Workflow for extreme-scale systems

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Outline

- Overview – context of workflow for science and engineering
- Workflow environments
- Expressing workflows – tools and programming models
- Workflow issues for extreme scale
- IO performance envelopes for workflow
- Expressing workflows in Swift
- Hands-on workflow examples and exercises using Swift
  - Language basics
  - Running on a cluster
  - Running on a cloud
  - Running on a supercomputer
  - Multi-machine workflows
  - Scaling up with Swift/Turbine: in memory and inter-language
  - More advanced (self-paced) workflows exercises and experiments
Definitions

- **Workflow**: the execution of a set of application programs
  - Often for a diverse set of application programs
  - Often with logical and physical dependencies
    - Logical: data dependencies
    - Physical: resource dependencies (space, processor, solution priorities)
  - Scripting is one way to implement workflows (Ad-hoc, Parallel libraries, Swift)
  - Generation of engine-specific input is another (DAGMan, Pegasus, Galaxy, Kepler)
- **Scripting**: higher-level dynamic programming
  - J. Ousterhout: “Scripting: Higher level programming for the 21st century”
- **High throughput computing (HTC)**
- **Many-task computing (MTC)**
- **Dataflow**
- **Data parallel vs. task parallel**
  - Workflow is almost always task-parallel at its outer levels
  - SPMD: typified by MPI
  - MPMD: multiple programs, multiple data – more typical of workflow
Definition of MTC Applications

- Many-task Computing applications assemble existing parallel or sequential programs
- Those programs read and write data to a filesystem
- Applications often have multiple stages
- Task dependencies between stages are in the form of file production and consumption
- Can have very high rates (e.g., hundreds per second) of very short tasks (minutes seconds)

Slide courtesy of Zhao Zhang
When do you need workflow?
Typical application: protein-ligand docking for drug screening

$O(10)$ proteins implicated in a disease

$O(100K)$ drug candidates

Tens of fruitful candidates for wetlab & APS

Work of M. Kubal, T.A. Binkowski, And B. Roux
Numerous many-task workflow applications

A. Simulation of super-cooled glass materials
B. Protein folding using homology-free approaches
C. Climate model analysis and decision making in energy policy
D. Simulation of RNA-protein interaction
E. Multiscale subsurface flow modeling
F. Modeling of power grid for OE applications
TARGET RESOURCES

- System types
  - Clouds
  - Clusters (campus, department)
  - Petascale HPC systems
  - Grids (OSG, LCG, ...)
  - Multi/many-cores – 256 core nodes!

- Patterns
  - A single big HPC machine
  - HPC Machine with attached resources
  - Extend campus cluster with cloud
  - Many HPC machines
  - Many combinations of above
Workflow client can send HPC work to Cray and analysis work to campus cluster and/or resource aggregator.
Workflow patterns and issues

- Parameter sweeps
- Ensembles
- Data analysis
- Scaling studies
- Specialized patterns: uncertainty quantification, branch and bound
- Programming an application from libraries of applications
- Dataflow vs control flow
  - Ultimately, workflow is essentially dataflow
  - The difference is who writes and thinks about the dataflow
- Pipelining and concurrency (and how dataflow is good at this)
- Workflow manager drives application (outer workflow, inner scripts)
- Workflow manager embedded in application (outer scripts, inner workflow)
PROGRAMMING MODELS

- MPI, OpenMP, Hybrid
- Map reduce
- Record processing (with functions) vs file processing (with apps)
- Generating workflows for other engines
- Dynamically interpret the workflow
- Script mode (for Blue Gene, Cray systems)
- Dependent job processing
A *partial* sampler of workflow tools

- **High throughput tools**
  - Condor
  - Cluster schedulers / local resource managers (PBS, SGE, Cobalt, LSF, LL, SLURM,...)

