

Embrace the Full Stack

The simulation process
from submission to submission

Matt Young
University of New Hampshire

2019 CEDAR Workshop
Software Engineering for Heliophysics

What I plan to talk about

Lessons I've learned so far about
using simulations as a tool

Habits and code I've developed that I
hope will help someone else

Some components of the full
simulation stack and why we need to
treat the process as a whole

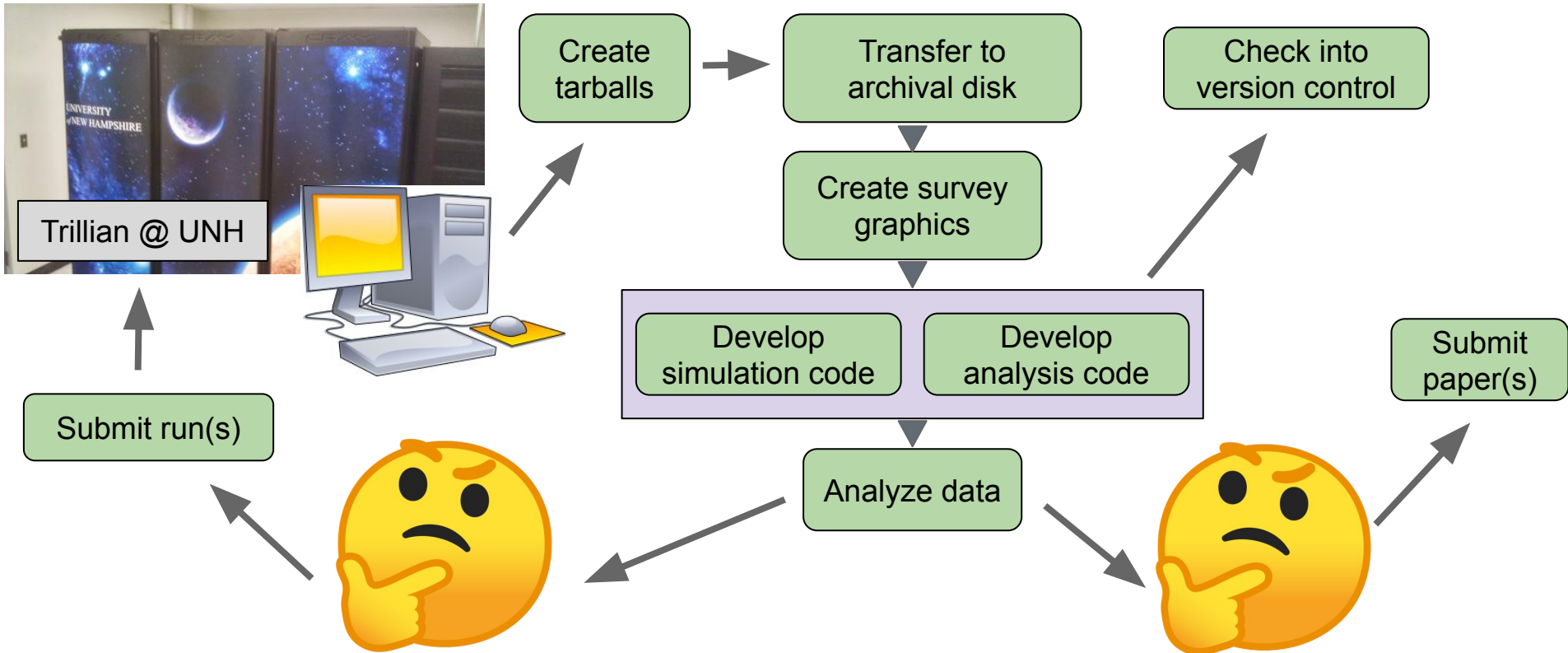
What I don't plan to talk about

Details of the hardware or software

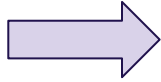
Choice of computing languages

Science results (in depth)

The “full stack”



Science!



A run by any other name.

I used to do this and it overwhelmed me:

```
matthew:simulations>> ls -l  
Bz0_0.50-Ey0_0.35-nui_3000-Ti_300-isothermal-no_gradient  
Bz0_0.50-Ey0_0.50-nui_3000-Ti_500-adiabatic-big_gradient  
Bz0_0.50-Ey0_0.70-nui_3000-Ti_300-adiabatic-big_gradient
```

Now I do this and it doesn't overwhelm me:

```
matthew:simulations>> ls -l  
README.md  
run000  
run001  
run002  
  
matthew:tests>> ls -l  
05Feb2019-000  
17Jun2019-000  
17Jun2019-001  
README.md
```

Log: It's better than bad – it's good.

