Parsl & funcX: Build and test challenges

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Parsl: A Python parallel scripting library

https://parsl-project.org

https://github.com/Parsl/parsl

Apps define opportunities for parallelism

- Python apps call Python functions
- Bash apps call external applications
- Implemented using decorators

Apps can be run remotely

Apps are asynchronous - return “futures”, a proxy for a result that might not yet be available

Apps run concurrently respecting dataflow dependencies. Natural parallel programming!

Parsl scripts are independent of where they run. Write once run anywhere!

```
pip install parsl
```

```
@python_app
def hello ():
    return 'Hello World!'

print(hello().result())
```

```
Hello World!
```

```
@bash_app
def echo_hello(stdout='echo-hello.stdout'):
    return 'echo "Hello World!"'

echo_hello().result()

with open('echo-hello.stdout', 'r') as f:
     print(f.read())
```

```
Hello World!
```

Try parsl via binder: https://parsl-project.org/binder

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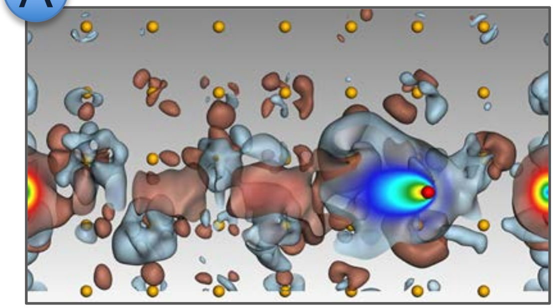
Parsl is being used in a wide range of scientific applications

- **A** Machine learning to predict stopping power in materials
- **B** Protein and biomolecule structure and interaction
- **C** LSST simulation and weak lensing using sky surveys
- **D** Cosmic ray showers in QuarkNet
- **E** Information extraction to classify image types in papers
- **F** Materials science at the Advanced Photon Source
- **G** Machine learning and data analytics in materials

A



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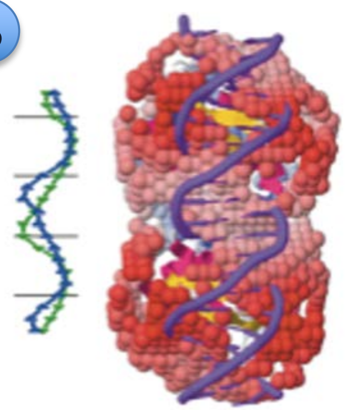

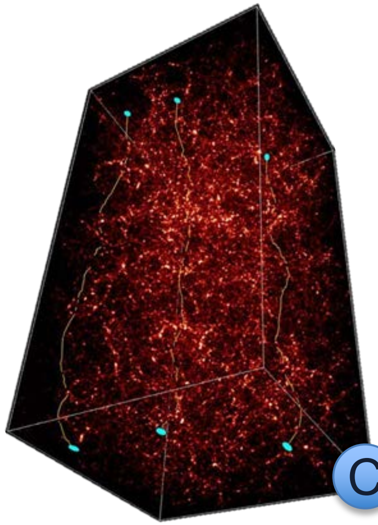

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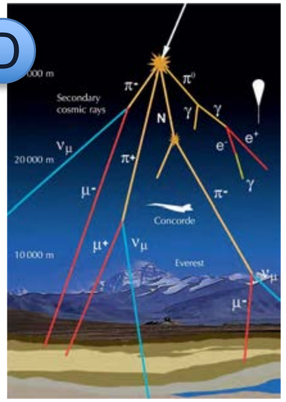

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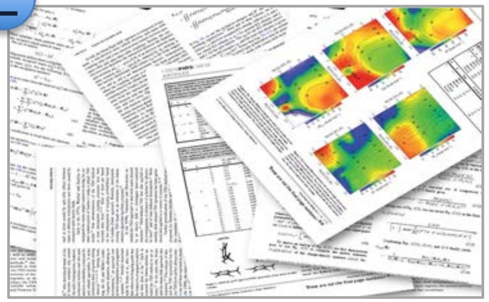

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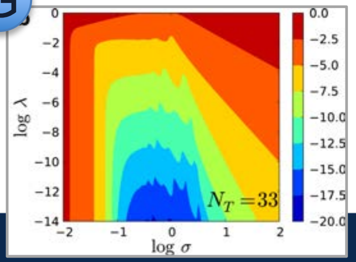