- **Workflow task dependency managers**
  - DAGMan
  - Schedulers with job dependencies

- **Integrated dependency and data management**
  - Pegasus

- **Dataflow languages**
  - Dryad, Ciel, Swift

- **Big data solutions**
  - Hadoop, Spark, Zookeeper, Uzi

- **Multicore tools**
  - GNU Parallel

- **Languages with parallel support**
  - Py_nnn, Java_nnn, Haskell, R, MATLAB => PSOM, Parallel BASH (Walker)
A sampler of workflow tools - part II

- Interactive workflow frameworks
  - Galaxy
  - Taverna
  - Kepler
  - LONI Pipeline (neuroscience)
  - Microsoft Workflow manager
  - Airivata

- Science gateways
Parallel BLAST as a workflow

Based on script of D. Matthog by Z. Zhang, L. Gahelha


**BLAST STAGE TASKS, INPUTS, OUTPUTS, AND INPUT AND OUTPUT SIZE**

<table>
<thead>
<tr>
<th>Stage</th>
<th># Tasks</th>
<th># In</th>
<th># Out</th>
<th>In (MB)</th>
<th>Out (MB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>fastasplitn</td>
<td>1</td>
<td>1</td>
<td>N</td>
<td>4039</td>
<td>4039</td>
</tr>
<tr>
<td>formatdb</td>
<td>N</td>
<td>N+M</td>
<td>N*M</td>
<td>4039</td>
<td>4400</td>
</tr>
<tr>
<td>blastp</td>
<td>N*M</td>
<td>N+M</td>
<td>N*M</td>
<td>73<em>N</em>M</td>
<td>2.4<em>N</em>M</td>
</tr>
<tr>
<td>merge</td>
<td>M</td>
<td>N*M</td>
<td>M</td>
<td>2.4<em>N</em>M</td>
<td>4.8*M</td>
</tr>
</tbody>
</table>
Can workflow scale?

BLAST workflow lags MPI BLAST by ~ 5%

Two fundamental problems in scaling workflow

- **Task rate**
  - 60,000 cores / 60 sec/task = 1,000 tasks per second!

- **Data management**
  - 1K tasks / sec may generate 5GB/sec – not so bad if blocked efficiently
  - 1K tasks / sec may generate 2,000 files / sec – not so easy
Multi-level scheduling: pilot jobs can improve task rate performance

- Pilot jobs are long-running meta-jobs
  - allocate compute resources and run many smaller jobs
- PANDA
  - Widely used on OSG and LCG by the ATLAS physics collaboration
- GWMS using Condor Glide-Ins
  - A generalized solution widely deployed on OSG
- SAGA and Bigjob
  - Obtaining good results on XSEDE resources
- Java CoG Coasters
  - Allocates/frees resources based on demand
  - Peaks at 600 tasks per second
- Falkon
  - Research system reached 3,000 tasks per second and 1B tasks
Workflow patterns and data exchange

Filesystem Access Patterns:
- File Creation
- File Open
- 1-to-1 Read
- N-to-1 Read
- Few-to-1 Read
- 1-to-1 Write

Measuring MTC Envelope:

- **Target platform**
  - GPFS deployed with ANL Intrepid BlueGene/P
  - Several metadata servers, but only one for each directory
  - 128 IBM x3545 file servers, each with two 2.6-GHz Dual Core CPUs and 8 GB RAM
  - We use I/O nodes as GPFS clients. (Ratio between I/O nodes and CPU cores – 1:256)

- **Experimental setup**
  - Metadata operation: \{create, open\} \times \{1, 2, 4, 8, 16, 32, 64, 128, 256\} clients
  - I/O: \{read, write\} \times \{1 KB, 128 KB, 1 MB, 16 MB\} \times \{1, 2, 4, 8, 16, 32, 64, 128, 256\} clients
  - Total number of operations fixed at 8192 at each scale
  - All files are in one directory

Performance envelope research and slides by Zhao Zhang
Measuring MTC Envelope

- Metadata Operation Throughput

![Graph showing Metadata Operation Throughput over scale (Number of GPFS Clients)]
Measuring MTC Envelope

- 1-to-1 Read
MTC Envelope vs. Scale
Performance guide for workflows

- MTC Envelope expressed as heat maps: (shown here for write ops)

- Use throughput heat map when files are small, and use bandwidth heat map when files are large.

