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Resource Management for Dynamic Function Distribution with Parsl and Work Queue

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ParSl / FuncX Workshop, 27 October 2021



Parsl + Work Queue for Scalable Apps

<http://parsl-project.org>



Productive parallel programming in Python

Use Parsl to create parallel programs comprised of Python functions and external components. Execute Parsl programs on any compute resource from laptops to supercomputers.

Don't miss ParslFest Oct 3-4!

Join us for ParslFest, the first Parsl community meeting, to be held at the University of Chicago



Try Parsl

Use Binder to run Parsl tutorials in hosted Jupyter notebooks. No installation required!

Try now »



Install Parsl

Pip install Parsl or checkout Parsl from source.

Quickstart »



Contribute

View, fork, and contribute to the open source Parsl on GitHub.

View source »

Powerful Pythonic Workflow Programming Model

<http://ccl.cse.nd.edu>

Work Queue: A Scalable Master/Worker Framework

Work Queue is a framework for building large master-worker applications that span thousands of machines drawn from clusters, clouds, and grids. Work Queue applications are written in C, Perl, or Python using a simple API that allows users to define tasks, submit them to the queue, and wait for completion. Tasks are executed by a standard worker process that can run on any available machine. Each worker calls home to the master process, arranges for data transfer, and executes the tasks. The system handles a wide variety of failures, allowing for dynamically scalable and robust applications.

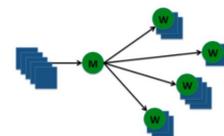
Work Queue has been used to write applications that scale from a handful of workstations up to tens of thousands of cores running on supercomputers.

Examples include [Lobster](#), [NanoReactors](#), [ForceBalance](#), [Accelerated Weighted Ensemble](#), the [SAND genome assembler](#), the [Makeflow workflow engine](#), and the [All-Pairs](#) and [Wavefront](#) abstractions. The framework is easy to use, and has been used to teach courses in parallel computing, cloud computing, distributed computing, and cyberinfrastructure at the University of Notre Dame, the University of Arizona, and the University of Wisconsin - Eau Claire.

For More Information

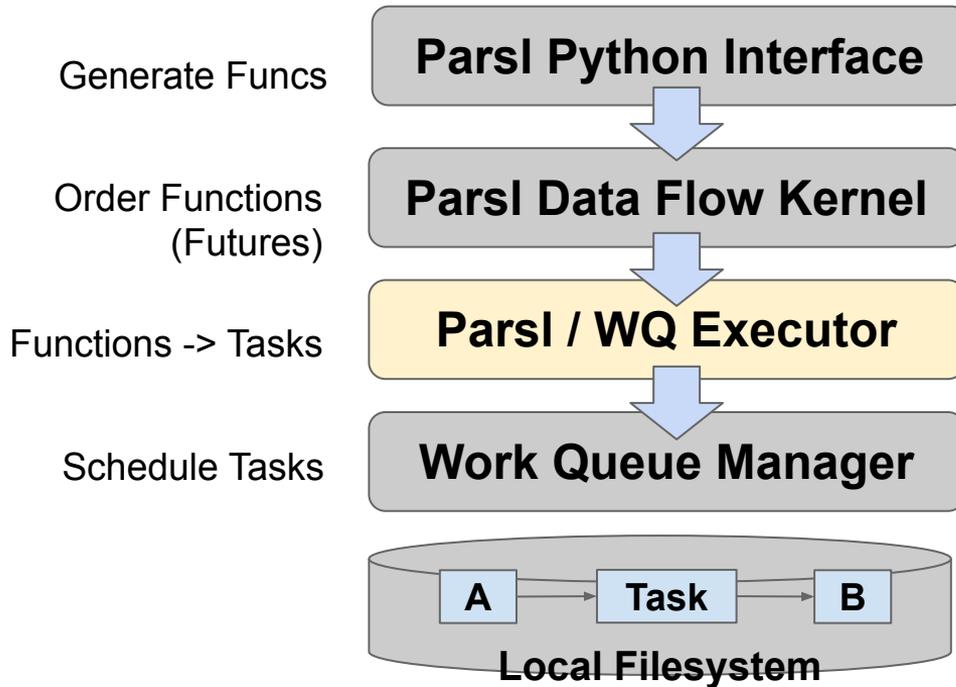
- [Work Queue User's Manual](#)
- [Work Queue API \(C | Perl | Python\)](#)
- [Work Queue Example Program \(C | Perl | Python\)](#)
- [Work Queue Status Display](#)
- [Download Work Queue](#)
- [Getting Help with Work Queue](#)

Work Queue



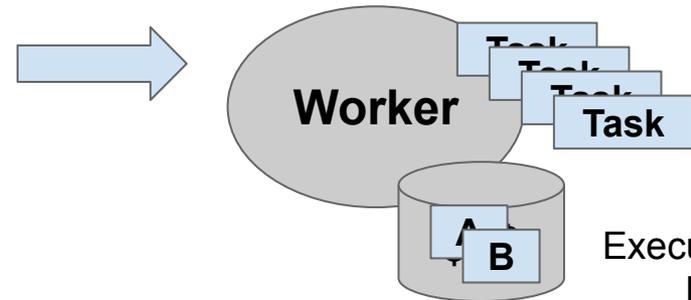
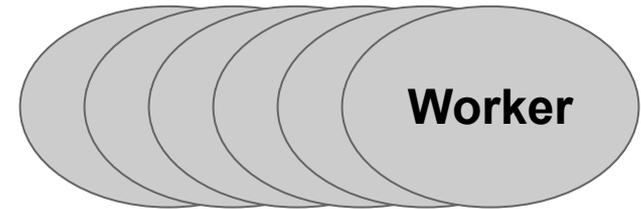
Scalable, Portable, Robust Distributed Execution

System Architecture



**Thousands of Workers
on National Cyberinfrastructure**

HTCondor, PBS, SLURM, Amazon,
Blue Waters, OSG, XSEDE...



