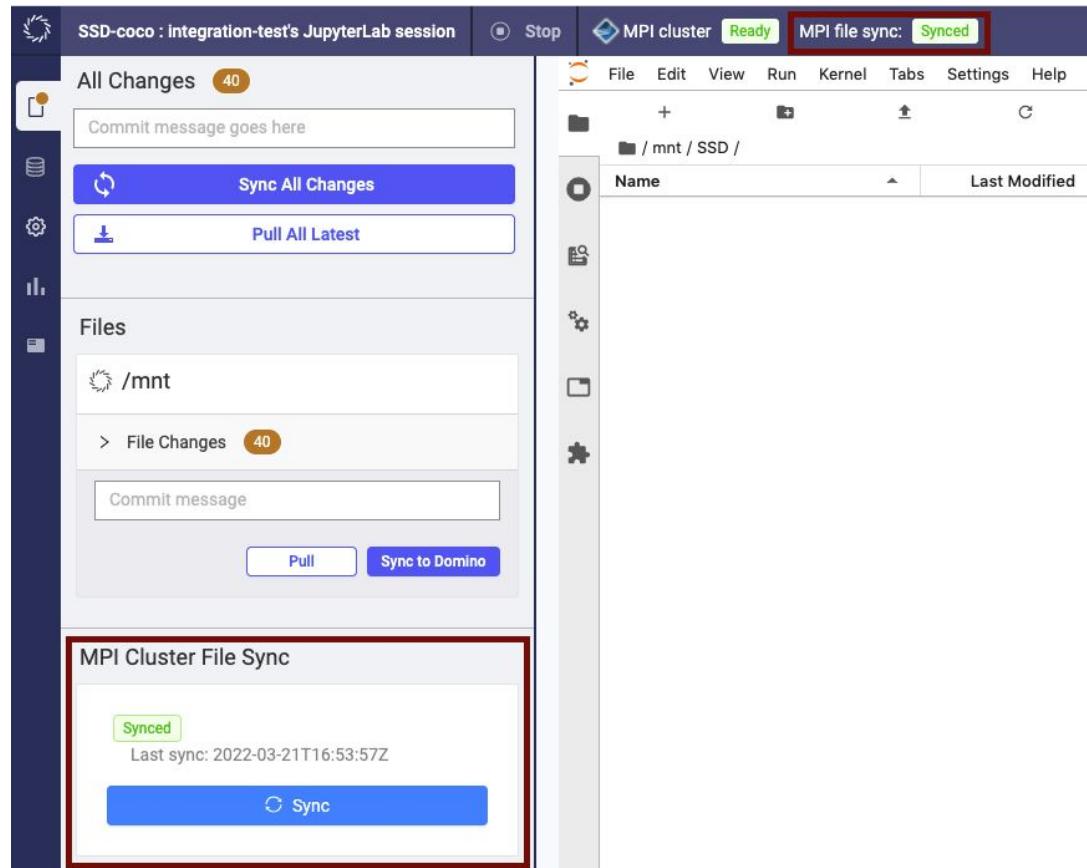
Launch an MPI Cluster

- MPI clusters do *not* have a scheduler node
- Choose number of workers and their resources
- Add temporary local storage if needed: mounted to /tmp



Workspace

- There is no MPI user interface (as with other clusters)
- Files must be manually synced to worker nodes if changed after Workspace starts
- Domino datasets are automatically mounted to worker nodes



Connect to the MPI cluster

Default configurations

- A hostfile is created with the name of the worker nodes, located at /domino/mpi/hosts
- Hosts are set to all workers. This does not include the Workspace/Job container.
- Slots are based on the CPU/GPU cores in the selected worker hardware tier. The minimum is one.
- Defaults are set for mapping (socket) and binding (core)

Connect to the MPI cluster - Workspaces

Submit `mpirun` jobs within Workspace

You can supply arguments for the `mpirun` command as described in the [Open MPI docs](#), including:

- `--x <env>`: This controls the settings to distribute an existing environment variable to all workers
- `--hostfile <your hostfile>`: Specify a new hostfile with custom slots.
- `--map-by <core>`: Map to the specified object.
- `--bind-to socket`: Bind processes to the specified object.

