Parsl: A Parallel Scripting Library for Python

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http://parsl-project.org
Scientific Workflows

- Most analyses require execution of many applications in a particular order
  - Binaries, scripts, Python functions, etc.
- Write once, execute many times
- Data flow (rather than control flow)
  - Applications can only execute when data dependencies are met
  - Often represented as a directed acyclic graph (DAG)
When do you need automated workflow?
Example application: protein-ligand docking for drug screening

- $O(10)$ proteins implicated in a disease
- $O(100K)$ drug candidates

$X$

= 1M docking tasks...

...then hundreds of detailed MD models to find 10-20 fruitful candidates for wetlab & APS crystallography
When do you need automated Workflow in machine learning?

Example application: predicting material design

Train/Validate  $f(x)$  Predict

$O(Ms)$ of data used to train model

$O(2M)$ evaluation of possible designs
When do you need automated workflow in online experiments?

Example application: cement hardening experiments

\( O(Ms) \) of images per day (2,000 projections per second, 2,048 x 2,048 pixels)
When do you need automated workflow in interactive science?
Example application: QuarkNet cosmic ray eLab

O(1M) cosmic ray events

Collect Data

Identify shower candidates

Curate

Analyze

Detector

Detector
Workflow requirements

Usability and ease of workflow expression

Ability to leverage complex architecture of HPC and HTC systems (fabric, scheduler, hybrid node/programming models), individually and collectively

Ability to integrate high-performance data services and volumes

Make use of the system task rate capabilities from clusters to extreme-scale
**Parsl: Parallel scripting in Python**

Annotate functions to make Parsl apps
- Bash apps call external applications
- Python apps call Python functions

Apps run concurrently respecting data dependencies via futures. Natural parallel programming!

Parsl scripts are independent of where they run. Write once run anywhere!
Expressing a many task workflow in Parsl

1) Wrap the protein docking code:

```python
@App('bash', dfk)
def dock(p, c, minRad, maxRad):
    return 'dock.sh {0} {1} {2} {3}'.format(p, c, minRad, maxRad)
```
Expressing a many task workflow in Parsl

2) Execute the protein docking workflow:

```python
for p in proteins:
    for c in ligands:
        structure[p][c] =
            dock(p, c, minRad, maxRad)

scatter_plot = analyze(structure)
```
The Swift parallel scripting language

- 10+ years of development
- C-like language with implicit parallelism
- Applied in dozens of scientific domains
- Data management, multi-site execution, coasters, etc.
- We are leveraging lessons and components to build Parsl

```swift
type file;

app (file c) simulation (int sim_steps, int sim_range, int sim_values)
{
    simulate "--timesteps" sim_steps "--range" sim_range "--nvalues" sim_values
    stdout=filename(c);
}

app (file c) analyze (file s[])
{
    stats filenames(s) stdout=filename(c);
}

int nsim = toInt(arg("nsim","10"));
int steps = toInt(arg("steps","1"));
int range = toInt(arg("range","100"));
int values = toInt(arg("values","5"));

file sims[];

foreach i in [0:nsim-1] {
    file simout <single_file_mapper; file=strcat("output/sim_",i,".out")>
    simout = simulation(steps,range,values);
    sims[i] = simout;
}

file stats<"output/average.out">;
stats = analyze(sims);
```
Dynamic dataflow execution

Parsl

Parsl host: login node, laptop, ...

Data servers

Scripts

Apps

Globus

Amazon web services
Parsl is Python

- Use Python libraries natively
- Stage Python data transparently
- Integrates with Python ecosystem

```
pip3 install parsl
```
Interactive supercomputing with Jupyter notebooks

- Parsl can be used from within a Jupyter notebook
- Visualization of Parsl graph in notebook
- Soon: transparent pass through of authentication tokens from JupyterHub
- Investigating support for JupyterLab
Parsl scripts are execution provider independent

- The same script can be run locally, on grids, clouds, or supercomputers
  - Works directly with the scheduler (no HTC-like setup)
- A single script may use many execution providers
- Parsl builds on libsubmit
  - https://github.com/Parsl/libsubmit
- Currently supported execution providers:
  - Local, Cloud (AWS, Azure, private), Slurm, Torque, Condor, Cobalt
Parsl supports a variety of execution models

