Building Apptainer Containers on Demand Using Globus Compute

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About me…

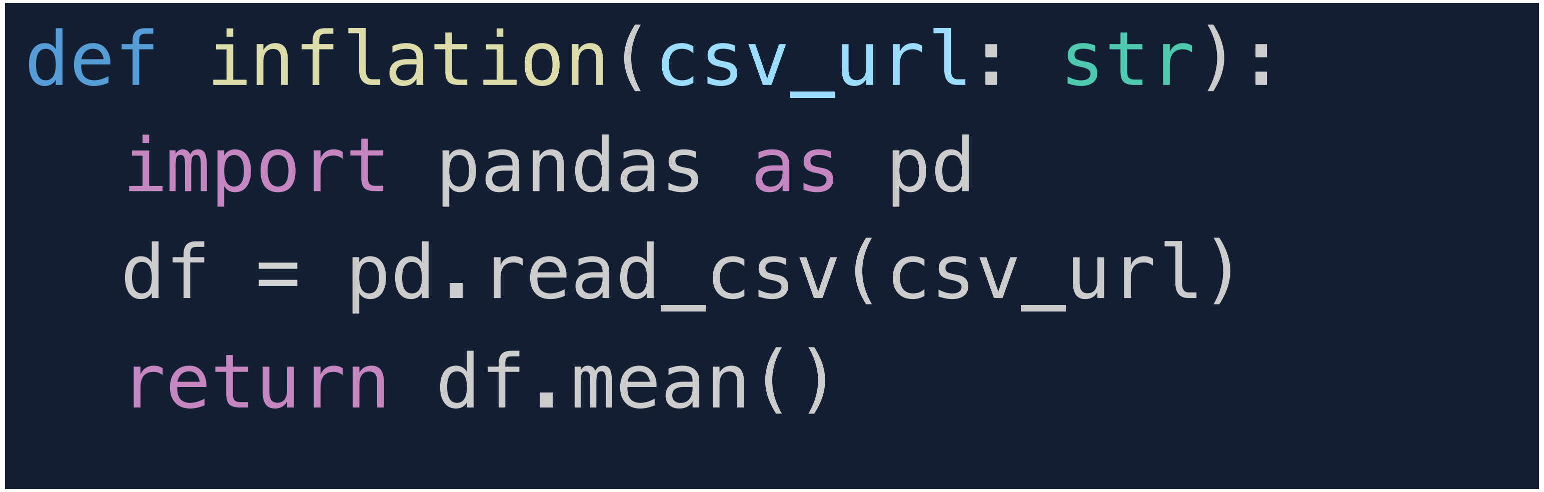
- Sr Research Software Engineer at NCSA
- Background in IT Consulting in Industry
- Contributor to
  - Globus Compute
  - Garden
  - Institute for Research and Innovation in Software for High Energy Physics (IRIS-HEP)
  - Data Management Consulting

Overview

- Dependency management in Globus Compute
- Lessons learned from Container Service
- Introducing the custom-image-builder library
- Try it out!