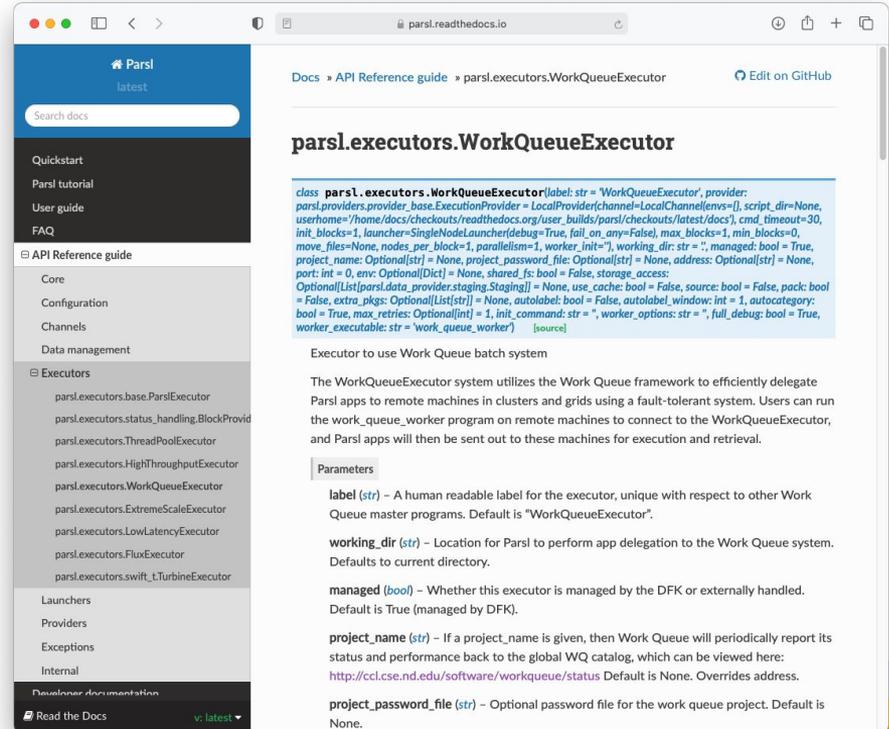
Execute Tasks
Remotely
on Local Disk

Configuring Parsl + WQ

```
import parsl

from parsl.executors import WorkQueueExecutor

config = parsl.config.Config(
    executors=[
        WorkQueueExecutor(
            label="wq-parsl-app",
            port=9123,
            project_name="wq-parsl-app",
            shared_fs=False,
            full_debug = True,
        )
    ]
)
```



The screenshot shows a web browser displaying the Parsl documentation for the `parsl.executors.WorkQueueExecutor` class. The page includes a search bar, navigation links, and a table of contents. The main content area shows the class definition with its parameters and a description of the executor's functionality.

parsl.executors.WorkQueueExecutor

```
class parsl.executors.WorkQueueExecutor[label: str = 'WorkQueueExecutor', provider:
parsl.providers.provider_base.ExecutorProvider = LocalProvider(channel=LocalChannel(lenvs=), script_dir=None,
userhome='/home/docs/checkouts/readthedocs.org/user_builds/parsl/checkouts/latest/docs', cmd_timeout=30,
init_blocks=1, launcher=SingleNodeLauncher(debug=True, fail_on_any=False), max_blocks=1, min_blocks=0,
move_files=None, nodes_per_block=1, parallelism=1, worker_init='', working_dir: str = '', managed: bool = True,
project_name: Optional[str] = None, project_password_file: Optional[str] = None, address: Optional[str] = None,
port: int = 0, env: Optional[Dict] = None, shared_fs: bool = False, storage_access:
Optional[List[parsl.data_provider.staging.Staging]] = None, use_cache: bool = False, source: bool = False, pack: bool
= False, extra_pkgs: Optional[List[str]] = None, autolabel: bool = False, autolabel_window: int = 1, autocategory:
bool = True, max_retries: Optional[int] = 1, init_command: str = '', worker_options: str = '', full_debug: bool = True,
worker_executable: str = 'work_queue_worker'] [source]
```

Executor to use Work Queue batch system

The WorkQueueExecutor system utilizes the Work Queue framework to efficiently delegate Parsl apps to remote machines in clusters and grids using a fault-tolerant system. Users can run the `work_queue_worker` program on remote machines to connect to the WorkQueueExecutor, and Parsl apps will then be sent out to these machines for execution and retrieval.

Parameters

- label (str)** – A human readable label for the executor, unique with respect to other Work Queue master programs. Default is "WorkQueueExecutor".
- working_dir (str)** – Location for Parsl to perform app delegation to the Work Queue system. Defaults to current directory.
- managed (bool)** – Whether this executor is managed by the DFK or externally handled. Default is True (managed by DFK).
- project_name (str)** – If a project_name is given, then Work Queue will periodically report its status and performance back to the global WQ catalog, which can be viewed here: <http://ccl.cse.nd.edu/software/workqueue/status> Default is None. Overrides address.
- project_password_file (str)** – Optional password file for the work queue project. Default is None.

Common Challenges

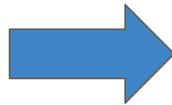
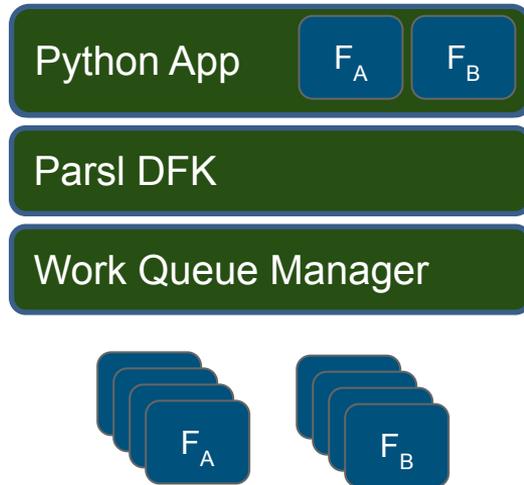
Two common problems of scaling up:

- What resources should be assigned to a function call?
- What software dependencies does this function need?