**1-to-1 Read Performance**

**I/O Performance Prediction:**
Some engineering problems and research challenges for extreme workflow

- Engineering
  - Diversity of interfaces, hard to tame and test, hard to abstract
  - Inter-language bindings and data interchange – challenge to usability
  - Integration with extreme-scale networks, runtimes and language stacks

- Research
  - Economics and policy-based scheduling
  - Retry/recovery of large distributed task and data graphs
  - Power management
  - Load balancing
  - Programming models: integration of dataflow and big-data techniques and tools
**GEMTC: GPU Enabled Many-Task Computing**

**Motivation:** Support Many-Task Computing on Accelerators

**Goals:**
1) MTC support
2) Improved programmability
3) MTC efficiency
4) MIMD on SIMD
5) Increase concurrency 12X (16 -> 192 (12x))

**Approach:**
1) Design, implement middleware:
   1) manages GPU
   2) spread host/device
   3) Workflow system support (Swift/T)

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- Parallel scripting language for clusters, clouds & grids
  - For writing loosely-coupled scripts of application programs and utilities linked by exchanging files
  - Can call scripts in shell, python, R, Octave, MATLAB, ...

- Swift does 3 important things for you:
  - Makes parallelism transparent – with functional dataflow
  - Makes basic failure recovery transparent
  - *Makes computing location transparent* – can run your script on multiple distributed sites and diverse computing resources (from desktop to petascale)

→ *this is what we’ll show today*
Language-driven: *Swift* parallel scripting

Swift runs parallel scripts on a broad range of parallel computing resources.

Submit host (login node, laptop, Linux server)

Data server

Application Programs

Swift script

Clouds:
Amazon EC2,
XSEDE Wispy, ...
Programming model: all execution driven by parallel data flow

(int r) myproc (int i)
{
    j = f(i);
    k = g(i);
    r = j + k;
}

- f() and g() are computed in parallel
- myproc() returns r when they are done

- This parallelism is *automatic*
- Works recursively throughout the program’s call graph
Encapsulation enables distributed parallelism

Encapsulation is the key to transparent distribution, parallelization, and automatic provenance capture.
app( ) functions specify cmd line argument passing

**To run:**
```
psim -s 1ubq.fas -pdb p -t 100.0 -d 25.0 >log
```

**In Swift code:**
```
app (PDB pg, File log) predict (Protein seq, Float t, Float dt)
{
    psim "-c" "-s" @pseq.fasta "-pdb" @pg
        "-t" temp "-d" dt;
}
```

Protein p <ext; exec="Pmap", id="1ubq">;
PDB structure;
File log;

(structure, log) = predict(p, 100., 25.);
foreach sim in [1:1000] {
    (structure[sim], log[sim]) = predict(p, 100., 25.);
}
result = analyze(structure)
Nested parallel prediction loops in Swift

1. Sweep()
2. {
3.   int nSim = 1000;
4.   int maxRounds = 3;
5.   Protein pSet[ ] <ext; exec="Protein.map">;
6.   float startTemp[ ] = [ 100.0, 200.0 ];
7.   float delT[ ] = [ 1.0, 1.5, 2.0, 5.0, 10.0 ];
8.   foreach p, pn in pSet {
9.       foreach t in startTemp {
10.          foreach d in delT {
11.              ItFix(p, nSim, maxRounds, t, d);
12.          }
13.       }
14.    }
15. }
16. Sweep();
Spatial normalization of functional run

Dataset-level workflow

- reorientRun
  - random_select
    - alignlinearRun
      - resliceRun
        - softmean
          - alignlinear
            - combinewarp
              - reslice_warpRun
                - strictmean
                  - binarize
                    - gsmoothRun

