Building Modular Parsl Workflows in Parallel Works

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A Google Cloud Partner

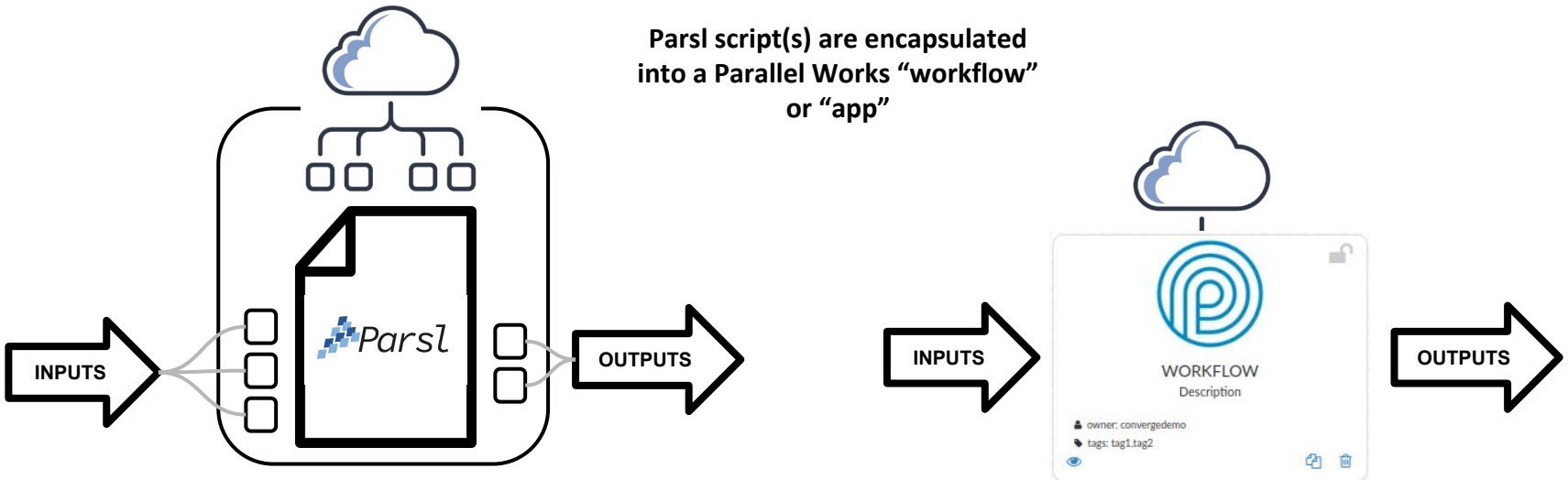
Outline

1. **Workflows in Parallel Works**

2. **Modular workflows**
   a. Motivation
   b. Sweep_CSV
   c. Pipeline

3. **Wrapping Parsl Apps**: SimpleBashRunner

Workflows in Parallel Works

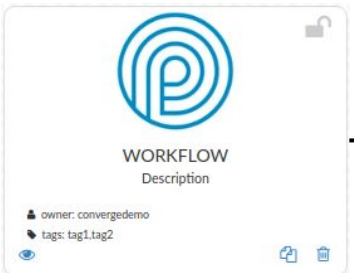


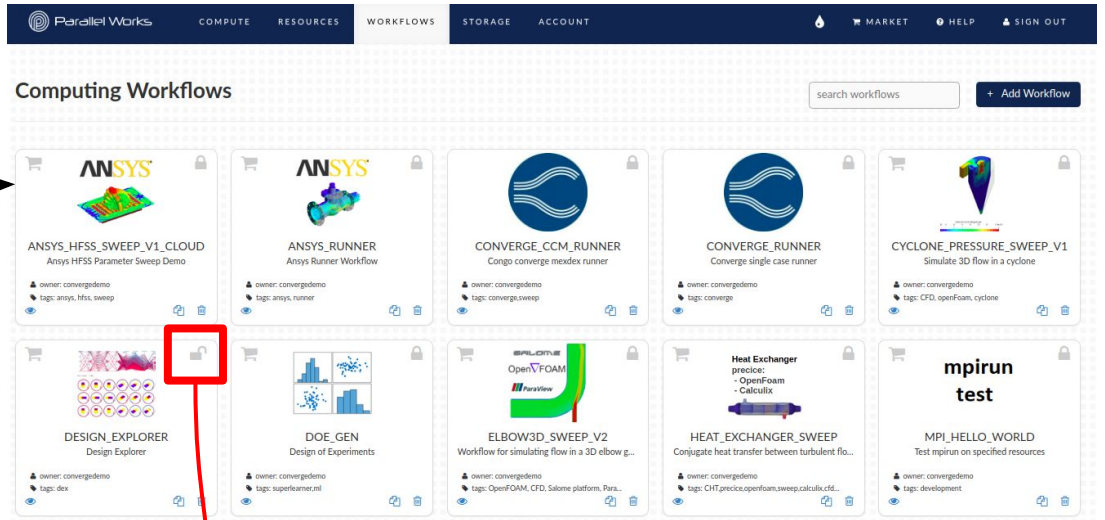
Parallel Works

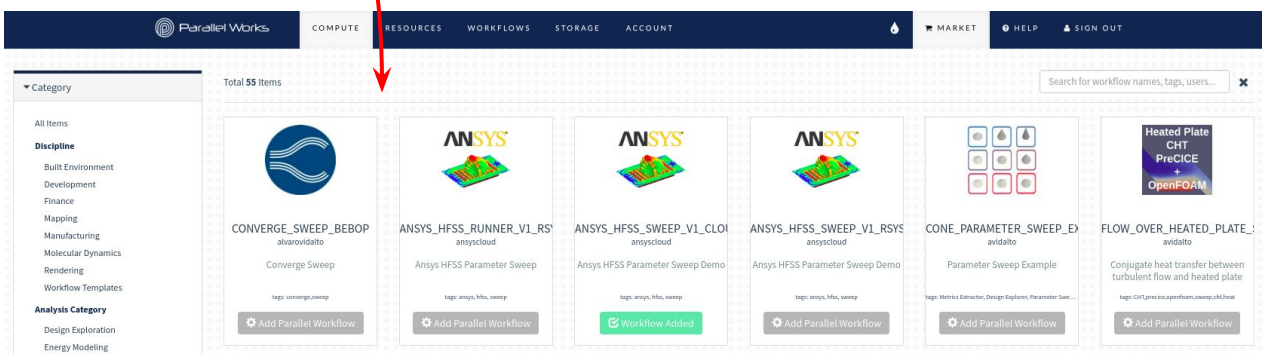
Workflows in Parallel Works

Use Parallel Works to:

- Develope
- Execute
- Share







Parallel Works

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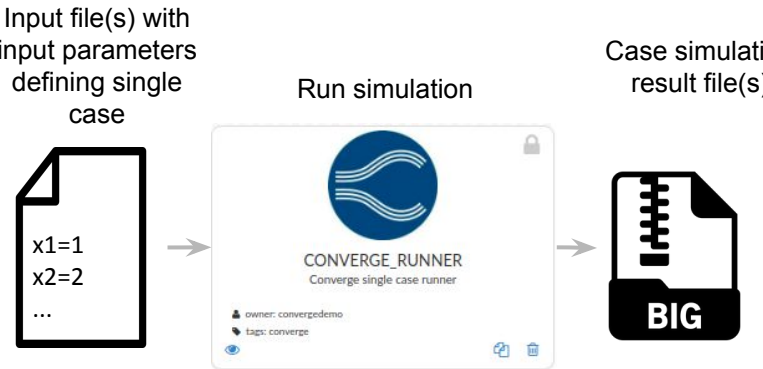
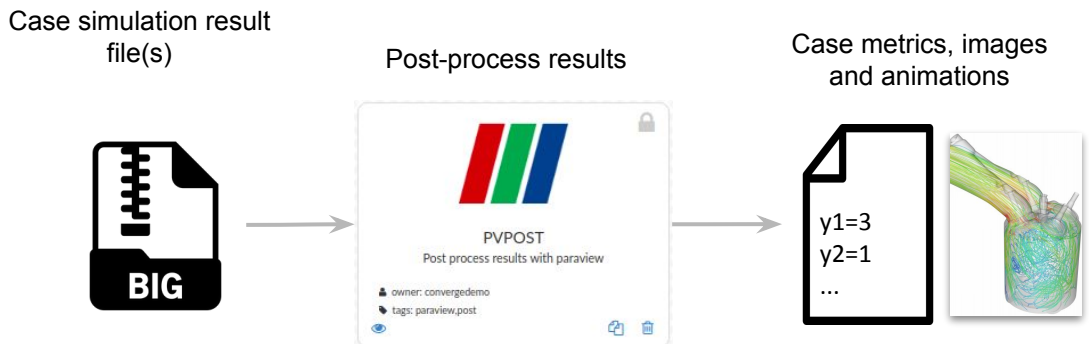
Modular Workflows: Motivation

Typical simple workflow



Post-process results with another workflow?



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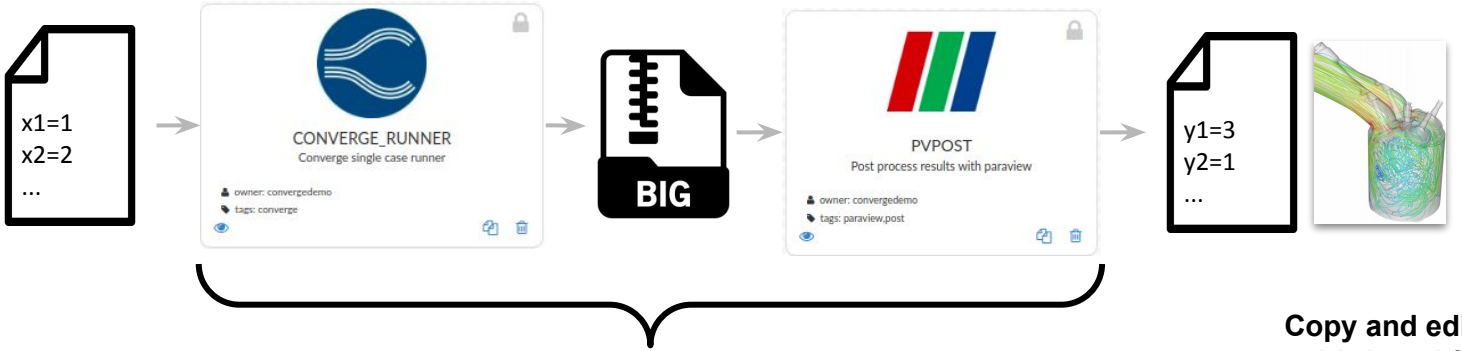
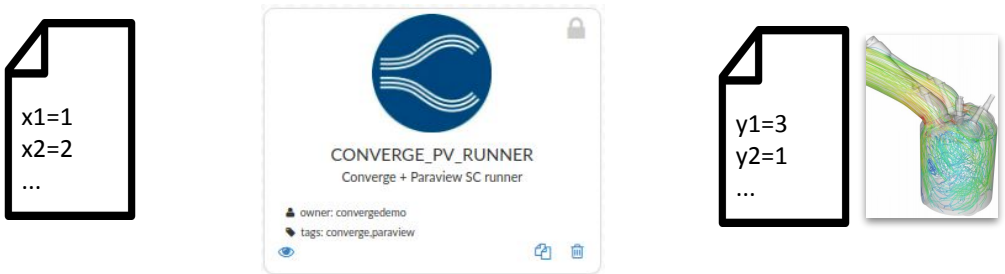
Modular Workflows: Motivation





Run and post-process in the same workflow?