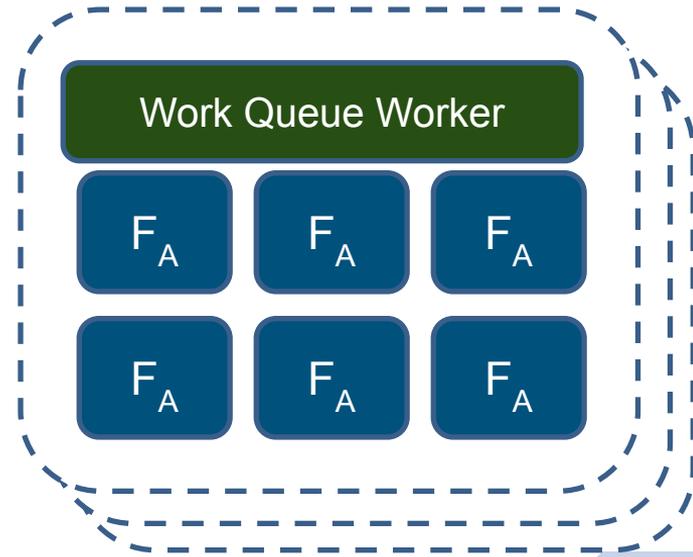
How can we solve these problems automatically at runtime, without requiring the user to make advance declarations?

A decorative yellow arrow pointing to the right, located in the bottom right corner of the slide.

Packing Functions Into Manycore Nodes



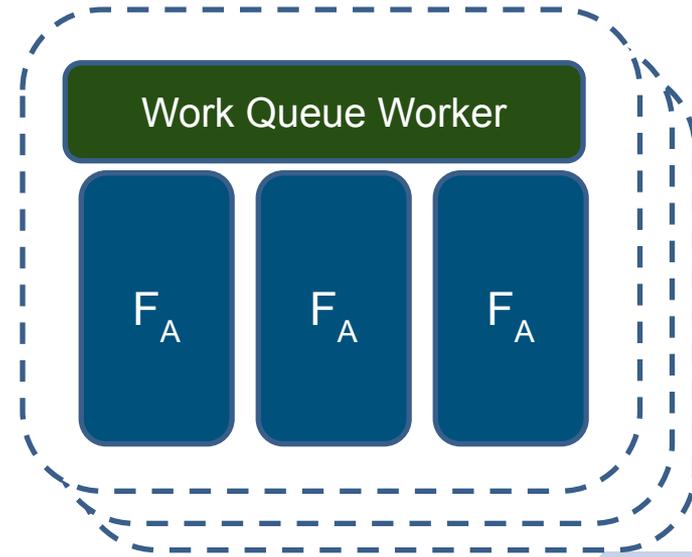
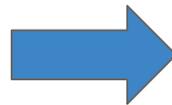
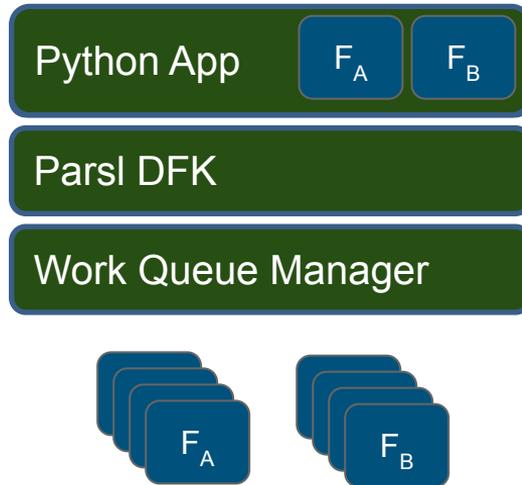
Allocate 2GB per Function A?



12 cores and 12 GB RAM

Packing Functions Into Manycore Nodes

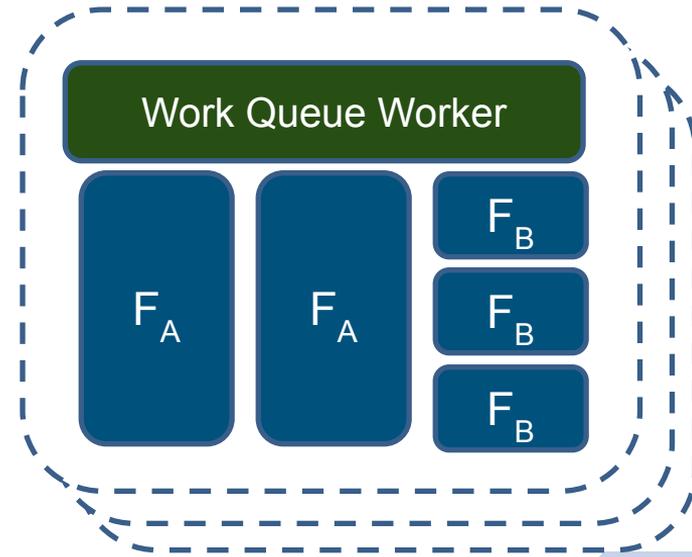
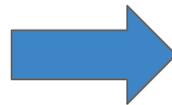
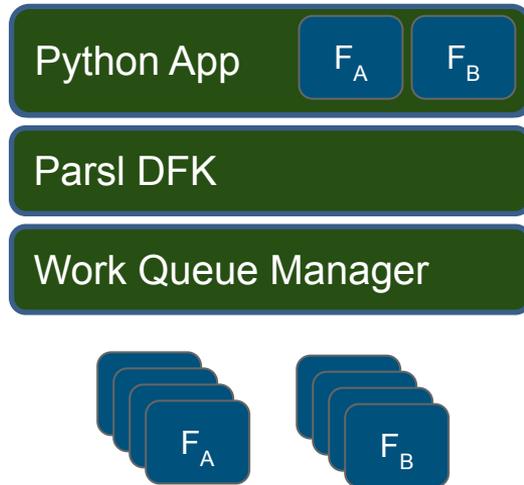
Allocate 4GB per Function A?