When in doubt, keep track of parameters in a log file rather than in file names



Encoding parameters in file names



Recording parameters in a log file

Primary source.

```
File Edit Options Buffers Tools Insert Help
#!/bin/bash

#PBS -M matthew.young@unh.edu
#PBS -m abe
#PBS -l nodes=4:ppn=32
#PBS -l walltime=10:00:00

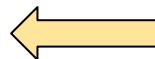
BVH=/mnt/lustre/lus0/home/space/myoung/bv_hybrid
RUN=data/project06/run006/

cd $BVH/src
tar -cvf $BVH/$RUN/src.tar *.c */*.c *.h makefile

cd $BVH/$RUN
aprun -n 128 ./ych.out > out
```

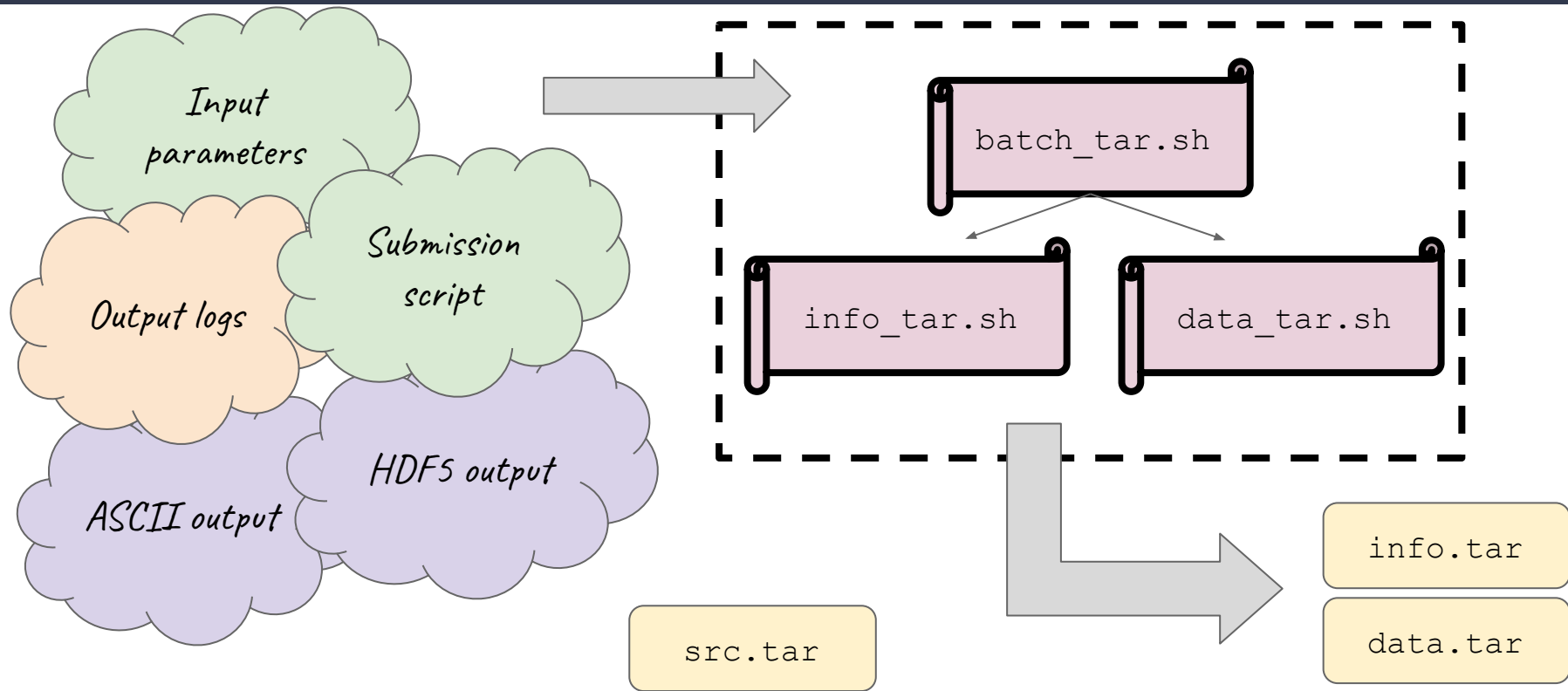
← Submit

- Example submission script.
- Machine-dependent, so don't worry about the details.
- Before the script submits the run, it archives the src directory.
- Allows me to rebuild the state that produced these results.



Archive (tar) the source

Play ball.



What do you Expect?

Expect is a program that interacts with other programs according to a script that you give it.