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funcX: Portable serverless computing for science

https://funcx.org

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

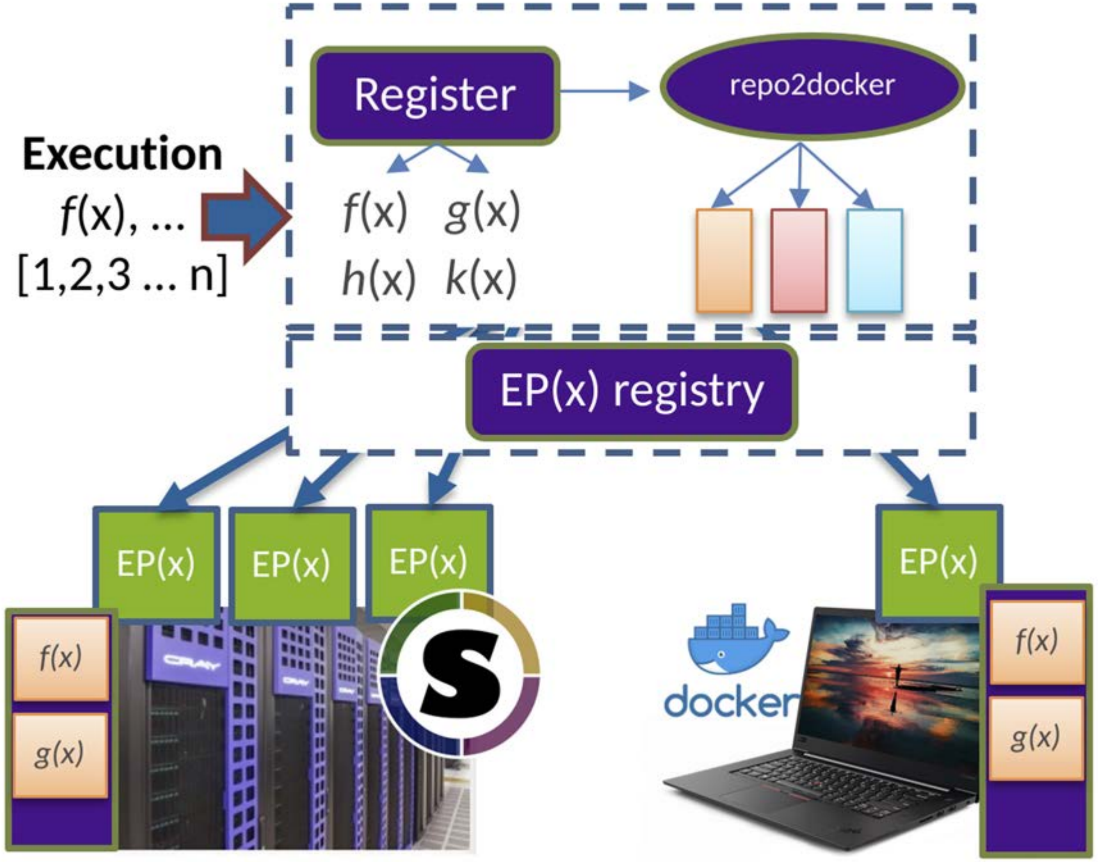
Remove barriers to using diverse and distributed infrastructure

Functions:

- Register once, run anywhere
- Can associate a container for encapsulation
- Authn/z (via Globus Auth) for user execution
- Add Globus group to a function to share it

Endpoints:

- Lightweight agent that can be deployed by users
- Abstracts underlying resource and elastically scales to demand



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funcX use cases

Metadata extraction (Xtract)

- Metadata extractors implemented as funcX functions; either distribute metadata extraction tasks to data or bring data to the cloud & act on it

Machine Learning inference (DLHub)

- Performs on-demand machine learning inference tasks, with inference requests routed to a funcX function executed within a model's container, using funcX endpoints on Kubernetes clusters that dynamically scale containers to serve ML models

Synchrotron Serial Crystallography & X-ray Photon Correlation Spectroscopy

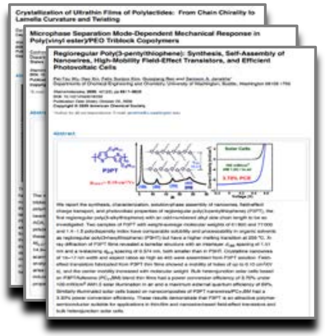
- High throughput analysis: as data are collected at the beamline, they are moved to ALCF and funcX functions are triggered to perform analyses