Expanded (10 volume) workflow

- reorient
  - alignlinear
  - reslice
    - softmean
    - combinewarp
    - reslice_warp
      - strictmean
      - binarize
      - gsmooth
(Run snr) **functional** ( Run r, NormAnat a, 
  Air shrink )
{
  Run yroRun = **reorientRun**( r , "y" );
  Run roRun = **reorientRun**( yroRun , "x" );
  Volume std = roRun[0];
  Run rndr = **random_select**( roRun, 0.1 );
  AirVector rndAirVec = **align_linearRun**( rndr, std, 12, 1000, 1000, "81 3 3" );
  Run reslicedRndr = **resliceRun**( rndr, rndAirVec, "o", "k" );
  Volume meanRand = **softmean**( reslicedRndr, "y", "null" );
  Air mnQAAir = **alignlinear**( a.nHires, meanRand, 6, 1000, 4, "81 3 3" );
  Warp boldNormWarp = **combinewarp**( shrink, a.aWarp, mnQAAir );
  Run nr = **reslice_warp_run**( boldNormWarp, roRun );
  Volume meanAll = **strictmean**( nr, "y", "null" )
  Volume boldMask = **binarize**( meanAll, "y" );
  snr = **gsMOOTHRun**( nr, boldMask, "6 6 6" );
}
Dataset mapping example: fMRI datasets

```plaintext
type Study {
  Group g[];
}

type Group {
  Subject s[];
}

type Subject {
  Volume anat;
  Run run[];
}

type Run {
  Volume v[];
}

type Volume {
  Image img;
  Header hdr;
}
```

On-Disk Data Layout

Swift’s in-memory data model

Mapping function or script
Nested loops can generate massive parallelism

Protein folding example:

Sweep( )
{
    int nSim = 1000;
    int maxRounds = 3;
    Protein pSet[ ] <ext; exec="Protein.map">;
    float startTemp[ ] = [ 100.0, 200.0 ];
    float delT[ ] = [ 1.0, 1.5, 2.0, 5.0, 10.0 ];
    foreach p, pn in pSet {
        foreach t in startTemp {
            foreach d in delT {
                ItFix(p, nSim, maxRounds, t, d);
            }
        }
    }
}

Sweep();

10 proteins x 1000 simulations x 3 rounds x 2 temps x 5 deltas = 300K tasks
Centralized evaluation can be a bottleneck

Had this (Swift/K):

For extreme scale, we need this (Swift/T):
Parallel evaluation of Swift/T in ExM

Swift/T: Large-scale application composition via distributed-memory data flow processing
Swift/T programs run as an SPMD MPI program using ADLB
Swift/T: High-level model

- Script-like global-view programming with “leaf tasks” - function calls in C, C++, Fortran, Python, R, or Tcl
- Leaf tasks can be MPI programs, etc.
- Distributed, scalable runtime manages tasks, load balancing, data movement
- User function calls to external code run on 1000’s of workers
- Like master-worker but with the expressive Swift language to control progress
MPI process architecture for parallel evaluation in Swift/T
Parallel evaluation in action

```java
int X = 100, Y = 100;
int A[][];
int B[];
foreach x in [0:X-1] {
    foreach y in [0:Y-1] {
        if (check(x, y)) {
            A[x][y] = g(f(x), f(y));
        } else {
            A[x][y] = 0;
        }
    }
    B[x] = sum(A[x]);
}
```

(To simplify diagram, array references are not shown for the loops above)
Pervasive implicit parallelism with automatic pipelining

```plaintext
blob models[], res[];

foreach m in [1:N_models] {
    models[m] = load(sprintf("model%i.data", m));
}

foreach i in [1:M] {
    foreach j in [1:N] {
        // initial quick evaluation of parameters
        p, m = evaluate(i, j);
        if (p > 0) {
            // run ensemble of simulations
            blob res2[];
            foreach k in [1:S] {
                res2[k] = simulate(models[m], i, j);
            }
            res[i][j] = summarize(res2);
        }
    }
}

// Summarize results to file
foreach i in [1:M] {
    file out<printf("output%i.txt", i)>
    out = analyze(res[i]);
}
```