Dependency Management in GC

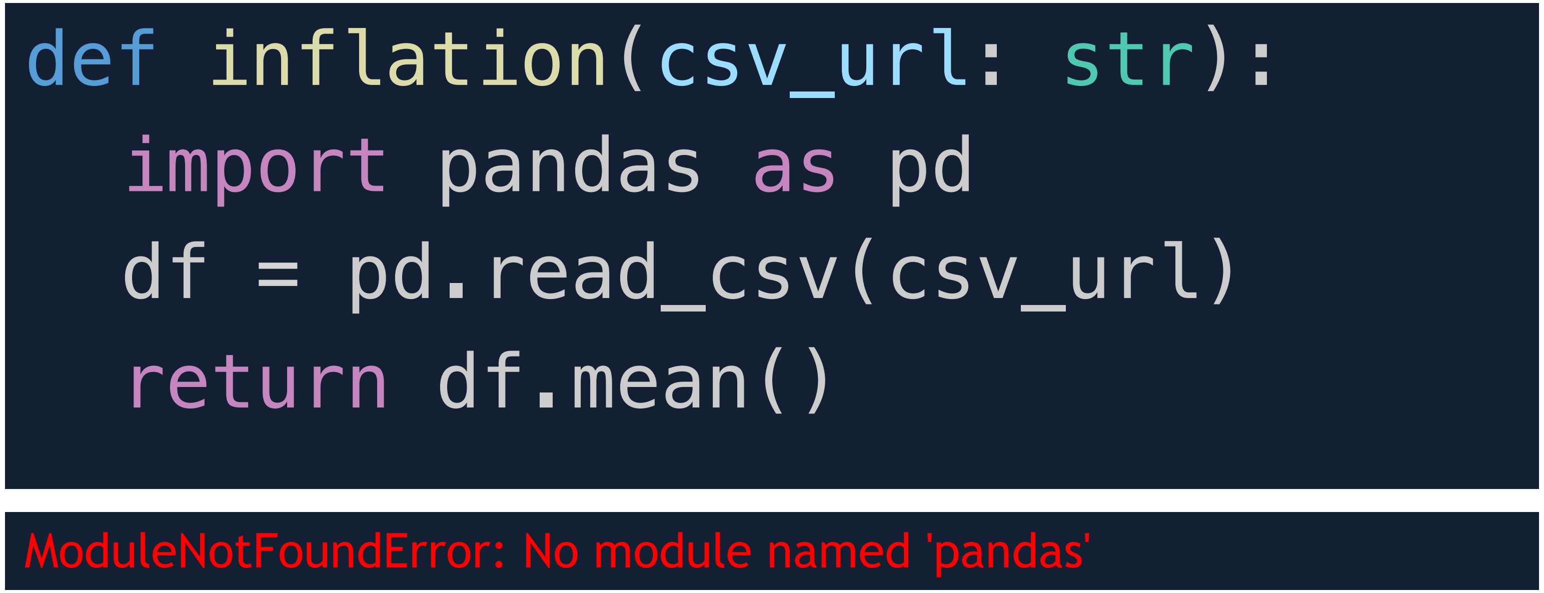
- Imports must sit inside the function
- The worker in the endpoint must have all dependencies installed



```
def inflation(csv_url: str):
  import pandas as pd
  df = pd.read_csv(csv_url)
  return df.mean()
```

Dependency Management in GC

- Imports must sit inside the function
- The worker in the endpoint must have all dependencies installed

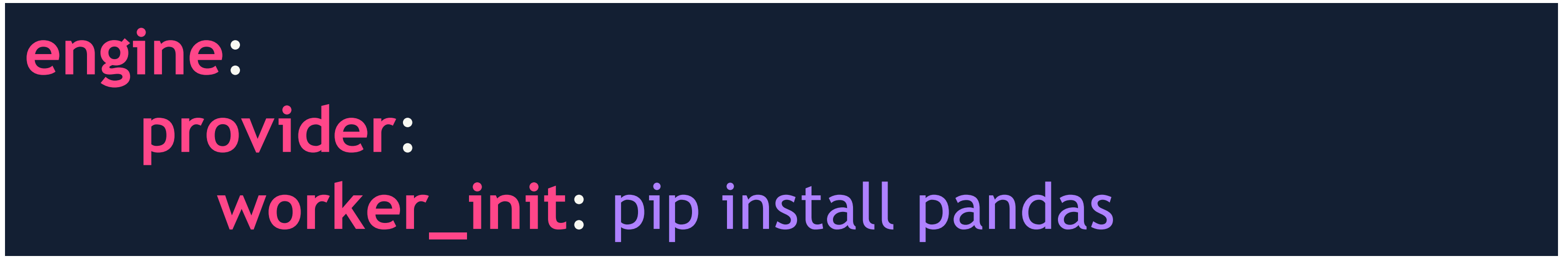


```python
def inflation(csv_url: str):
  import pandas as pd
  df = pd.read_csv(csv_url)
  return df.mean()
```

```
ModuleNotFoundError: No module named 'pandas'
```

Current Solution

- In the endpoint configuration



```
engine:
    provider:
        worker_init: pip install pandas
```

Drawbacks

- Hardcoded
- Each unique environment requires its own endpoint
- Opaque

Container Service

- Service deployed inside Globus Compute Cluster
- Accepts repo2docker style container spec
- Builds on demand
- Publish to DockerHub
- Conveniently integrated with Globus Compute container objects