Connect to the MPI cluster - Workspaces

Code example:

To add `--bind-to none`, which specifies that a training process should not be bound to a single core, and `--map-by slot`, use:

```
mpirun \
    --bind-to none \
    --map-by slot \
    python my-training.py
```

Using Python API for Open MPI

- Python API exists and must be installed on both the workspace and clusters by indicating so in the two environments
- Python wrapper requires very little knowledge of Open MPI
- Documentation can be found here: [Documentation \(mpi4py\)](#)
- For our ‘hello world’ example we will Calculate Pi



Demo Using MPI – Calculate Pi

Submitting a File to the MPI Cluster

- Calculate Pi will use a basic Monte Carlo Method as we have done with our other distributed compute methods
- Code available in C and Python
- Example uses mpi4py API to submit the MPI code to run on Domino
 - Requires a file that is to be submitted to the MPI cluster
 - Requires a command line interface to submit file using python API
 - Very similar to how MPI works with supercomputing applications
- Other methods include using shell files to submit R or Python code

GPUs in Domino

GPUs

Perform multiple, simultaneous computations enabling the distribution of training processes

Large number of simple cores vs a few complicated cores (CPU)

Note that GPUs can have a bandwidth bottleneck issue - transferring large amounts of data to the GPU can be slow

- Optimizing this process is covered in the tutorial notebooks

NVIDIA and Domino

GPUs available as hardware tiers

⊖ Hardware tier

Tier	Core	RAM	Cost
Small	1 core	4 GB RAM	\$0.0011/min
Large	6 cores	28 GB RAM	\$0.0064/min
Medium	2 cores	8 GB RAM	\$0.0021/min
NGC	1 core	10 GB RAM	\$0.00/min
XLarge	64 cores	256 GB RAM	\$0.051/min
GPU (1 V100) - Global	6 cores	28 GB RAM	\$0.051/min
GPU (2 V100s)	6 cores	28 GB RAM	\$0.102/min
spark-gpu-k8s	6 cores	24 GB RAM	\$0.051/min
GPU (1 V100) Ray	4 cores	20 GB RAM	\$0.00/min

NGC containers available with Domino configurations or can be made automatically compatible

PyTorch

Image	URI
	https://ngc.nvidia.com/catalog/containers/nvidia:pytorch

Domino registry path: `quay.io/domino/ngc-pytorch:20.12-py3`

Versions: Ubuntu 18.04, CUDA 11

Base Image: `docker pull nvcr.io/nvidia/pytorch:21.02-py3`

Notes: N/A

Start from a custom base image
Use a custom Docker or container image URI from a registry like NGC

FROM `nvcr.io/nvidia/tensorflow:21.11-tf2-py3`

Automatically make compatible with Domino
You can review and update this configuration later

System Utilization

- While a model is training, you may want to confirm that it's making full use of your hardware.
- If it isn't, that's a sign that you can do things like train larger batches, a larger model, or do more things in parallel.
- `nvidia-smi` shows information about the GPUs in your system and their memory/processor usage.
- `top` is a commonly-used linux command showing the most active processes.

System Utilization

- You may occasionally need to clear cached data from the GPU between model trainings
- `torch.cuda.empty_cache()`

Optimization

In software development, it's good to put effort into making something faster when you know that the part you are working on is the bottleneck.

`line_profiler` is a great Jupyter extension to profile functions line-by-line:

```
%load_ext line_profiler
```

Optimization

It's best practice to use a command like the one below instead of hard-coding GPUs, so your code can still run (very slowly!) on a cpu-only machine:

```
device = 'cuda' if torch.cuda.is_available() else 'cpu'  
print('Using {} device'.format(device))
```



Optimizing GPUs Demo

Advanced Course Summary



Great Job! You've completed this course!
The main learning points from this course are:

- Setting your project up for success
- Git integration, git-based projects and importing a git repo
- Domino Environments, Custom Images and Best Practices
- Benefits and Use Cases for On-Demand Distributed Computing in Domino
- Ray, Dask and MPI Integration, Distributed Computations
- GPUs Provide Performance and Optimization in Domino

Advanced Course Summary



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- GPUs Provide Performance and Optimization in Domino



Thank you!

Any Questions?

Help us improve! Please fill out our post-training survey here:

http://bit.ly/domino_training_survey

Code Repository: https://github.com/jddavis1000/Rev3_Advanced_Data_Science