3 Workflows:

1. **CONVERGE_RUNNER**
2. **PVPOST**
3. **CONVERGE_PV_RUNNER**

Copy and edit blocks of code to make a third workflow:

- **Pros:**
  - Workflow is self contained
- **Cons:**
  - Hard to maintain
  - Need to update many workflows
  - Too many workflows
  - Hard to test
  - Slow development
  - More code
  - ...

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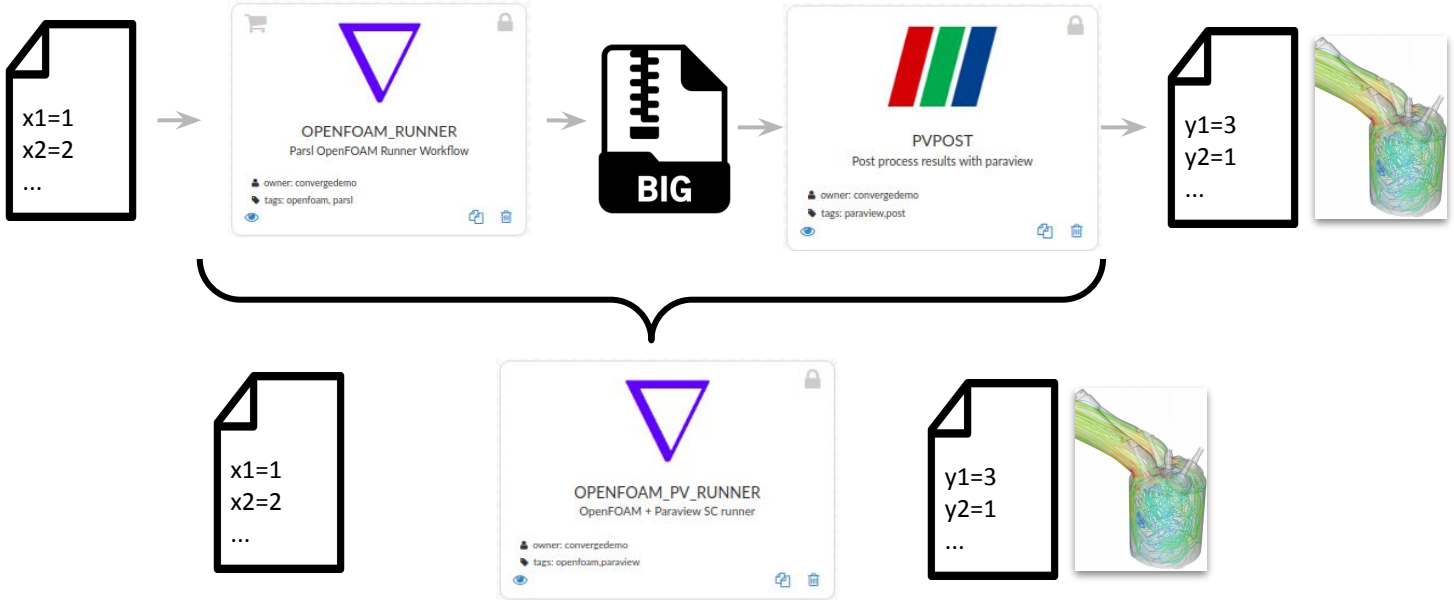
Modular Workflows: Motivation



Use a different CFD tool?

5 Workflows:

1. **CONVERGE_RUNNER**
2. **PVPOST**
3. **CONVERGE_PV_RUNNER**
4. **OPENFOAM_RUNNER**
5. **OPENFOAM_PV_RUNNER**

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Modular Workflows: Motivation

Run different cases in parallel and merge results?

AND MORE...

1. **CONVERGE_RUNNER**
2. **PVPOST**
3. **CONVERGE_PV_RUNNER**
4. **OPENFOAM_RUNNER**
5. **OPENFOAM_PV_RUNNER**
6. **CONVERGE_PV_SWEEP**
7. **OPENFOAM_PV_SWEEP**
8. **...**

one workflow for every compatible software tool and workflow topology combination

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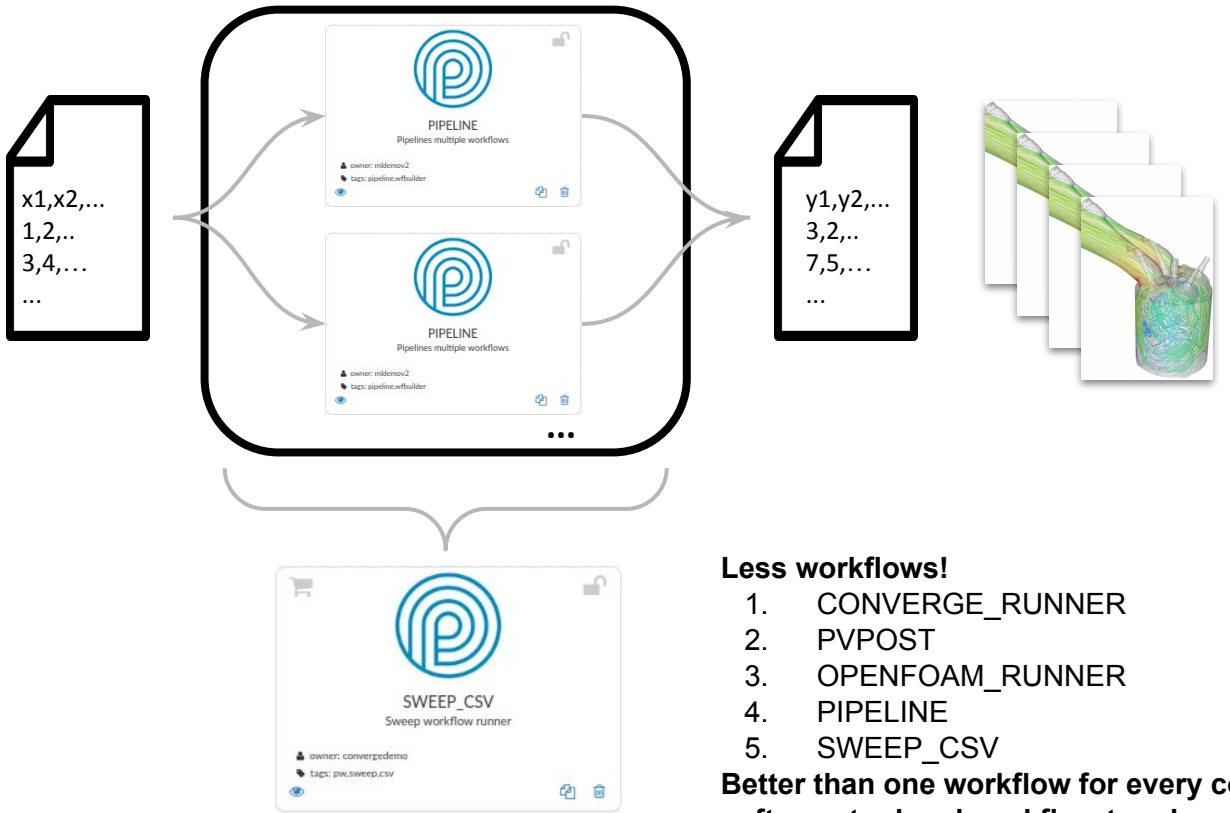
Modular Workflows: Motivation