12 cores and 12 GB RAM

Packing Functions Into Manycore Nodes

Mix Function A and Function B?



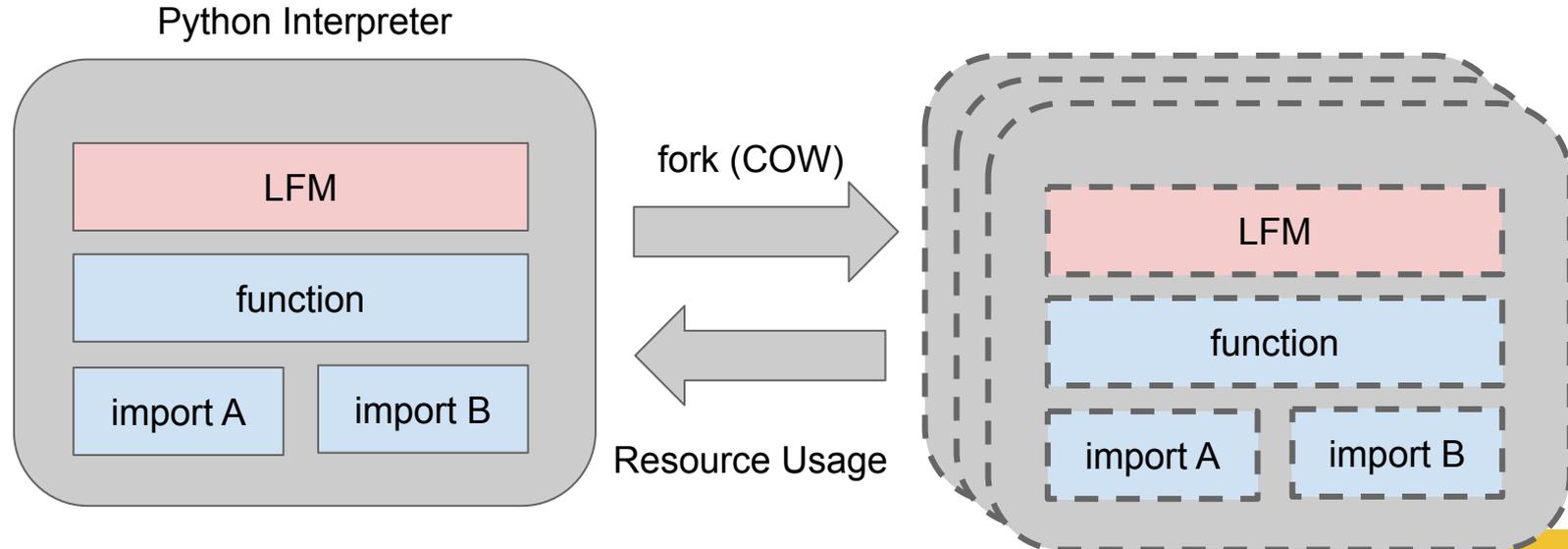
12 cores and 12 GB RAM

How to measure a single function call?



Ben Tovar

LFM - Lightweight Function Monitor



Lightweight Function Monitors (LFMs)

Activate LFMs with an import and the `@monitored` keyword

```
In [7]: from resource_monitor import monitored
        from time import sleep
```

```
In [12]: # declare a function to be monitored with the @monitored() decorator

@monitored()
def my_function_1(wait_for):
    sleep(wait_for)
    return 'waitied for {} seconds'.format(wait_for)

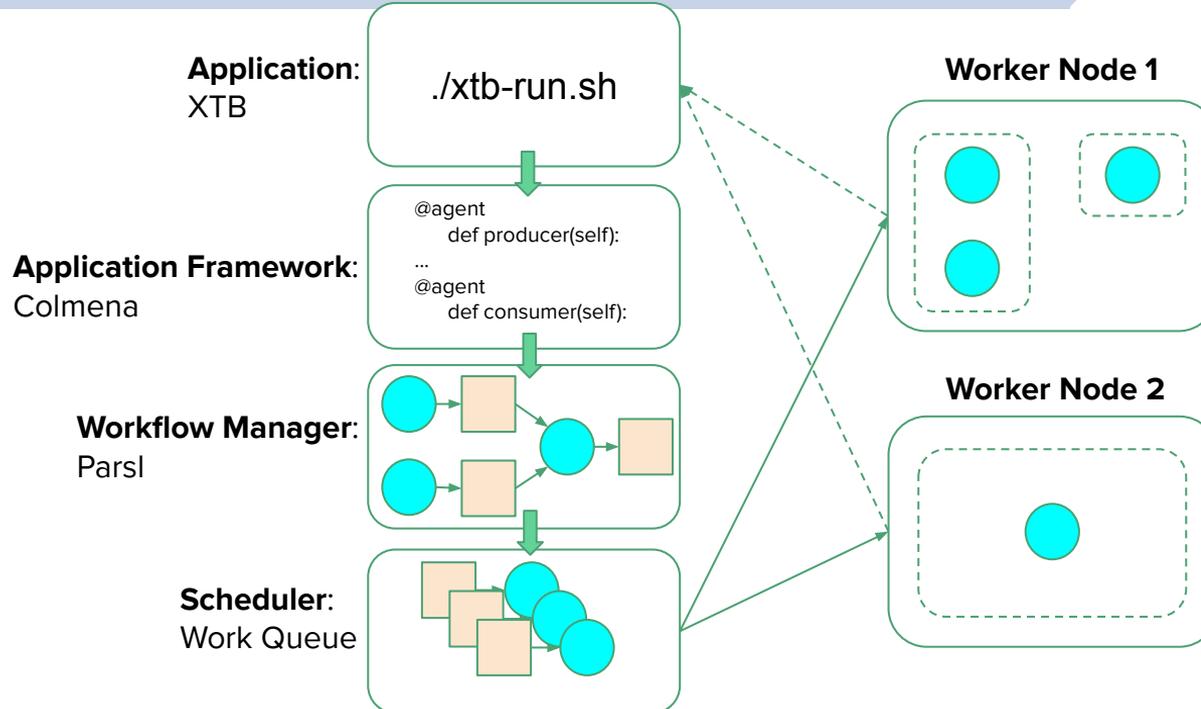
(result, resources) = my_function_1(.1)
print(result, '{}'.format({'memory': resources['memory'], 'wall_time': resources['wall_time']}))

waitied for 0.1 seconds {'memory': 49, 'wall_time': 101689}
```

