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HPC WORKFLOW MANAGEMENT WITH CHAPEL

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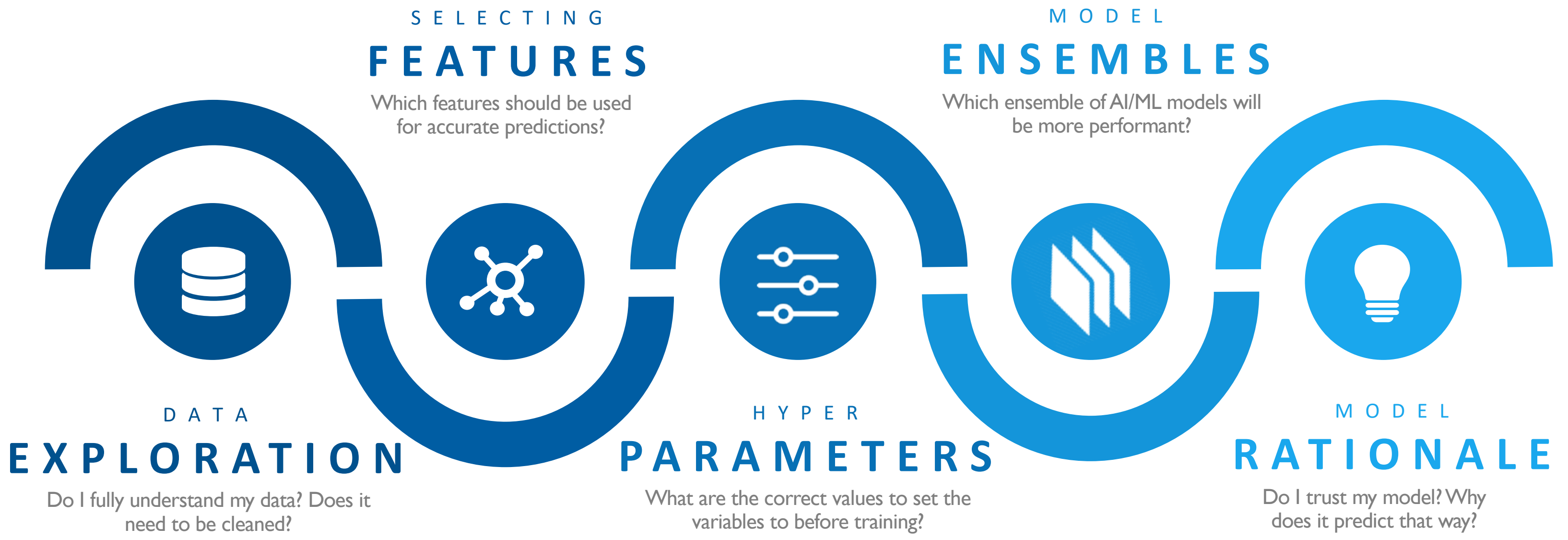
MOTIVATION

- Coordinating many monolithic applications is a challenge for the HPC user community
  - This impacts scientists across many domains such as astronomy, computational chemistry, and bioinformatics
- These workflows often begin as a simple shell script or collection of scripts
  - Depending on the complexity of the workflow, this may become unwieldy
  - Users can adopt a workflow framework or code their workflow in a more advanced programming language
- This talk will explore Chapel as a language to write HPC workflows

BACKGROUND: CRAY HPO

- The patterns explored in this talk are motivated by those found in Cray HPO
  - They are not a comprehensive list of workflow patterns
- Cray HPO is a hyperparameter optimization framework developed at HPE
- Background on hyperparameter optimization (HPO):
  - In data science, a model is trained on a dataset
  - Parameters are internal values in the model that are used to make predictions, e.g. slope and offset in y=mx+b
  - Hyperparameters are external values that impact how the model is trained, e.g. learning rate in SGD
  - Hyperparameter optimization is a process of tuning hyperparameters to minimize a metric, e.g. 1-accuracy
  - There is a wide breadth of HPO strategies: grid, random, genetic, bayesian, and more advanced variations


SELECTING FEATURES
Which features should be used for accurate predictions?
MODEL ENSEMBLES
Which ensemble of AI/ML models will be more performant?
DATA EXPLORATION
Do I fully understand my data? Does it need to be cleaned?
HYPER PARAMETERS
What are the correct values to set the variables to before training?
MODEL RATIONALE
Do I trust my model? Why does it predict that way?