Build workflows as Python modules that can be imported by other workflows

- **Pipelining**
- **CSV Sweep**
- **Optimization**
- **Active Learning**
- **...**

Advantages:

- Fast development
- Easy to maintain
- Less workflows
- Less code
- ...

Less workflows!

1. CONVERGE_RUNNER
2. PVPOST
3. OPENFOAM_RUNNER
4. PIPELINE
5. SWEEP_CSV

Better than one workflow for every compatible software tool and workflow topology combination

Parallel Works

Modular Workflows: main.py

Create a workflow script (main.py) that can be:

1. Executed directly

runs:

python main.py

in */pw/jobs/job_num/*

2. Imported by other workflows

```
imported_workflow = wfbuilder.import_workflow(workflow_name)
```

Main parts:

1. **Run workflow function(s): Imported and executed by other workflows**
   - **Do not wait for futures inside these functions**
     - If imported cannot be executed multiple times in parallel
   - **To be compatible with wfbuilder module**
     - Inputs:
       i. (Required) **wf_pwargs**: Python Namespace with functions IO
       ii. (Optional) **wf_dir**: Workflow directory for intermediate IO, logs, etc.
     - Outputs:
       i. **Dictionary of objects with a .result() method were keys are output parameter names**

2. **Only when executed directly**:
   - Load Parsl configuration
   - Load and preprocess IO
   - Run workflow function(s)
   - **Wait for results**

3. **Only when imported** → Build workflow as module

4. Execute always

sample main.py script

```
import parsl
from parslpw import pwconfig, pwargs

# RUN WORKFLOW FUNCTION
def run_workflow(wf_pwargs, wf_dir = "./workflow"):
    # Workflow code HERE
    # ...
    # ...
    # Return dictionary where keys are output parameter names and values objects with .result() method or dictionaries in the same format
    return out_futs

if __name__ == "__main__":
    # Workflow executed directly
    # Write code HERE
    # ...
    import module_sample
    # ...
    # Load Parsl configuration
    parsl.load(pwconfig)
    # Run workflow
    out_futs = run_workflow(pwargs)
    # Wait for results
    wfbuilder.wfconn.wait_for_futs(out_futs)

else:
    # Workflow imported by other workflow
    # Write code HERE
    # ...
    if not os.path.isdir("module_sample"):
        shutil.copytree("/pw/workflows/workflow/module_sample", "module_sample")
    import module_sample
    # ...
```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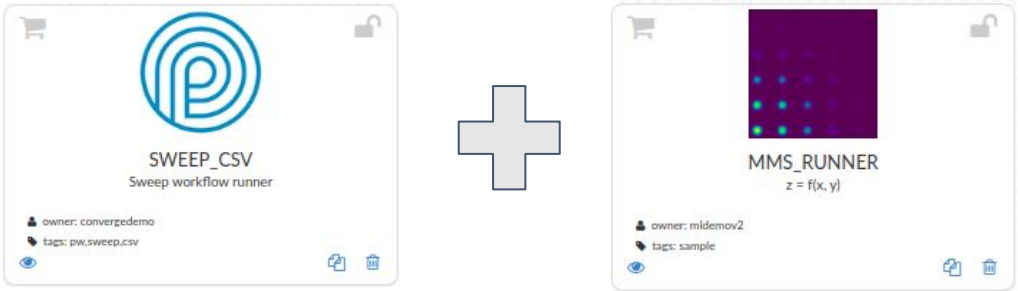
Modular Workflows: SWEEP_CSV

Example 1: **SWEEP_CSV(MMS_RUNNER)** (“placeholder workflow”)



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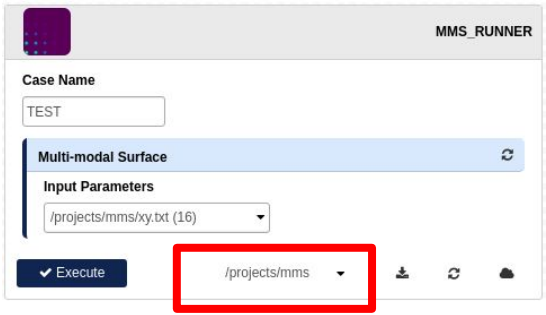
Modular Workflows: SWEEP_CSV

MMS:

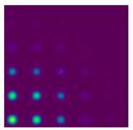


NAMESPACE:

```
pwargs.casename = "TEST"
pwargs.in_mms = "/pw/projects/mms/xy.txt"
pwargs.out_mms = "/pw/project/mms/mms-TEST-date-time.txt"
```

in_mms

```
x 0.0404
y 0.5454
```



MMS_RUNNER
z = f(x, y)

out_mms

```
x=0.0404
y=0.5454
z=0.8123
```

main.py script

```
import sys
import os,shutil
import parsl
from parslpw import pwconfig,pwargs

if not os.path.isdir("wfbuilder"):
    shutil.copytree("/pw/modules/wfbuilder", "wfbuilder")
import wfbuilder

def run(wf_pwargs, wf_dir = "mms_runner"):
    os.makedirs(wf_dir,  exist_ok=True)
    print("MMS_RUNNER INPUTS:")
    print(wf_pwargs)
    # Define runner
    runner = wfbuilder.pwrunners.SimpleBashRunner(
        cmd = "/bin/bash mms/mms_eval.sh",
        cmd_arg_names = ["in_mms", "out_mms"],
        inputs = {
            "in_mms": wfbuilder.Path(wf_pwargs.in_mms),
            "scripts": wfbuilder.Path("/pw/workflows/mms_runner/./mms"),
        },
        outputs = {"out_mms": wfbuilder.Path(wf_pwargs.out_mms)},
        logs = {
            "stdout": wf_dir + "/mms.out",
            "stderr": wf_dir + "/mms.err"
        }
    )
    return runner.run()

if __name__ == "__main__":
    # Runs only when executed (not when imported)
    parsl.load(pwconfig)
    case_fut = run(pwargs)
    case_fut["out_txt"].result()
```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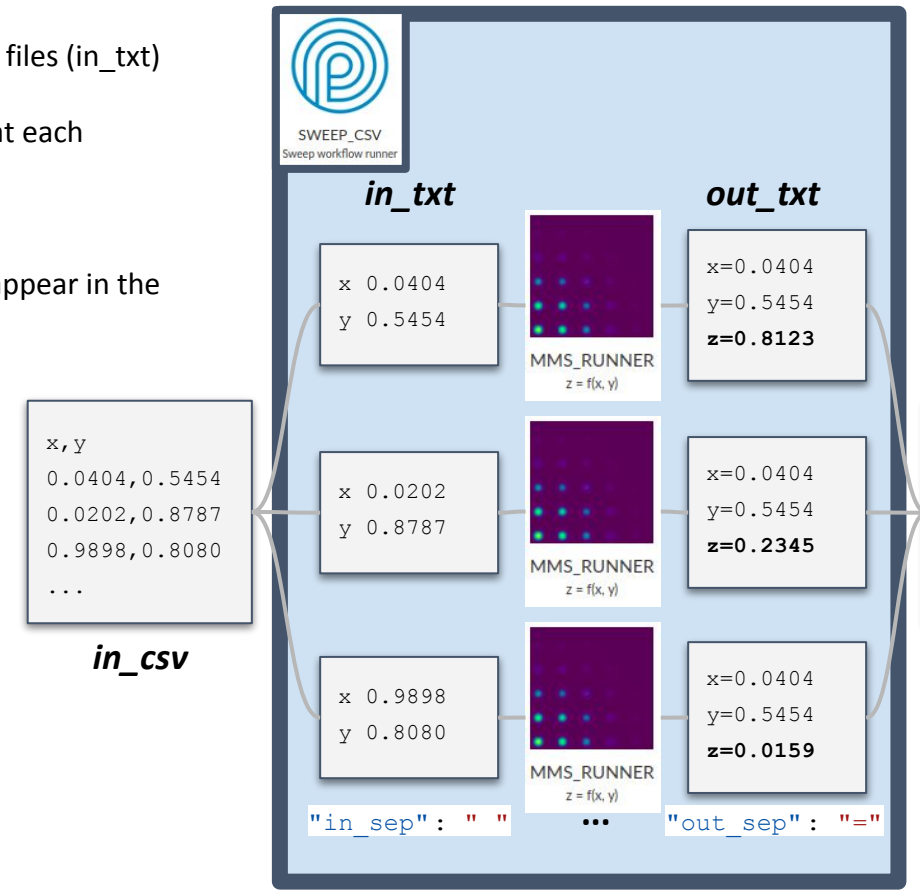
Workflow Building: SWEEP_CSV

SWEEP_CSV:

1. Splits a CSV (in_csv) file into several case inputs files (in_txt)

2. Submits “runner” workflows in parallel such that each workflow gets a case file. Compatibility:
   - Input and output files in the right format
   - Other inputs remain constant
   - Other outputs (images, logs, etc) need to appear in the workflow output directory (wf_dir)



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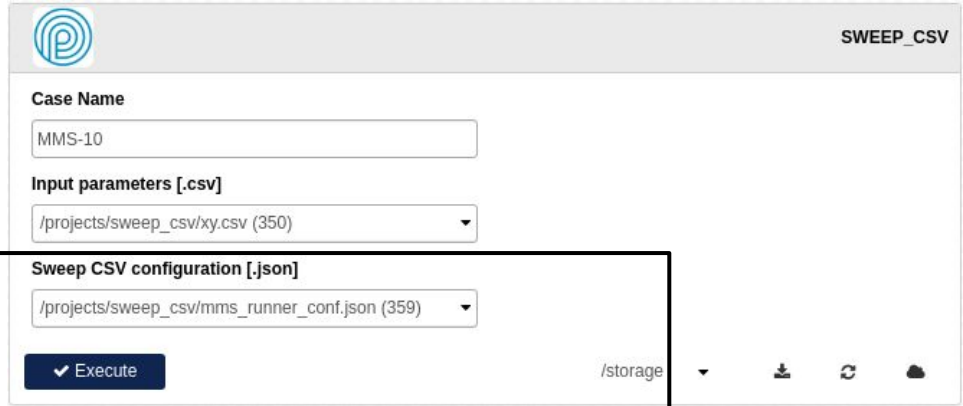
Workflow Building: SWEEP_CSV

