Argonne NATIONAL LABORATORY

# Federated HPC for On-demand Data Science

funcX

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globus labs

# The need for federated, on-demand HPC

1. Support a new class of workloads
   - Real-time, interactive, stream processing, next-gen instruments, ML training, on-demand inference
2. Democratize access to diverse resources
   - Simplify scaling up
   - Facilitate multi-site deployments
   - Standardize access to specialized resources
   - Abstract heterogeneous compute infrastructure
3. Enable fluid function execution across the computing continuum
   - Containers enable portability and sandboxing
   - Networks allow code and data to be sent anywhere

# Existing research computing infrastructure has significant barriers for use

- Complex queuing systems with unpredictable delays
- Coarse allocation blocks
  - Not designed for short-duration tasks with variable resource needs
- Steep learning curve and lack of portability
  - Translation to different schedulers (and update when they inevitably break)
  - Heterogeneous architectures
  - Different modules and source code
  - Different container technology


There is an impedance mismatch between many workloads and existing infrastructure available to scientific users

# Serverless computing

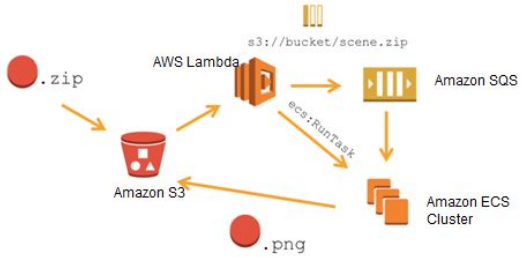
Provider runs infrastructure and manages allocation of resources

Function as a Service (FaaS)

- Pick a runtime (python/JS/R etc.)
- Write function code
- Run (and scale)

Low latency, on-demand, elastic scaling

Combine functions to solve complex problems

# funcX: creating a function serving ecosystem

**Functions:**

- Register once, run anywhere, any time

**Endpoints:**

- Dynamically provision resources, deploy containers, and execute functions
- Exploit local architecture/accelerators

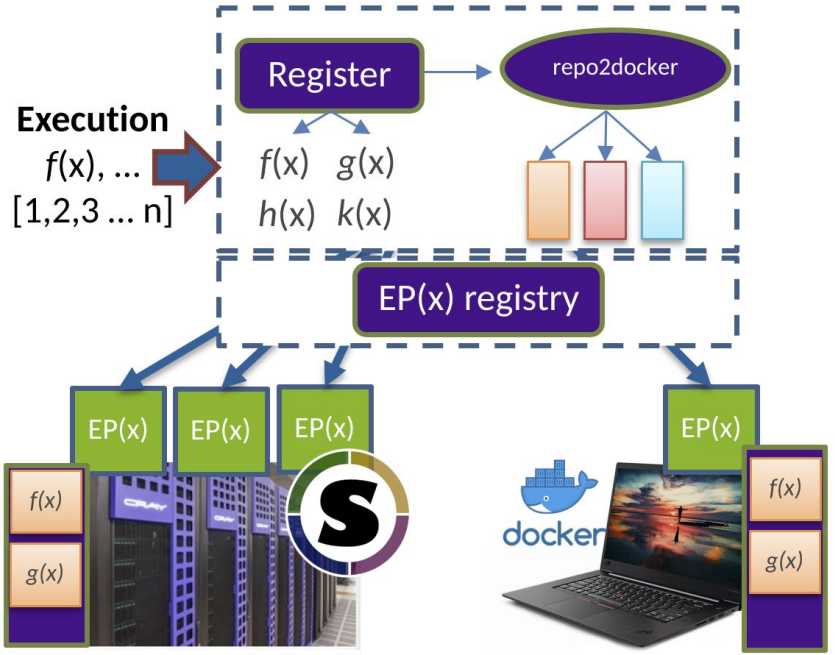
**funcX Service:**

- Register and share endpoints
- Register, share, run functions

Turn ***any*** machine into a function serving endpoint

Route functions to remote endpoints

- Closest, cheapest, fastest, accelerators
- …

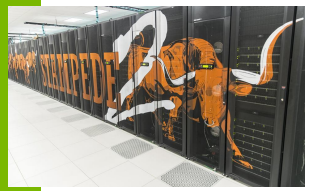


# Deploying a funcX endpoint

- Pip install funcX (e.g., using Conda)
- **Authenticate** and register with the funcX service
- Configure the endpoint for the local resources
- Examples: https://funcx.readthedocs.io/en/latest/endpoints.html#example-configurations

```
from funcx.config import Config
from parsl.providers import SlurmProvider
from parsl.launchers import SrunLauncher

config = Config(
    provider=SlurmProvider(
        'debug',
         launcher=SrunLauncher(),
         nodes_per_block=5,
         init_blocks=1,
         min_blocks=1,
         max_blocks=1,
         worker_init='source activate funcx',
         walltime='00:30:00',
    ),
    max_workers_per_node=28,
)
```