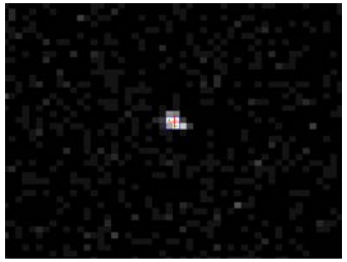
Quantitative Neurocartography

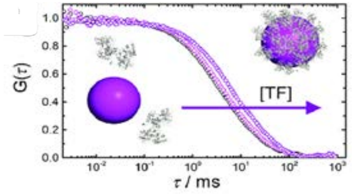
- Users invoke tasks on supercomputers via Automo library via funcX functions to create previews or perform full reconstructions w/ GB-TB of data

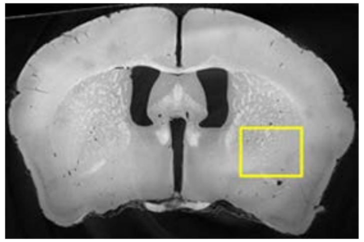
Real-time data analysis in High Energy Physics

- Aggregates histograms of analysis products in real time via Coffea framework using funcX backend to process 300m events in 9 min across 2 resources









Enabling portability in Parsl & funcX: *providers*

The same Parsl app or funcX function can be run locally, on grids, clouds, or supercomputers

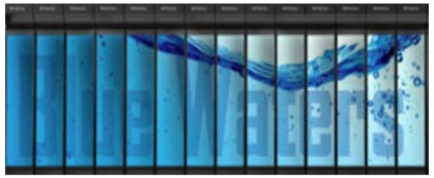
Config object specify how to run on resources; can be built by users, and are provided for common resources

- Includes: authentication method, scheduler choice, queue/job parameters, file transfer method