Workflow inputs:




```
{
    "import": ["mms_runner"],          (workflows to import)
    "runner":                          (workflow info)
        {
            "wfname": "mms_runner",    (name)
            "run_func": "run",         (run function)
            "in_sep": " ",             (input parameter name/value separation)
            "out_sep": "=",            (output parameter name/value separation)
            "in_excld": [],            (input parameter names to exclude from in_txt)
            "out_excld": [],           (output parameter names to exclude from out_csv)
            "wfparams": {              (parameters of the run_func)
                "in_mms": "in_txt",    (tagged input parameter to be replaced by the Sweep_CSV)
                "out_mms": "out_txt"   (tagged output parameter to be replaced by the Sweep_CSV)
                                        (other constant IO definitions may be added here)
            }
        }
}
```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Workflow Building: SWEEP_CSV

You need to wait and merge the results but you cannot do it inside the *run_csv* function:

- Return a *SweepFut* object with a *.result()* method that waits for the futures and merges all the case output files (out_txt) into a single CSV output file (out_csv)

Parts of the main.py script of SWEEP_CSV

```
class SweepFut():
    def __init__(self, rwf_fut_list, rwf_conn, wf_pwargs):
        self.rwf_fut_list = rwf_fut_list
        self.rwf_conn = rwf_conn
        self.wf_pwargs = wf_pwargs
    # METHOD TO WAIT AND MERGE RESULTS!
    def result(self):
        # Wait for results
        out_txt_paths = []
        for rwf_fut in self.rwf_fut_list:
            out_txt_paths.append(rwf_fut[ self.rwf_conn["out_txt"]].result().path)

        # Merge results in CSV
        wfbuilder.data_reformat.txts2csv(
            out_txt_paths,
            self.wf_pwargs.out_csv,
            exclude = self.wf_pwargs.runner["out_excld"],
            sep = self.wf_pwargs.runner["out_sep"],
        )
        return self.wf_pwargs.out_csv
```

Parts of the main.py script of SWEEP_CSV

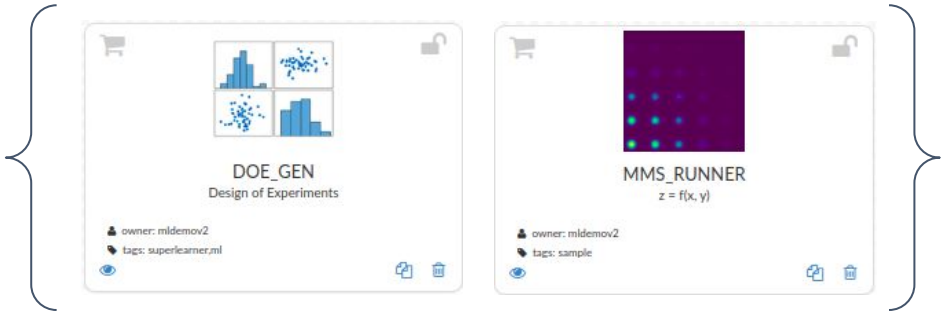
```
import os, sys, shutil, json
import parsl
from parslpw import pwconfig,pwargs
from copy import deepcopy
import inspect
if not os.path.isdir("wfbuilder"):
    shutil.copytree("/pw/modules/wfbuilder", "wfbuilder")
import wfbuilder

# Run CSV
def run_csv(wf_pwargs, wf_dir = "./sweep_csv"):
    os.makedirs(wf_dir, exist_ok = True)
    print("Sweep CSV wf_pwargs:", flush = True)
    print(wf_pwargs, flush = True)
    # RUNS SWEEP of MMS RUNNERs
    # DELETED CODE FOR SPACE
    return {"out_csv": SweepFut(rwf_fut_list, rwf_conn, wf_pwargs)}

if __name__ == "__main__":
    # This pwarg is only seen when executed from the form!
    with open(pwargs.sweepconf_json, 'r') as json_file:
        sweepconf = json.load(json_file)

    # Imported workflows
    if "import" in sweepconf:
        for wf_name in sweepconf["import"]:
            rwf = wfbuilder.pwimport.import_workflow(wf_name)

    # Add runner info to workflow arguments
    pwargs.runner = sweepconf["runner"]
    parsl.load(pwconfig)
    sweep_csv_fut = run_csv(pwargs)
    sweep_csv_fut["out_csv"].result()
```


Parallel Works

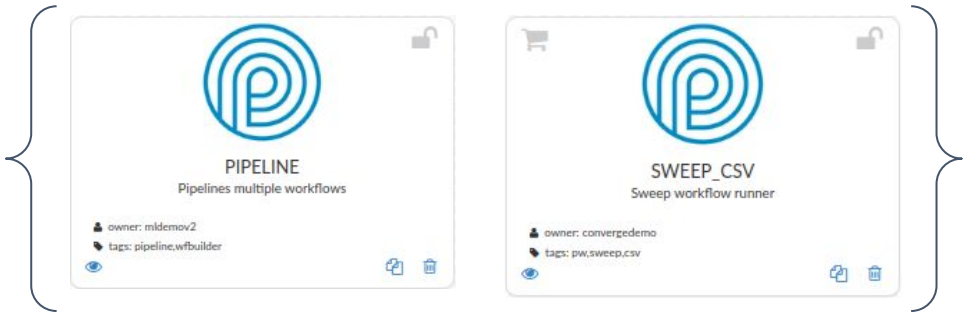
Workflow Building: PIPELINE

Example 2: **PIPELINE(DOE_GEN, SWEEP_CSV(MMS_RUNNER))**

Two base workflows



Two workflow topologies



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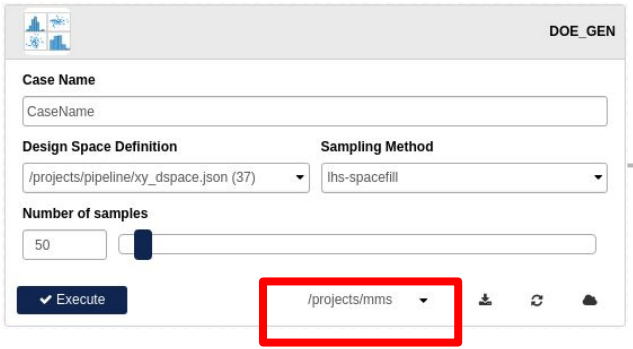
Workflow Building: PIPELINE