XSEDE


Google Cloud

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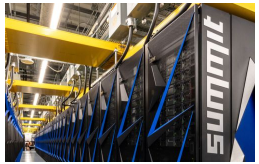



Open Science Grid


amazon web services

# Coding the computing continuum with funcX

**1. Define Python functions and register functions with funcX**

- Codes are serialized and stored on the cloud
- Registration returns a UUID for the function which is used for invocation

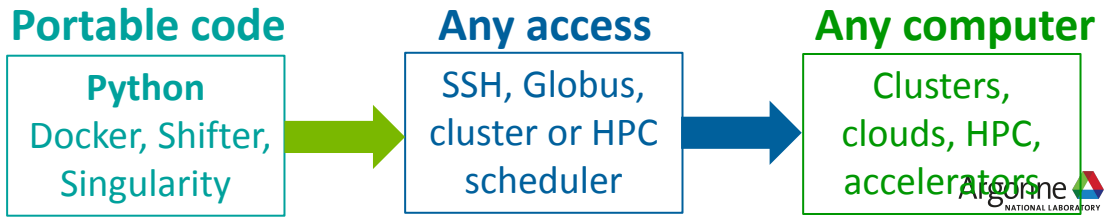
**2. Run the function on a specified endpoint**

- args* and kwargs* are serialized and sent to funcX
- Function code and inputs routed to endpoint

**3. Retrieve Results**

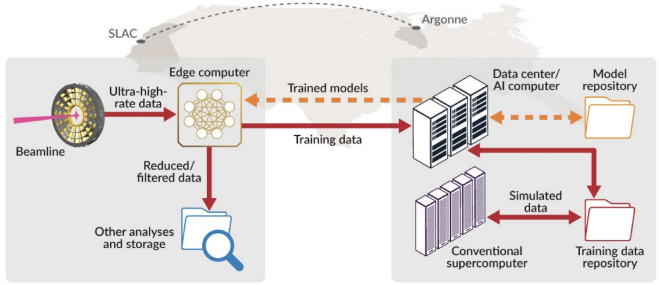
- Inspect status, wait on results, retrieve outputs

```
[1]: from funcx.sdk.client import FuncXClient
     fxc = FuncXClient()

[2]: def funcx_sum(items):
         return sum(items)

[3]: func_uuid = fxc.register_function(funcx_sum,
                                       description="A sum function")
     print(func_uuid)

     ce23d1c0-91f1-49df-a30b-0672453d8f9b

[4]: payload = [1, 2, 3, 4, 66]

     endpoint_uuid = '4b116d3c-1703-4f8f-9f6f-39921e5864df' # Tutorial endpoint

     res = fxc.run(payload, endpoint_id=endpoint_uuid, function_id=func_uuid)
     print(res)

     7508c2e7-3026-4ee3-95b3-25f7a605d893

[5]: fxc.get_result(res)

[5]: 76
```

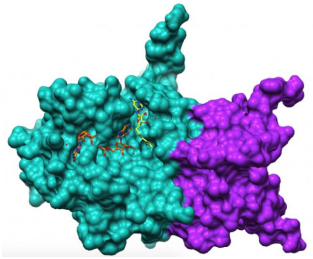


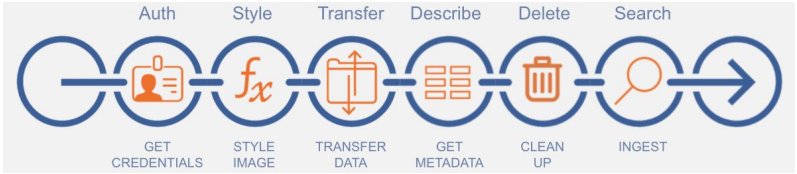
# Data Science with funcX

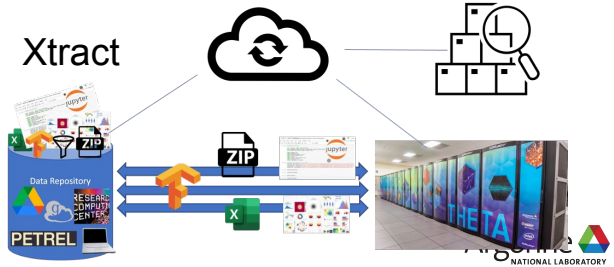
- Train ML models
- ML inference on-demand
- Distributed analysis pipelines
- Multi-site HPC campaigns
- Screening 180B molecules
- Solving covid structures
- Fitting as a Service tool for HEP
- Inverse spectroscopy at scale
- On-demand metadata extraction
- RuralAI and robots at the edge
- Delta: smart placement of tasks
- FLoX: federated learning on funcX




**DLHub**
Data and Learning Hub for Science





# Thanks!

https://funcx.org

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Join us on Slack: https://funcx.org/support.html