Example: Colmena-XTB Application



Thanh
Son Phung

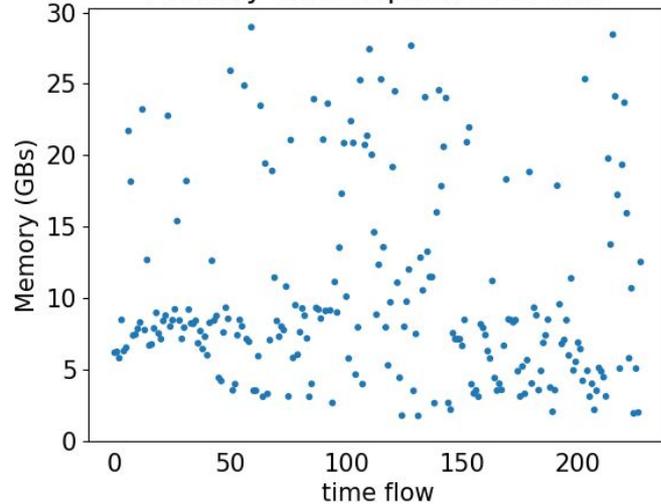


Tasks:

- Are of two types: inference and simulation
- Display significant differences in resource consumption

Memory Consumption of Colmena-XTB's Tasks

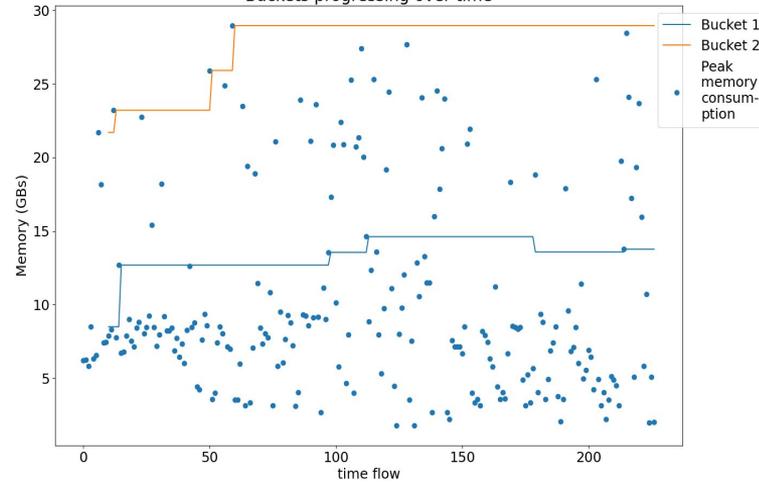
Memory consumption over time



Problem

Tasks can consume as low as 2 GBs or as high as 30 GBs of RAM!

Buckets progressing over time

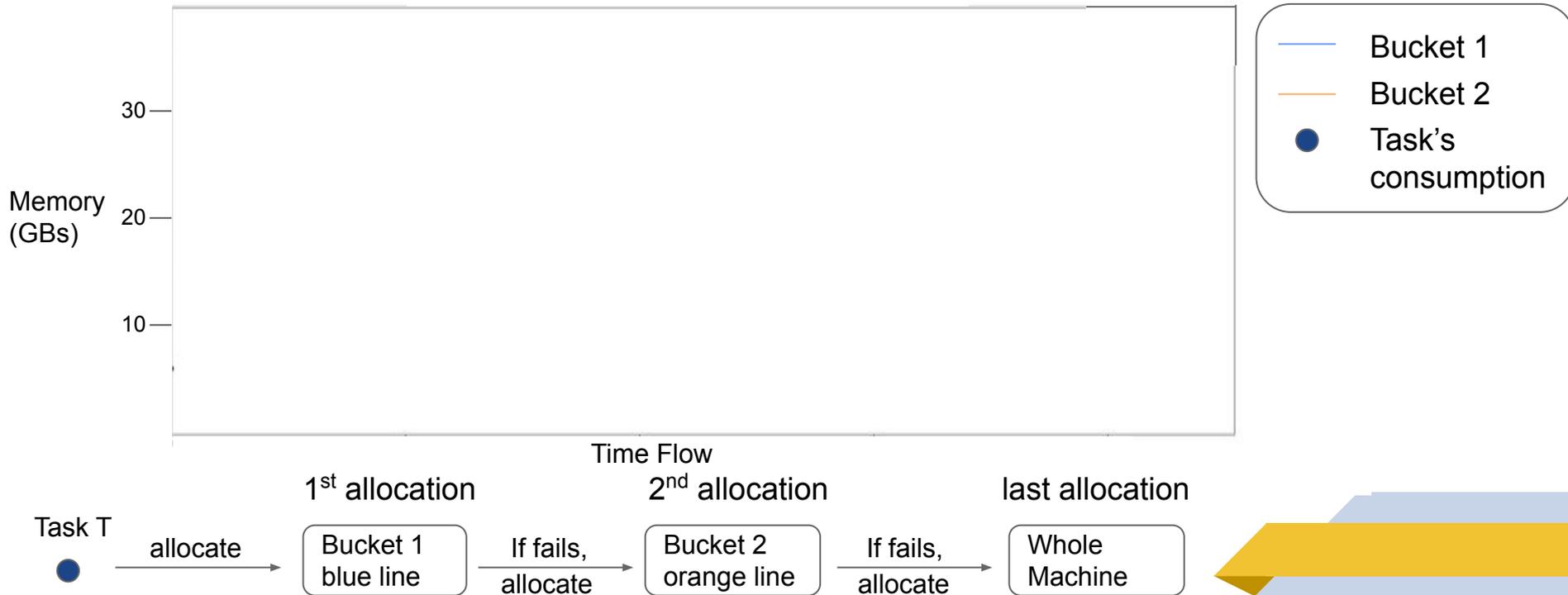


Solution

Bucket tasks with similar consumption and allocate new tasks accordingly.