Design of experiments:




```
# INPUTS:
pwargs.casename = "CaseName"
pwargs.dspace = "/pw/projects/pipeline/xy_dspace.json"
pwargs.method = "lhs-spacefill"
pwargs.num_samples = "50"
# OUTPUTS:
pwargs.out_csv = "/storage/mms/doe-CaseName-date-time.csv"
pwargs.out_png = "/storage/mms/doe-CaseName-date-time.png"
pwargs.out_html =
"/storage/mms/doe-CaseName-date-time.html"
```

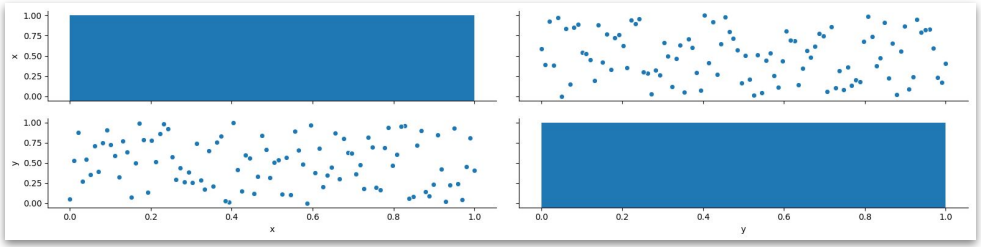
dspace

```
{
    "x": [0, 1],
    "y": [0, 1]
}
```

out_csv

```
x,y
0.0404,0.5454
0.0202,0.8787
0.9898,0.8080
...
```

out_png



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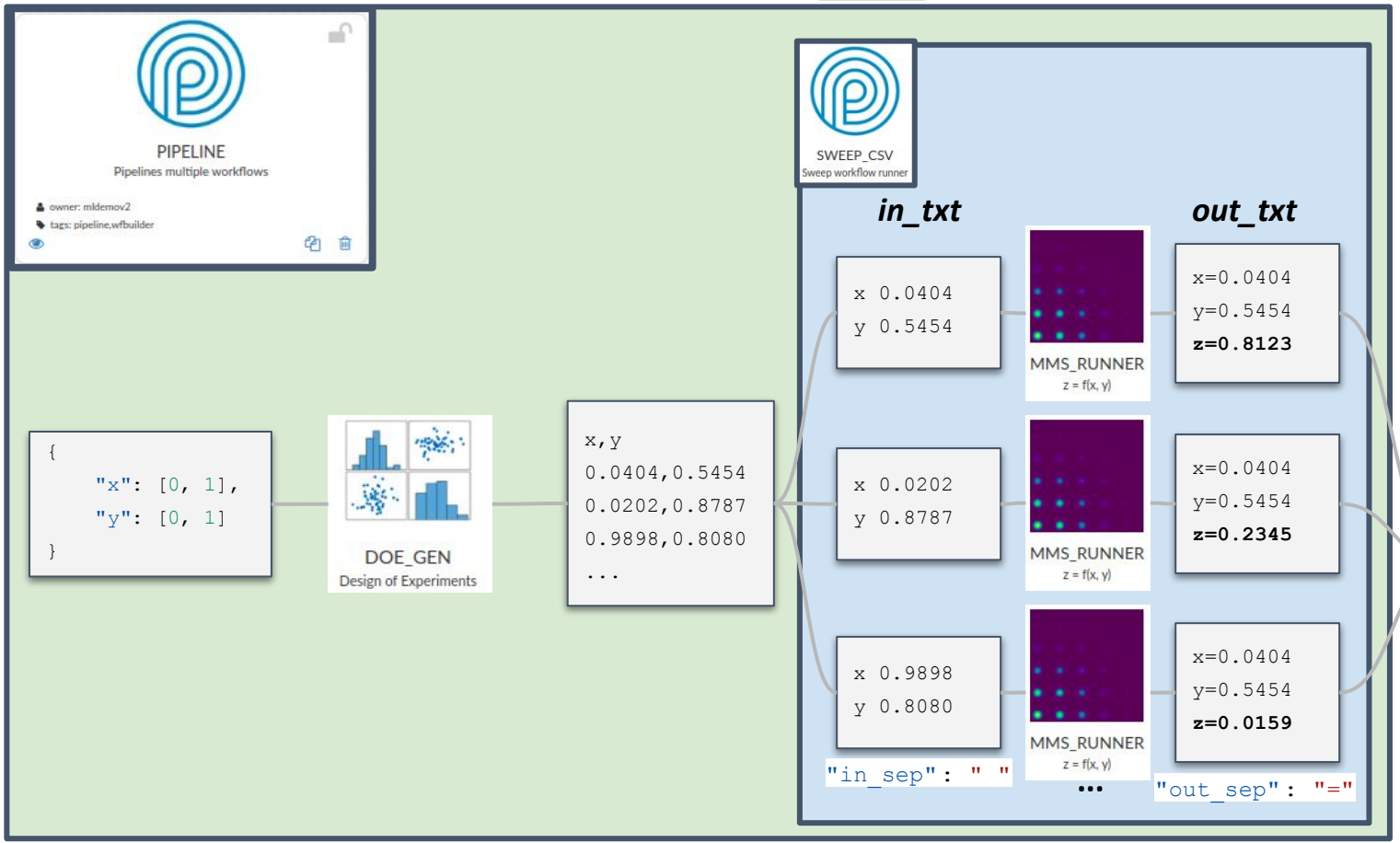
Workflow Building: PIPELINE



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Workflow Building: PIPELINE

PIPELINE:

- Runs a list of workflows in order piping the output of the previous workflows to the input of the next workflow(s)
- Only waits for the required DataFutures
- Returns a dictionary with remaining DataFutures and completed results

```
if __name__ == "__main__":
    # This pwarg is only seen when executed from the form!
    with open(pwargs.pipeconf_json, 'r') as json_file:
        pwargs.pipeconf = json.load(json_file)

    # Imported workflows!
    if "import" in pwargs.pipeconf:
        for wf_name in pwargs.pipeconf["import"]:
            rwf = wfbuilder.pwimport.import_workflow(wf_name)

    parsl.load(pwconfig)
    wfbuilder.wfconn.wait_for_futs(run_pipeline(pwargs))
```

main.py script of PIPELINE

```
# Run pipeline
def run_pipeline(wf_pwargs, wf_dir = "./pipeline"):
    os.makedirs(wf_dir, exist_ok = True)
    print("Pipeline wf_pwargs:", flush = True)
    print(wf_pwargs, flush = True)
    pipeconf = wf_pwargs.pipeconf
    wf_futs = {}
    for wi, wf_info in enumerate(pipeconf["pipeline"]):
        # Import workflow:
        wf = wfbuilder.pwimport.import_workflow(wf_info["wfname"])
        wf_run_func = getattr(wf, wf_info["run_func"])
        next_wf_pwargs = Namespace(**wf_info["wfparams"])
        if wi > 0:
            # Depends on the previous workflows
            # Get current workflow input from previous workflow outputs
            # Get workflow connections (dependencies)
            for pwi in reversed(range(wi)): # For previous workflow index (wfi)
                next_wf_pwargs, wf_conn = wfbuilder.wfconn.get_wf_pwargs(
                    vars(next_wf_pwargs),
                    pipeconf["pipeline"][pwi]["wfparams"]
                )
                # Make sure all dependencies are ready from previous workflows:
                for fut_key in wf_conn.keys():
                    wf_futs[pipeconf["pipeline"][pwi]["wfname"]][fut_key].result()
        # Run workflow:
        wf_futs[wf_info["wfname"]] = wf_run_func(next_wf_pwargs, wf_dir = wf_dir +
"/"
                                                 +
wf_info["wfname"])
        prev_wf_info = wf_info
    return wf_fut
```


Parallel Works

Workflow Building: PIPELINE

```
{
    "import": ["doe_gen", "sweep_csv", "mms_runner"],          (workflows to import)
    "pipeline": [                                              (list of workflows to execute serially)
        {                                                      (first workflow to run)
            "wfname": "doe_gen",                               (name)
            "run_func": "run_doe",                             (run function)
            "wfparams": {                                      (parameters of the run function)
                "dspace": "/pw/projects/pipeline/xy_dspace.json",
                "method": "lhs-spacefill",
                "num_samples": "50",
                "out_csv": "/pw/tmp/pipeline/xy.csv",
                "out_png": "/pw/tmp/pipeline/xy.png",
                "out_html": "/pw/tmp/pipeline/xy.html"
            }
        },
        {                                                      (second workflow to run)
            "wfname": "sweep_csv",                             (name)
            "run_func": "run_csv",                             (run function)
            "wfparams": {                                      (parameters of the run function)
                "in_csv": "out_csv",                           (tagged input parameter to replace with out_csv from the previous workflow(s))
                "out_csv": "/pw/tmp/pipeline/xyz.csv",
                "runner": {
                    "wfname": "mms_runner",
                    "run_func": "run",
                    "in_sep": " ",
                    "out_sep": "=",
                    "in_excld": [],
                    "out_excld": [],
                    "wfparams": {
                        "in_mms": "in_txt",
                        "out_mms": "out_txt"
                        }
                    }
            }
        }
    ]
}
```

Any workflow parameter value that corresponds to a workflow parameter key from a previous workflow will be replaced by the corresponding parameter value

Outline

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   a. Motivation
   b. Sweep_CSV
   c. Pipeline

3. Wrapping Parsl Apps: SimpleBashRunner

Wrapping Parsl Apps: SimpleBashRunner

Build wrappers around Parsl Apps to execute tasks every time a Parsl App is executed

SimpleBashRunner object:

- Runs a *bash_app*
- Builds and runs a bash command
  - *cmd cmd_args*
- IO are defined as dictionaries
- **Streams** standard output and error files from remote VM to local (PW)
- Run command as a given user
- Implements extra **logging** for debugging
- Writes resource information in the remote VM
- Returns a dictionary with the DataFutures

```
{
    "out_key_1": <DataFuture>,
    "out_key_2": <DataFuture>,
    ...
```

```
crunner = wfbuilder.pwrunners. SimpleBashRunner(
    cmd = "bash scripts/run.sh" ,
    cmd_arg_names = ["in_zip", "lic_server", "np", "out_zip"],
    inputs = {
        "in_zip": wfbuilder.Path(wf_pwargs.in_zip),
        "lic_server": wf_pwargs.lic_server,
        "np": wf_pwargs.np,
        "scripts": wfbuilder.Path( "/pw/workflows/converge_runner/./scripts" )
    },
    outputs = {
        "out_zip": wfbuilder.Path(wf_pwargs.out_zip)
    },
    logs = {
        "stdout":  wf_dir + "/std.out",
        "stderr":  wf_dir + "/std.err"
    },
    stream_host = "localhost",
    stream_port = os.environ[ 'PARSL_CLIENT_SSH_PORT' ],
    user = "cluster",
    write_pool_info = True
)
crunner_fut = crunner.run()
```

```
{"out_zip": <DataFuture at 0x7f2f638c11d0 state=pending>}
```

SUMMARY

Parsl App Wrappers:

- Run tasks every time a Parsl App is executed

Modular workflows:

- Built as a Python modules that can be executed directly or imported
- Workflow functions return futures and do not wait for results
- Only wait for results when executed directly (*if __name__ == “__main__”)*

Thanks for your attention!

Questions?

Contact:
alvaro@parallelworks.com