- Cray HPO essentially acts as a distributed workflow manager for tuning the hyperparameters

```
from crayai import hpo  # crayai.hpo implementation is written in Chapel

# Specify training kernel and the resources on which to execute HPO training
evaluator = hpo.Evaluator('python3 source/train.py’, workload_manager=‘slurm’, nodes=16)

# Specify hyperparameter search space
params = hpo.Params([['--lr', 0.001, (1e-5, 0.1)],
                     ['--optimizer', 'Adam', ['Adam', 'Adadelta', 'Nadam']]])

# Specify optimizer and its metaparameters
optimizer = hpo.GeneticOptimizer(evaluator,
                                 generations=10,
                                 pop_size=16,
                                 mutation_rate=0.15)

# Optimize hyperparameters, results are stored in a csv file
optimizer.optimize(params)
```

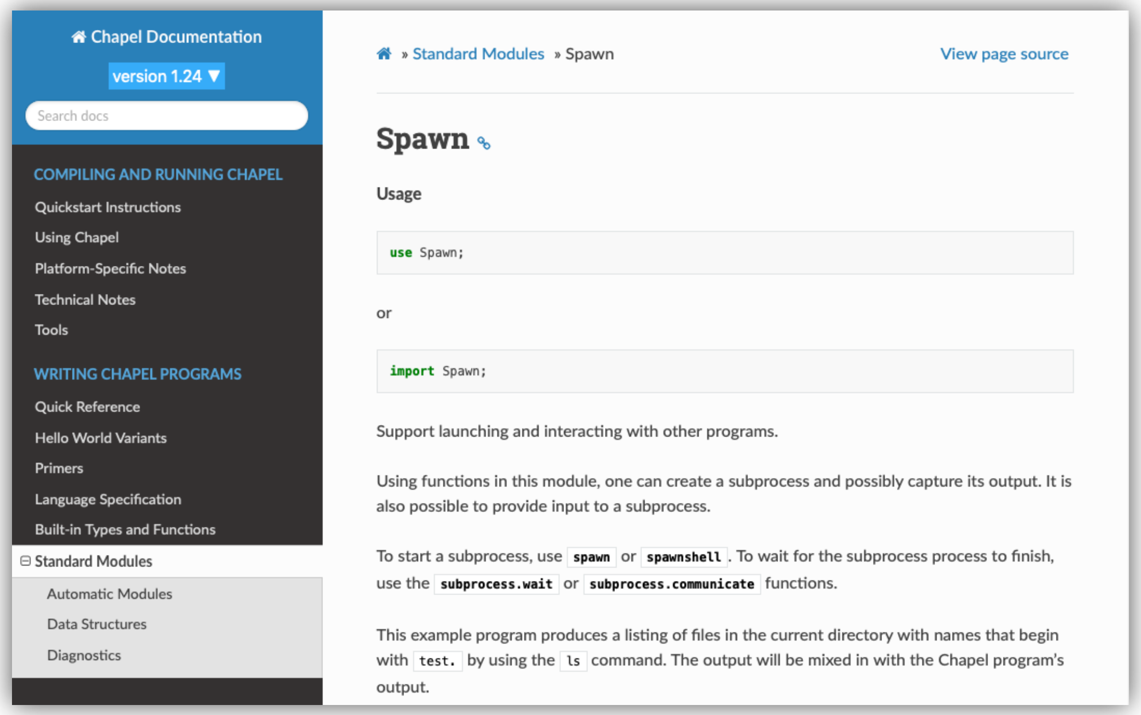
WORKFLOW BUILDING BLOCKS

LAUNCHING A SUBPROCESS

- Running other programs and interacting with their outputs is the basic building block of workflows
- In Chapel, running other programs can be done with the Spawn module:

```
use Spawn;

var process = spawn(['./run-simulation']);
```



Chapel Documentation
version 1.24
Search docs

COMPILING AND RUNNING CHAPEL
Quickstart Instructions
Using Chapel
Platform-Specific Notes
Technical Notes
Tools

WRITING CHAPEL PROGRAMS
Quick Reference
Hello World Variants
Primers
Language Specification
Built-in Types and Functions
Standard Modules
Automatic Modules
Data Structures
Diagnostics

» Standard Modules » Spawn   View page source

Spawn

Usage

```
use Spawn;
```

or

```
import Spawn;
```

Support launching and interacting with other programs.

Using functions in this module, one can create a subprocess and possibly capture its output. It is also possible to provide input to a subprocess.

To start a subprocess, use `spawn` or `spawnshell`. To wait for the subprocess process to finish, use the `subprocess.wait` or `subprocess.communicate` functions.

This example program produces a listing of files in the current directory with names that begin with `test.` by using the `ls` command. The output will be mixed in with the Chapel program's output.