Growing support for various schedulers and cloud vendors

Open Science Grid

amazon web services



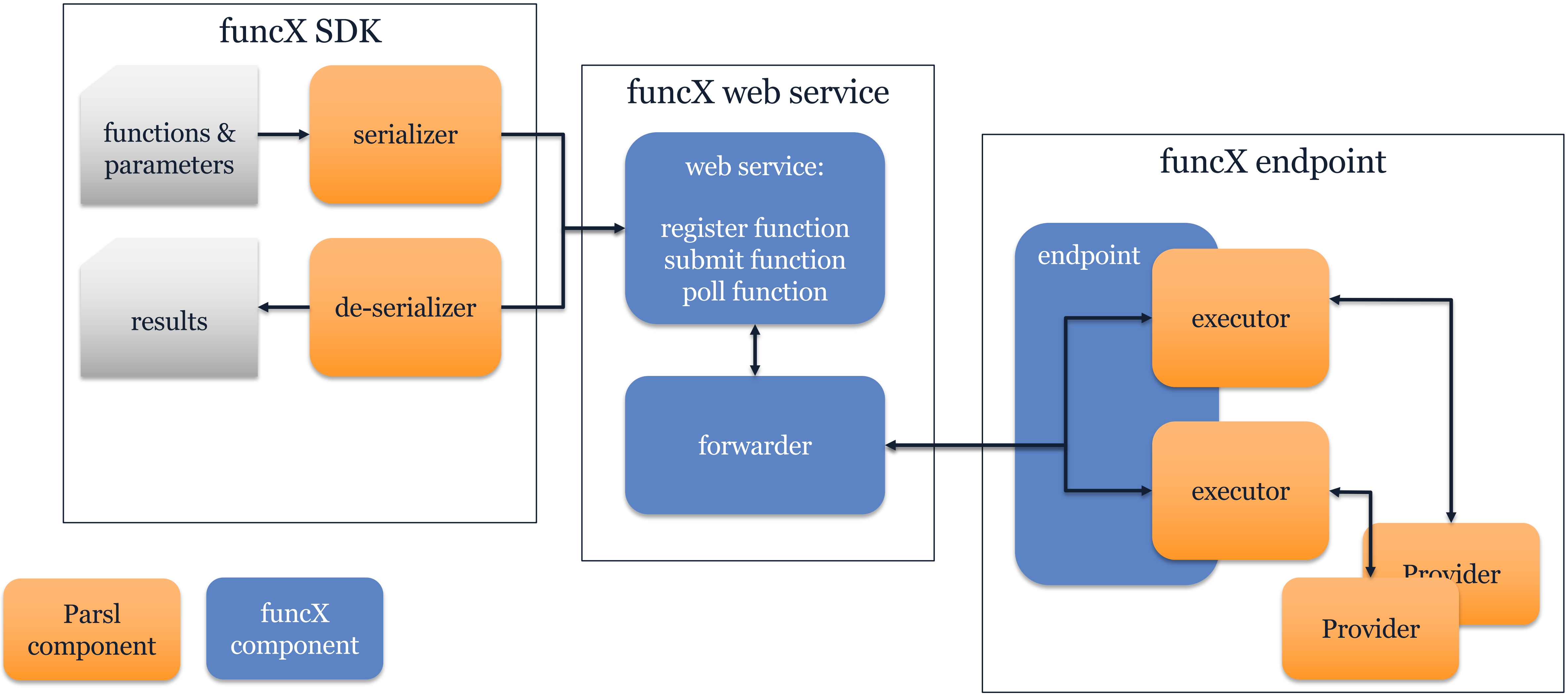
Google Cloud

XSEDE

⊟ Configuration

- How-to Configure
- Comet (SDSC)
- Cori (NERSC)
- Stampede2 (TACC)
- Theta (ALCF)
- Cooley (ALCF)
- Swan (Cray)
- CC-IN2P3
- Midway (RCC, UChicago)
- Open Science Grid
- Amazon Web Services
- Ad-Hoc Clusters
- Further help

funcX and Parsl



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Challenge: testing on real systems

- Traditional CI tries to provide a nice clean isolated environment for building software
- But we need a way to test on various HPC/cloud systems, with different schedulers, access, environments, configurations, etc.
  - We need to see how the system is set up in practice, and not be cleanly isolated from it in our CI
- Administrative/political problem:
  - In CI model, an unknown person, Sue, makes a PR to code, which triggers an attempt to run and test that code
  - As developers/maintainers, we also want to do this on a set of HPC platforms
  - HPC administrators: "Any random user can provide code and you want to automatically run it on my system? No!"

Challenge: debugging user problems

- Users have problems
- Sometimes they do things we don't expect
  - Can try to address through better documentation
- For Parsl, generally hard to know exactly what they are doing
    - We don't have access to the system they are using
    - We don't have access to their logs
    - Leads to lots of interactive discussion, very resource intensive, not scalable
- Sometimes they find bugs in our software that we can then fix, which they then need to download and install
- funcX's hybrid cloud/distributed architecture allows us to see errors that users are having, and sometimes fix things behind the scenes without needing to distribute new software

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Challenge: keeping our own software in sync

- In funcX we can struggle to keep many different things in sync: Python versions, SDK version, endpoint version. Mostly because we aren't always backwards compatible.
- We also need to sync with external dependency changes
- Keeping things in sync uses a huge amount of developer time and is even less glamorous than bug-fixing
- Hierarchy of developer excitement:
  new features > bug-fixing > packaging and release management

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Challenge: changing needs

- Initially, a newly developed product must move fast to be useful to its users
  - Requirements are discovered through use
- Later, a product must be stable be useful to its users
  - Moving too fast becomes a problem
- The "correct" balance changes over the project's lifetime

- This tension between experimental vs production isn't unique to software
- Also seen in hardware testbeds that initially don't want to support production science but eventually can be "frozen" by it

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Challenge: developer ecosystem

- Parsl funded by NSF award for initial development
  - That award is ending soon
  - How do we maintain what we've built?
    - Check/merge PRs, work with users, fix bugs, support new platforms, …
- Need for funding for core team (and others)
  - Can we depend entirely on support funding from projects that use Parsl?
    - These projects need software that works and that they can rely on
  - Are there any funding agencies that will support maintenance of existing software?
    - Funding agencies generally focus on novelty, but production software is infrastructure
    - CZI EOSS is a seemingly lonely example, and focuses on software with substantial life science impact
- And incentives for others
  - We can't easily do this by ourselves - we need systemwide changes
    - E.g., hiring and promotion policies that include software work
  - Even better, incentives encourage quality and support of contribution

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Helpful new technology: containers

- Packaging/distribution
  - One person who knows all the awkwardness and puts in the effort can be in charge of making a container image
    - An excellent machine readable way of sharing install knowledge (eg encapsulated in a Dockerfile) rather than an out-of-date wiki page that someone hacked together a while ago and no longer is right
  - Then that container image can be used in many places
    - * HPC systems have different container technology and are not as portable as one might think
- Debugging
  - Instead of getting error reports on software versions of unknown age, a user can give their container image and staff can recreate their problem on their laptop using their actual software installs

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Conclusion

- Software can be complicated, but the software itself is mostly not what makes build and test difficult
- Most difficulties are related to the environment, and lack of knowledge about it
- Normal CI on HPC has technical and policies issues
- Software as a service and containerization can help
- Also room for CS research to make this easier
- Still have to balance between changing features and stable software
- Additional difficulties are related to developer ecosystem issues
  - Funding for maintenance (it's not new and shiny, but we still need to support it)
  - Non-monetary incentives for contributors (and maintainers)

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