Cloud computing for neuroimaging

Sorry, what is this cloud thing again?

The cloud can be a lot of different things

- You are already doing cloud computing!
- Computers you can't touch
- Computers you rent
- A set of technologies and practices
- Focus on efficiency and automation

The merits of the cloud

The advantages of renting computers from a vendor

- Scalability
- Elasticity
- Frequent upgrades
- A dizzying array of services

The merits of the cloud

"Cattle, not pets"

- Portability
- Verifiability
- Explicit/Declarative configuration

But there are issues

- $$$
- Complexity
- Learning curve
- "I'm a brain scientist, not a dev-ops engineer!"

To the clouds!

Ultimately, we might not have a choice!

- Datasets that are too large to move (HCP: 80TB and 15 million files)
- "Bring the compute to the data" -- what does that mean?
- New kinds of hardware:
  - GPU
  - TPU
  - Quantum computing

Let's look at a few things in detail

- Starting a machine in the cloud
- Reading neuroimaging data in the cloud
- Processing data in the cloud (at scale!)
- Sharing computation and analysis through Binder

Processing data at scale

Cloudknot: scaling your existing (Python) code in the (AWS) cloud

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AWS Batch

Pros:

- Abstracts away infrastructure details
- Dynamically provisions AWS resources based on requirements of user-submitted jobs
- Allows scientists to run 100,000+ batch jobs

Cons

- AWS Web Console resists automation
- Requires learning new terminology
- Does not easily facilitate reproducibility

AWS Batch workflow

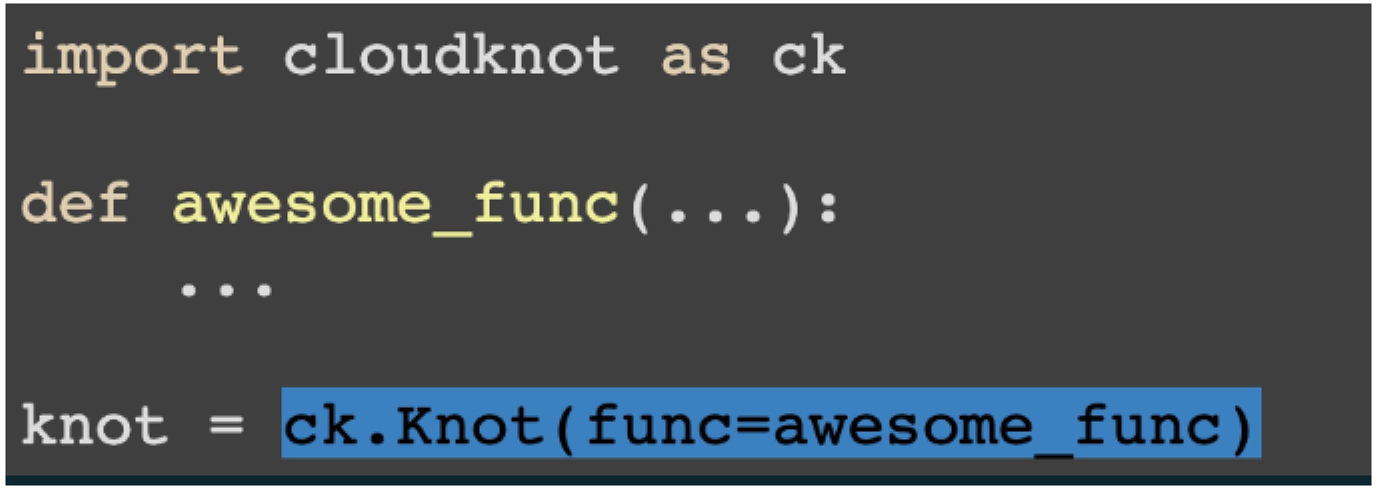
- Build a Docker image (local machine)
- Create an Amazon ECR repository for the image (web)
- Push the build image to ECR (local machine)
- Create IAM Roles, compute environment, job queue (web)
- Create a job definition that uses the built image (web)
- Submit jobs (web)

Cloudknot:

Implements Single Program Multiple Data (SPMD) parallelism

Where:

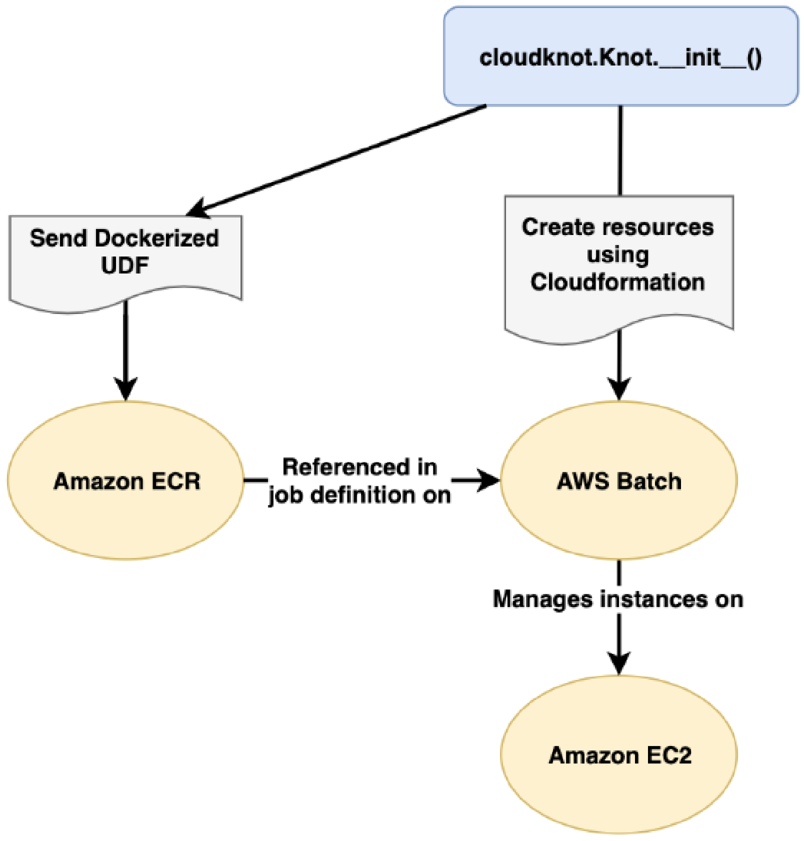
- Single program: Python function
- Multiple data: a sequence of arguments to this function



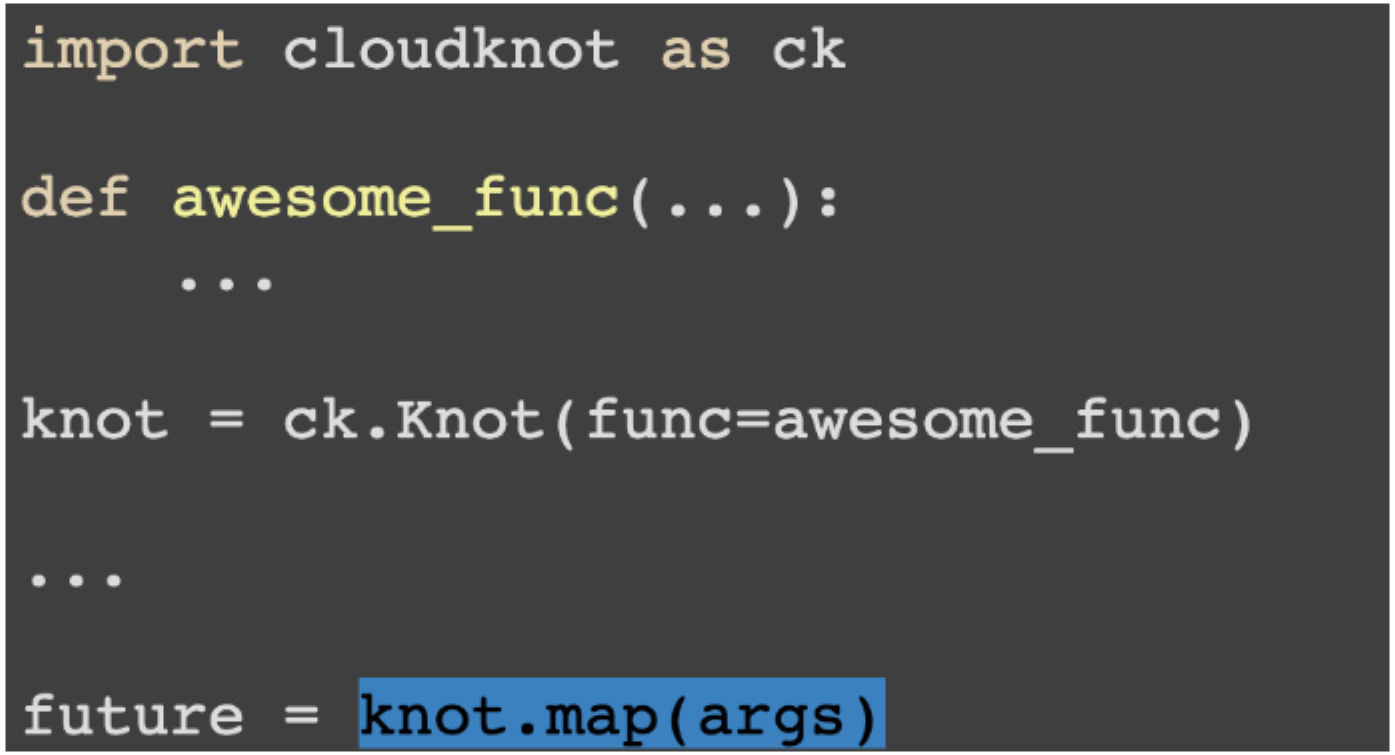
```
import cloudknot as ck

def awesome_func(...):
    ...

knot = ck.Knot(func=awesome_func)
```


cloudknot.Knot.__init__()
Send Dockerized UDF
Create resources using Cloudformation
Amazon ECR
Referenced in job definition on
AWS Batch
Manages instances on
Amazon EC2