LAUNCHING A SUBPROCESS

- Spawning a subprocess is a non-blocking operation.
  - Blocking on the completion of the program can be done with a ‘wait’ or ‘communicate’ call:

```
use Spawn;

var process = spawn(['./run-simulation’],
                     stdout=PIPE);
process.wait();
for line in process.stdout.readlines() {
  writeln(line);
}
```

LAUNCHING A DISTRIBUTED SUBPROCESS

For interacting with HPC workload managers and launchers, one can capture interface into a function:

```
use Slurm;

const jobid = salloc(numNodes=32, timeout=120);
var process = srun('./run-simulation', numNodes=32, id=jobid);
process.wait();
```

Abstracting away workload manager specifics enables portability across HPC systems:

```
use Jobs;

var job = new Job(workloadManager=Launchers.pbs, launcher=Launchers.aprun);
job.alloc(numNodes=32, timeout=120);
var process = job.run('./run-simulation', numNodes=32);
process.wait();
```

LAUNCHING SUBPROCESSES IN PARALLEL

- Launching subprocesses in parallel is necessary for many workloads
- The forall loop is the ideal construct for this functionality:
  - Creates a concurrent task mapped to available resources, such as cores, gpus, nodes, etc.

```
var simulationCommands: [1..n] string = getCommands(n);

forall simulationCommand in simulationCommands {
  var process = spawn(simulationCommand, stdout=PIPE, stderr=PIPE);
  process.wait();
}
```

  - Each task will block on the process.wait() call, allowing the subprocess to complete before starting a new one
  - This forall maps to the local available resources, i.e. number of cores on the machine

LAUNCHING DISTRIBUTED SUBPROCESSES IN PARALLEL

To map the number of concurrent tasks to the available distributed resources, use the iterator explicitly:

```
use Jobs;

config const nodesPerSim = 8;
config const numNodes = 128;

var job = new Job(workloadManager=Launchers.slurm);
var inputs: [0..<n] string = readInputs('inputs.txt');
const numParallelTasks = (numNodes / nodesPerSim):int;

job.alloc(numNodes, timeout=240);
forall i in simulationCommands._value.these(tasksPerLocale=numParallelTasks) {
  var process = job.run(simulationCommand, numNodes=nodesPerSim);
  process.wait();
}
```

This will allocate 128 nodes and run 16 concurrent tasks that each launch a process with 8 nodes

VARIABLE NUMBER OF NODES PER DISTRIBUTED APPLICATION

Varying the number of nodes in the distributed application requires tracking the available node pool

```
use ChapelLocks;
var nodesAvailable = numNodes;
var lock: chpl_LocalSpinlock;
...
forall i in simulationCommands._value.these(tasksPerLocale=numParallelTasks) {
  localNumNodes = randStream.getNext(1,8);
  waitForNodes(localNumNodes);
  var process = job.run(simulationCommand, numNodes=localNumNodes);
  process.wait();
}
```

VARIABLE NUMBER OF NODES PER DISTRIBUTED APPLICATION

```
proc waitForNodes(localNumNodes) {
  // Wait until nodes are available
  while true {
    lock.lock();
    if nodesAvailable >= localNumNodes {
      // Remove nodes from node pool
      nodesAvailable -= localNumNodes;
      lock.unlock;
      break;
    } else {
      lock.unlock();
      Time.sleep(1);
    }
  }
  // Add nodes back to node pool when done
  lock.lock();
  nodesAvailable += localNumNodes;
  lock.unlock;
}
```

PARSING OUTPUT

- I/O is an important component of any workflow application
- The output generated by the subprocess can be accessed through various mechanisms:
  - Parsing subprocess stdout
  - Parsing files generated by subprocess
  - Connecting with the subprocess and communicating in memory, e.g. over ZMQ
  - Writing results to a database from the subprocess

ADVANTAGES AND DISADVANTAGES OF CHAPEL

Advantages

- Modern programming language with modern features and productivity
  - Generics, type inference, native C/python interop, etc.
- Parallel constructs built into the language
  - Parallel loops, atomics, tasks, etc.
- Performance
  - Not always important in workflow space, but can be important for sufficiently large workflow programs
  - Some workflow tools use complex algorithms in their feedback loops, e.g. Bayesian optimization in HPO
- Compiling and statically linking produces a dependency-free binary

Disadvantages

- Compilation is time consuming
- Standard library and module ecosystem not as mature as other languages such as Python

ALTERNATIVE OPTIONS FOR BUILDING WORKFLOWS

- Shell scripting
- Other modern programming languages: Python, Julia, Go, Rust, etc.
- Workflow frameworks, such as Apache Airflow
- Domain-specific workflow frameworks, such as Bioclipse
- Domain-specific languages for workflow automation, such as swift scripting language

SUMMARY

- Developing HPC workflows is a challenged faced by many scientists and engineers
- Chapel has many appealing features making it a competitive choice for developing workflows
  - Modern PL features
  - Parallel constructs
  - Performance
  - Portability

THANK YOU