K-means Bucketing

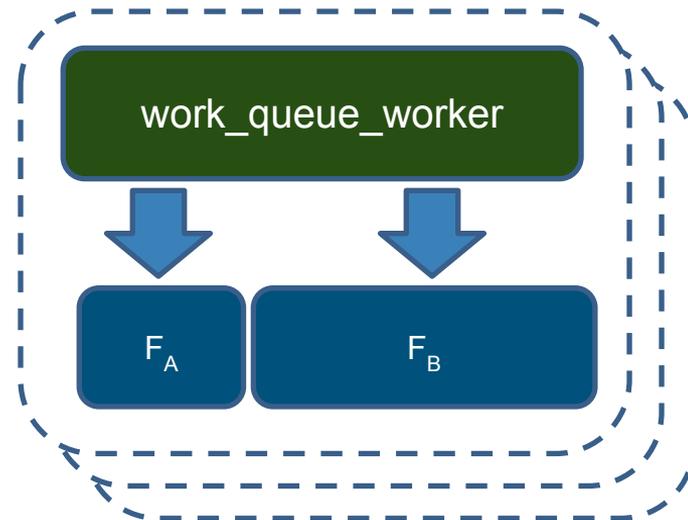
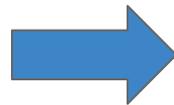
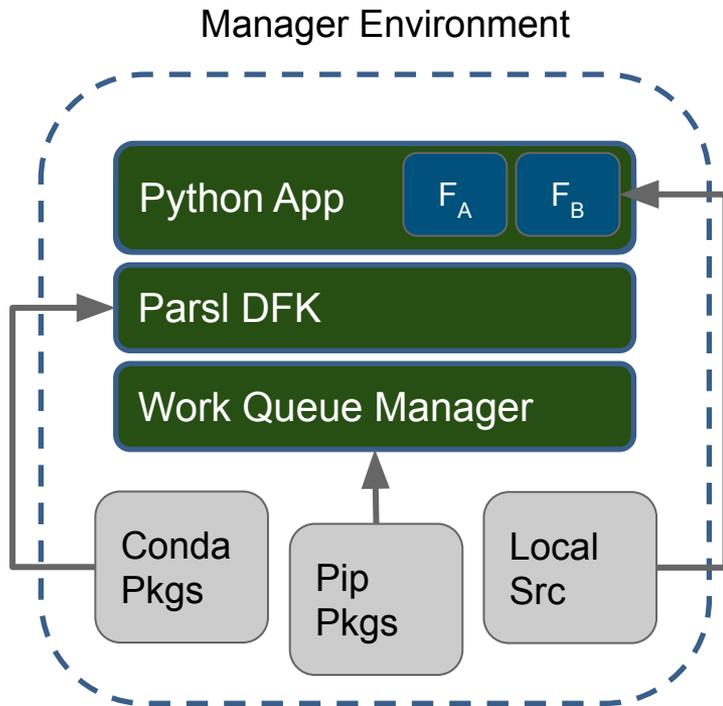
Buckets progressing over time



Run Time Dependency Management



Barry
Sly-Delgado



How do we ensure that all the tasks get a consistent, minimal environment matching the manager?

Poncho Toolkit

The Poncho Toolkit allows users to create and deploy self contained Python environments at user level in arbitrary distributed systems via a JSON specification file.

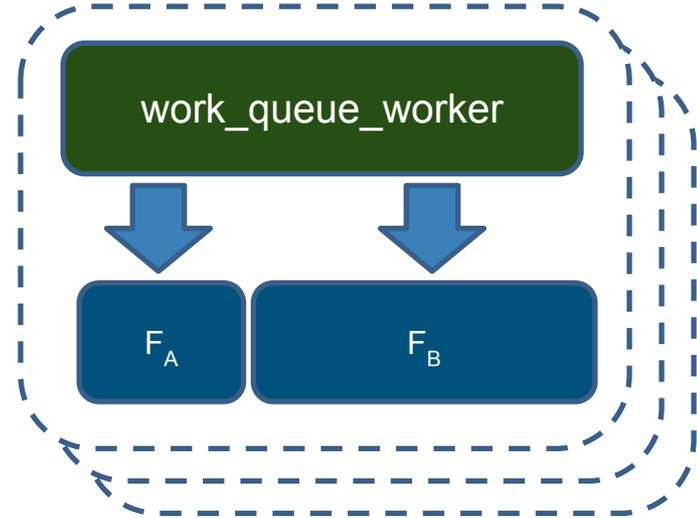
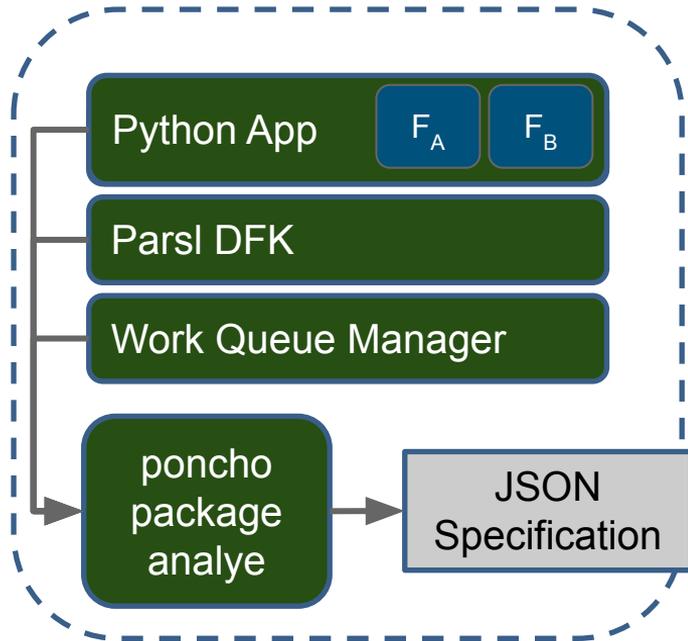
- `poncho_package_analyze`
- `poncho_package_create`
- `poncho_package_run`