Single Program



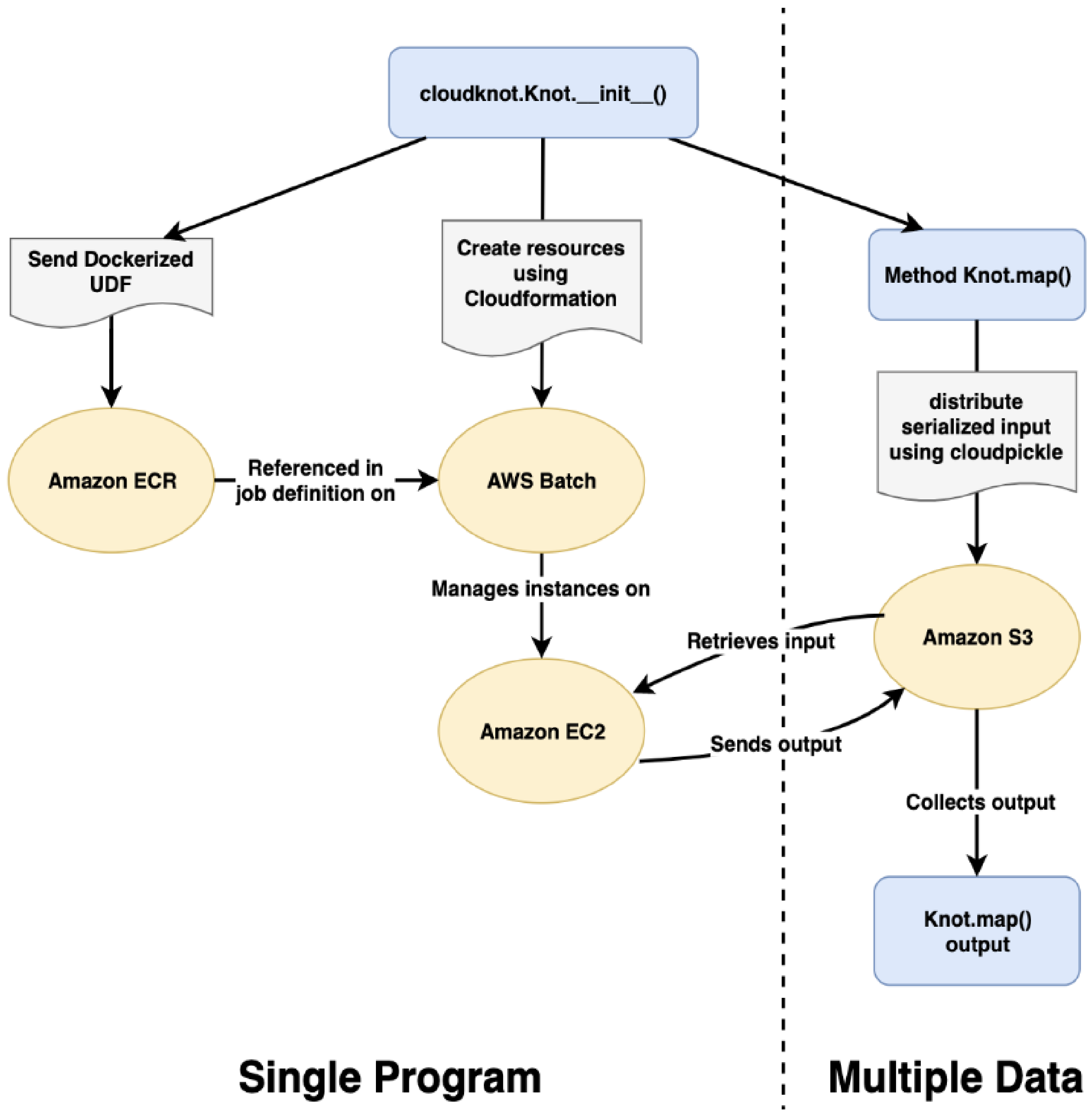
```
import cloudknot as ck

def awesome_func(...):
    ...

knot = ck.Knot(func=awesome_func)

...

future = knot.map(args)
```


cloudknot.Knot.__init__()
Send Dockerized UDF
Create resources using Cloudformation
Method Knot.map()
distribute serialized input using cloudpickle
Amazon ECR
Referenced in job definition on
AWS Batch
Manages instances on
Amazon S3
Retrieves input
Amazon EC2
Sends output
Collects output
Knot.map() output
Single Program
Multiple Data