- **Threads**  
  - Local execution
- **Ipython.parallel**  
  - Pilot job model
- **Swift/T**  
  - Extreme scale execution
- **New execution models can be added**
Multiple sites supported within a single script

- Common for apps to require different execution resources and environments
- Parsl apps may specify the site(s) on which they can be executed
  - Including remote and local execution

```python
@App('bash', dfk, sites=['Midway_SB'])
def tleap(input_file, inputs=[], outputs=[], stdout=None, stderr=None, mock=False):
    return '''module load amber/16; tleap -f %s'' % input_file

@App('bash', dfk, sites=['Midway_GPU'])
def pmemd_cuda(input_file=None, inputs=[], outputs=[], stdout=None, stderr=None, ref=True):
    if ref:
        r = '-ref {inputs[1]}"
    else:
        r = ""
    return '''software/amber-16-el6-x86_64+cuda-8.0/bin/pmemd.cuda -O -i %s -p {inputs[0]}'''
```
Elasticity

- Parsl DAGs are dynamic and grow over time
  - Results in variable workloads with variable resource requirements
- Parsl provides a user-oriented flow control model that:
  - Monitors waiting workload
  - Provisions resources within user-defined bounds according to a parallelism parameter
App caching (memoization)

- Parsl apps are often expensive to recompute
- In many development modes, results need not be recomputed
  - During development or interactive workflow
- Memoization optimizes execution by caching app results when called with the same inputs
- Parsl relies on user control to annotate deterministic functions

```python
@app('Python', dfk, cache=True)
def simulate(input_variable):
    return input_variable * 10
```

Cache

| Simulate(1) = 10 |
| Simulate(7) = 70 |
| Simulate(23) = 230 |
Fault tolerance and checkpointing

- **Failure modes:**
  - App failure, data error, node failure, etc.

- **Lazy vs immediate failure**

- **Simplest model: workflow level checkpointing**
  - Exploits app caching to save app results and reuse results for subsequent execution
    - Python objects and files

- **Extensible model for checkpointing to different persistent stores**

- **Enables automatic retry of workflows and re-execution from saved state**
Globus-based authentication and authorization

- A&A is hard today
  - 2FA, X509, etc.
- Building native app integration to provide embedded access to Globus (and other) services
- Using scoped access tokens, refresh tokens, delegation support
- Developing support for (semi-transparent) SSH-based authentication to compute resources
Globus data management

- Adding support for transparent high performance and reliable data movement to/from repositories, laptops, supercomputers, ...
  - Initially Globus, then HTTP
- Support for site-specific DTNs
- Compliments node-specific staging and caching models

```python
parsl_file = File(globus://EP/path/file)
```
Large-scale applications using Parsl

A. Machine learning to predict stopping power in materials

B. Protein and biomolecule structure and interaction

C. Information extraction to discovery facts in publications

D. Materials science at the Advanced Photon Source

E. Cosmic ray showers as part of QuarkNet

F. Weak lensing using sky surveys

G. Machine learning and data analytics
Parsl in action: materials science

**Stopping Power**: a “drag” force experienced by high speed protons, electrons, or positrons in a material

**Areas of Application**
- Nuclear reactor safety
- Magnetic confinement / inertial containment for nuclear fusion
- Solar cell surface adsorption
- Medicine (e.g., proton therapy cancer treatment)
- Critical to understanding material radiation damage

André Schleife and Cheng-Wei Lee (UIUC)
2016 ALCF INCITE Project
“Electronic Response to Particle Radiation in Condensed Matter”
Computing Stopping Power with TD-DFT

Stopping power (SP) can be accurately calculated by time-dependent density functional theory (TD-DFT)

- Excellent agreement with experiment
- Can vary orientation, projectile, material
- Highly parallelizable

But we need many results
- Direction dependence
- Effect of defects
- Many more materials