You can work with it natively in a shell script or use the `pexpect` module within Python

I can automate secure file transfer with `scp`, so I only need to enter my password once.

```
def main(
    user=None,
    remote_host=None,
    remote_paths=None,
    data_names=None,
    local_paths=None,
    timeout=None,
):
    """main function for expect_scp.py."""
    password = getpass.getpass()
    command = "scp"
    for remote_path, local_path in zip(remote_paths, local_paths):
        local_path = Path(local_path)
        remote_path = Path(remote_path)
        if not local_path.is_dir():
            if local_path.exists():
                local_path.rename(f"{local_path}.bak")
            local_path.mkdir(parents=True, exist_ok=True)
        else:
            pass
        for data_name in data_names:
            spawn_str = (
                f"{command} {user}@{remote_host}:"
                f"{remote_path}/{data_name} "
                f"{local_path}/{data_name}"
            )
            child = pexpect.spawn(spawn_str, encoding="utf-8")
            ret = child.expect(["Password: ", pexpect.EOF])
            if ret == 0:
                child.sendline(password)
                child.logfile = sys.stdout
                child.expect(pexpect.EOF, timeout=timeout)
                print(child.logfile)
                child.close()
            else:
                print(f"received EOF")
    return None
```

expect_scp.py

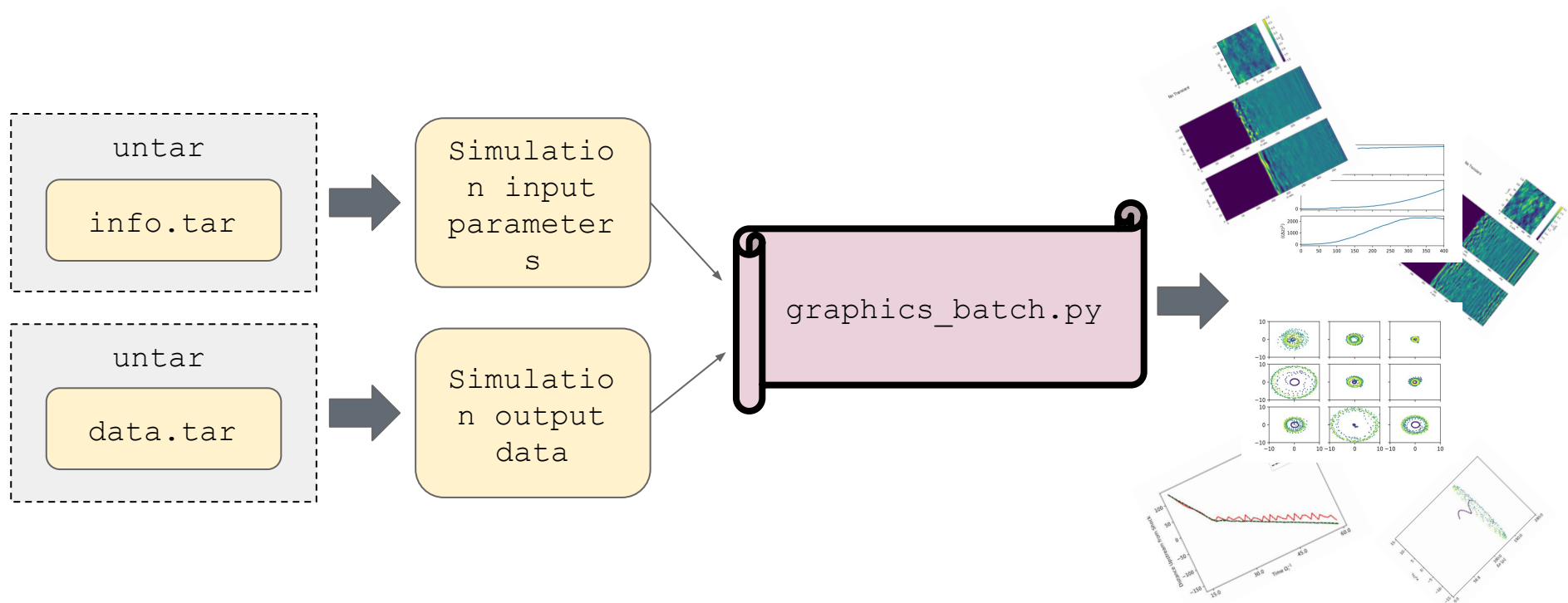
Securely save user password

Establish the local (destination) and remote (source) paths

Declare the command to execute

Send the command and submit the password automatically

First light.



Summary

The entire simulation "stack", from run submission, through managing the data set and versioning our code, to analyzing results and producing graphics *is* our tool, rather than a set of loosely connected tasks with differing priorities

Running numerical simulations.

Developing code to further science.

Embracing the full stack