<https://cctools.readthedocs.io/en/latest/poncho/>

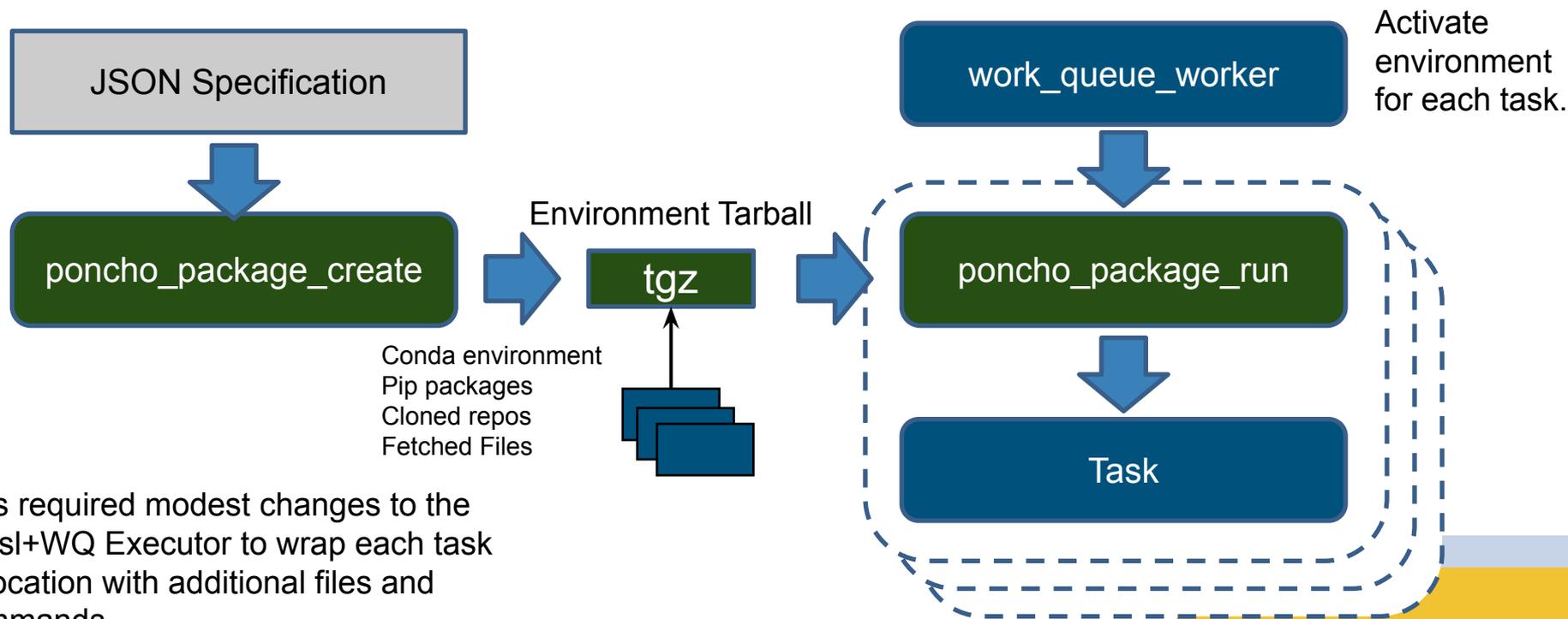
```
"conda":{
  "channels":[
    "defaults",
    "conda-forge"
  ],
  "packages":[
    "ndcctools=7.3.0",
    "parsl=1.1.0",
  ]
},
"pip": [
  "topcoffea"
]
"git": {
  "DATA_DIR": {
    "remote": "http://.../repo.git"
  }
}
```