TD-DFT is costly, so use ML too
Parsl enables straightforward parallelization

\[ \Delta H_f = -1.0 \]

\[ \Delta H_f = -0.5 \]
LSST: Dark energy weak lensing

- Large Synoptic Survey Telescope (LSST): 10-year sky survey delivering 200 PB of production images
- Small to large scale workflows needed to 1) process images and 2) perform analyses of processed images
- Weak lensing analyses can determine the structure of dark matter, measure the expansion rate of the universe, etc.
LSST: Dark energy weak lensing

```python
@App("bash", dfk)
def doTomoBinning (d_des, f_wcl, ntomo=None, zbins=None, ctomo=0, cneff=1, omdeg=None, prefix=None, 
                   inputs=[], outputs=[], stdout=None, stderr=None):
    cmd_line = 'export PYTHONPATH=desweprs:$PYTHONPATH
{0}/bin/doTomoBinning.py --input {1} --ntomo {ntomo} --zbins {zbins} --ctomo {ctomo} --cneff {cneff} --omdeg {omdeg} --prefix {prefix}
...'

@App("bash", dfk)
def TreeCorr (config_file, output_file):
    # Call doTomoBinning
    fu_db, data_db = doTomoBinning(d_wlpipe, # Directory containing apps
                                    "{0}/wcl/doTomoBinning-{1}.wcl".format(d_wlpipe, dataset), # WCL file
                                    ntomo=nbtomo, zbins=zbins, omdeg=omdeg, prefix=prefix, # Various args
                                    outputs=['%s-neff.txt' % fileprfx] + ['"{0}\gg_z{1}.fits"'.format(fileprfx,i) for i in range(1,nbtomo+1)
                                       stdout='tomobinning.out', stderr='tomobinning.err') # Logging etc.

    # Call TreeCorr on combinations
    # ... Calculate 2pcf for Xpm
    # ... Xpm cross correlations
    gg_outputs = []
    for comb in combinations(range(1, nbtomo+1), 2):
        print("Launching TreeCorr GG on %s\%s\%s" % comb)
        filename=fileprfx+'\gg_\%s\%s.out' % comb
        fu_tc, data_tc = TreeCorr("\%s\%s\%s.yaml" % d_wlpipe,
                                 cmd_options = 'ra_col="RA" dec_col="DEC" ra_units="degrees" dec_units="degrees" g1_col="S_1" g2_col="S_2"
                                 inputs=[data_db[comb[0]], data_db[comb[1]]], # Pass in the input data futures from TomoBinning
                                 min_sep=thetamin, max_sep=thetamax, nzbins=nteta, bin_slop=bin_slop, # Args
                                 outputs=[filename], # Specify output files
                                 stdout='\gg1_tcorr.\%s\%s.out' % comb, stderr='\gg1_tcorr.\%s\%s.err' % comb)
        gg_outputs.extend(data_tc)
```

https://github.com/Parsl/DESC_WeakLensing
Demo
Parsl provides 4 important benefits:

- Intuitive programming model in Python
  
  *Integrates with the Python ecosystem*

- Makes parallelism more transparent
  
  *Parallel dataflow programming*

- Makes computing location more transparent
  
  *Runs your script on multiple distributed sites and diverse computing resources (desktop to petascale) with transparent data movement*

- Enables provenance capture
  
  *Tasks have recordable inputs and outputs*
Conclusion: parallel workflow scripting is practical, productive, and necessary, at a broad range of scales

- Parsl takes a highly successful parallel scripting model and brings it to Python
  - No porting of existing scripts to other languages
  - Support for both Python and external app functions
- Already applied to numerous MTC and HPC application domains
  - Attractive for data-intensive applications
  - And several hybrid programming models
- Deep integration with growing ecosystem:
  - Globus, Python, Jupyter, workflow library, ...

Workflow through implicitly parallel dataflow is productive for applications and systems at many scales, including on highest-end systems
Parsl Resources

- Getting started
  - [http://try-parsl.parsl-project.org](http://try-parsl.parsl-project.org)

- Parsl tutorial
  - [https://github.com/Parsl/parsl-tutorial](https://github.com/Parsl/parsl-tutorial)

- Documentation
Questions?

http://parssl-project.org

Try Parsl: http://try.parssl-project.org