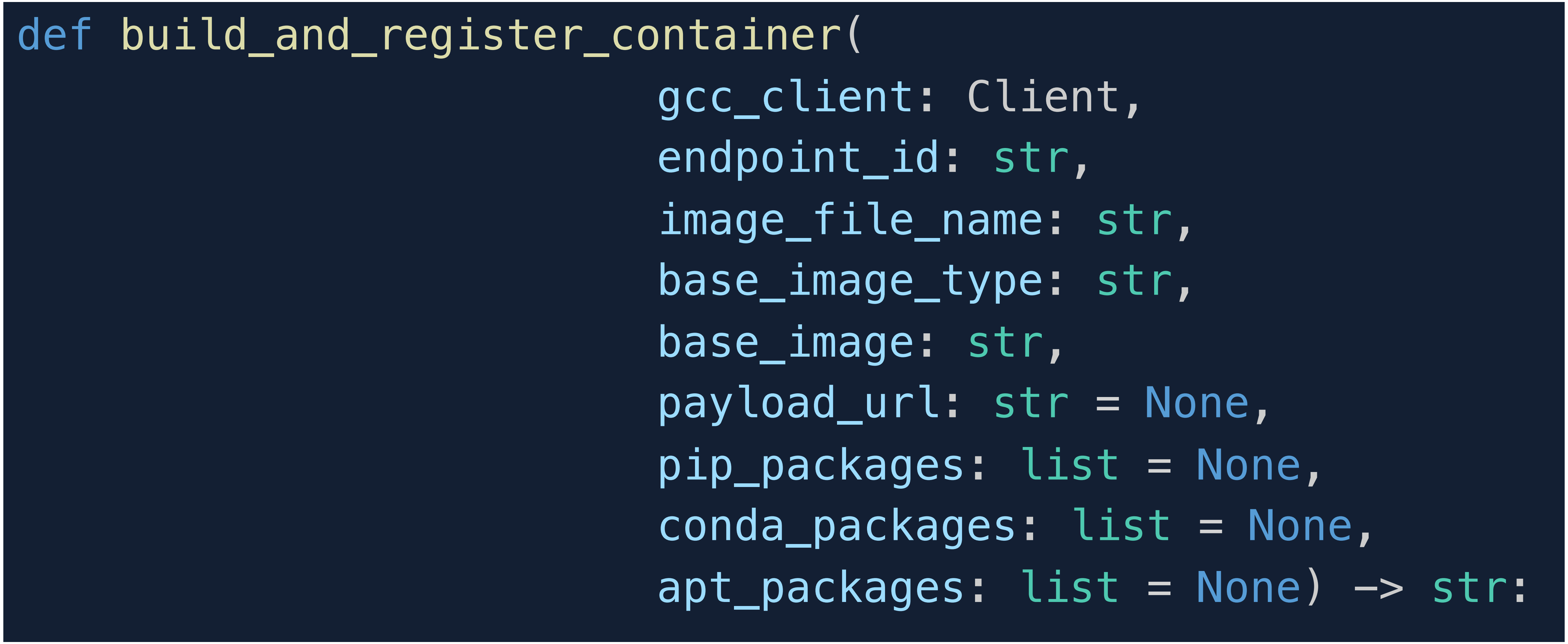
Container Service: Lessons Learnt

- Very convenient for users
- Unbounded compute requirement
- Difficult to manage docker image repository
- Only works on Kubernetes based endpoints

Enter the Custom-Image-Builder

- Pip installable library
- Runs as Globus Compute Task on any endpoint
- Accepts repo2docker style container spec
- Writes out an apptainer env file
- Executes apptainer build
- Registers container

Build and Register Container



```python
def build_and_register_container(
                         gcc_client: Client,
                         endpoint_id: str,
                         image_file_name: str,
                         base_image_type: str,
                         base_image: str,
                         payload_url: str = None,
                         pip_packages: list = None,
                         conda_packages: list = None,
                         apt_packages: list = None) -> str:
```

Example

```
image_builder_endpoint = "5cdc5147-378c-4ed9-8ede-25fa3614e6aa"
gcc_client = Client()

container_id = build_and_register_container(gcc_client=gcc_client,
                                    endpoint_id=image_builder_endpoint,
                                    image_file_name="my-pandas-image",
                                    base_image_type="docker",
                                    base_image="python:3.8",
                                    pip_packages=["pandas"])

with Executor(endpoint_id=image_builder_endpoint,
              container_id=container_id) as ex:
   fut = ex.submit(my_function)
```

Try it out!

```
% pip install custom-image-builder
```

Current caveats

- *Only works with globus-compute-endpoint 2.2.0*
- *Requires python 3.9*

Gratitude

- Ben Blaiszik
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- KJ Schmidt
- Owen Price Skelly
- Steve Wangen

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Find Out More….

https://pypi.org/project/custom-image-builder/

https://github.com/ncsa/CustomImageBuilder

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