Run Time Dependency Management

Manager Environment

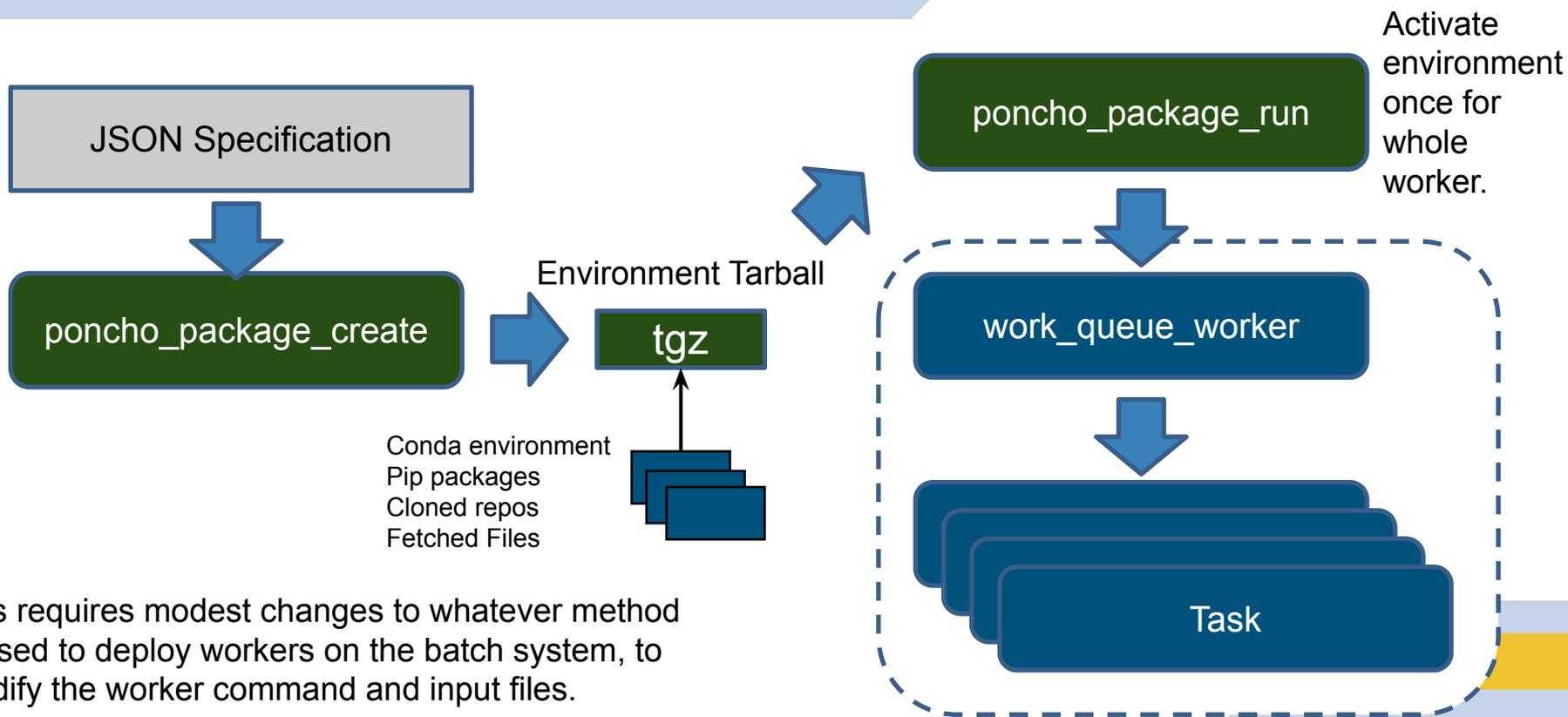


Package per Task



This required modest changes to the Parsl+WQ Executor to wrap each task invocation with additional files and commands.

Package per Worker



This requires modest changes to whatever method is used to deploy workers on the batch system, to modify the worker command and input files.

First Look: Orders of Magnitude

poncho_package_create

Application	No Versions Specified	All Versions Specified
TopEFT	2940s	170s
SHADHO	257s	159s

poncho_package_run

Application	Size compressed	Size unpacked	Unpack Time
SHADHO	438MB	1.4GB	12s
TopEFT	594MB	2GB	21s
Colmena-XTB	1.4GB	4.8GB	46s

Next Steps...

- Do we really need all this code just to run a function? (maybe)
- Understanding the dependencies **actually used** by a function execution, and how they evolve over time.
- Extending dependency detection to other kinds of resources: databases, executables, file system resources...
- Closing the loop on application configuration: capture discovered resource configurations from multiple runs and use to predict future runs.
- Conveying known application categories from top to bottom through software stacks.

End to End Integration Testing

All workflows

Showing runs from all workflows

Q Filter workflow runs	
341 workflow runs	Event ▾ Status ▾ Branch ▾ Actor ▾
 CI-Daily CI-Daily #160: Scheduled	 16 hours ago ...  3m 39s
 CI-Daily CI-Daily #159: Scheduled	 2 days ago ...  3m 44s
 drop conda-pack from coffea.sh (comes fr... CI-Daily #158: Commit 7f26ea3 pushed by btovar main	 2 days ago ...  4m 43s
 update python for parsl, drop conda-pack f... CI-Daily #157: Commit 0b66cc3 pushed by btovar main	 2 days ago ...  30m 4s
 CI-Daily CI-Daily #156: Scheduled	 3 days ago ...  30m 25s
 CI-Weekly CI-Weekly #25: Scheduled	 4 days ago ...  30m 0s
 CI-Daily CI-Daily #155: Scheduled	 4 days ago ...  30m 27s

End-to-end daily test that simply installs parsl+workqueue and runs a trivial example out of the manual to see if it gets the right result.

conda-forge dropped support for python 3.6, resulting in attempts to install taking forever while conda tries to solve an unsolvable dependency problem!

For More Information...

Quick Start:

```
conda install -c conda-forge python=3.9 ndcctools parsl
```

<https://cctools.readthedocs.io>

<https://ccl.cse.nd.edu/software/workqueue>

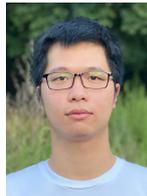
btovar@nd.edu



bslydelg@nd.edu



tphung@nd.edu



dthain@nd.edu



The image displays three overlapping screenshots of the CTools Documentation website. The top screenshot shows the 'Work Queue User's Manual' page, with a navigation menu on the left listing sections like 'GETTING STARTED', 'SOFTWARE', and 'Work Queue'. The middle screenshot shows the 'Poncho Packaging Utilities' page, with a similar navigation menu. The bottom screenshot shows the 'Resource Monitor User's Manual' page, featuring an 'Overview' section that describes the `resource_monitor` tool and its capabilities. The navigation menu in all screenshots includes options like 'About', 'Installation', 'Getting Help', 'SOFTWARE', 'Makeflow', 'Work Queue', 'JX Language', 'Resource Monitor', 'Parrot', 'Chirp', 'Catalog Server', 'Poncho', 'Commands', 'Example', 'Specification File', 'RESEARCH PROTOTYPES', and 'AWE'.