(a) Declarative Swift/T code

(b) Visualization of parallel execution for $M = 2$, $N = 2$, $S = 3$
Swift/T toolchain and runtime environment
Inside the Swift/T “stc” compiler

STC Compiler

- Optimization
- Post-processing: Ref. Counting & Value. Passing
- Normalization
- Code Generator

Swift/T Script

Frontend

Distributed Executor

Tcl Script w/ runtime library calls
Operation reduction optimizations by stc

- (a) Sweep ($10^7$ combinations)
- (b) Fibonacci ($n = 24$)
- (c) Sudoku (100x100 board)
- (d) Wavefront (100x100 array)
- (e) Simulated Annealing (125 iterations, 100-way objective function parallelism)
1. \( a = f1(); \quad b = f2(a); \)
2. \( c, d = f3(a, b); \quad e = f4(f5(c)); \)
3. \( f = f4(f5(d)); \quad g = f6(e, f); \)

(a) Swift code fragment

(b) Unoptimized version, relying on shared data flow variables to pass data and runtime data dependency tracking

(c) After wait pushdown and elimination of shared variables in favor of parent-to-child data passing

(d) After pipeline fusion merges tasks
Task priority can be specified to reduce tail effects

- Variable-sized tasks produce trailing tasks: addressed by exposing task priorities at language level
Performance results:
10 Cray XE MC-12 24-Core nodes,
2 control nodes, 8 worker nodes (240 cores total)

Fig. 11: Throughput at different optimization levels measured in application terms: tasks/sec, or annealing iterations/sec.
Example execution

- Code

- Engines: evaluate dataflow operations

- Workers: execute tasks

  - Task put
  - Notification
  - Task put
ADLB: Asynchronous Dynamic Load Balancer

- Developed previously by Lusk and Butler
- Pure MPI task distributor
- Uses client-server model with multiple servers for scalability
- Servers can share work
- Originally, supported just Put() and Get() on tasks
- We added Store(), Retrieve(), Subscribe(), etc. on data for data-dependent processing

Supports calls to native libraries

- Including MPI libraries

- Top-level dataflow script
  sweep.swift

- user1.c
  wrapper

- user2.f
  wrapper

- user3.cpp
  wrapper

- Swift/T runtime
  Task distribution / Data store

- MPI
Application: Power Grid Modeling (PIPS)

Swift/T (and the many-task, dataflow model) complements existing application workflows.
Application: Branch-and-Bound (Minotaur)

Minimize some function via recursive search, allow only for integer solutions

Builds a new, scalable application from pre-existing components
Visualization of Swift/T execution

- User writes and runs Swift script
- Notices that native application code is called with nonsensical inputs
- Turns on MPE logging – visualizes with MPE

![Graph showing process rank and time]

- **PIPS task computation**
  - Store variable
  - Notification (via control task)

Blue: Get next task
Retrieve variable

Server process (handling of control task is highlighted in yellow)

- Color cluster is task transition:
- Simpler than visualizing messaging pattern (which is not the user’s code!)
- Represents Von Neumann computing model – load, compute, store
Debugging Swift/T execution

- Starting from GUI, user can identify erroneous task
  - Uses time and rank coordinates from task metadata

- Can identify variables used as task inputs

- Can trace provenance of those variables back in reverse dataflow

Aha! Found script defect. ← ← ← (searching backwards)
Swift is a parallel scripting system for grids, clouds and clusters
  – for loosely-coupled applications - application and utility programs linked by exchanging files

Swift is easy to write: simple high-level C-like functional language
  – Small Swift scripts can do large-scale work

Swift is easy to run: contains all services for running Grid workflow - in one Java application
  – Untar and run – acts as a self-contained Grid client

Swift is fast: uses efficient, scalable and flexible “Karajan” execution engine.
  – Scaling close to 1M tasks – .5M in live science work, and growing

Swift usage is growing:
  – applications in neuroscience, proteomics, molecular dynamics, biochemistry, economics, statistics, and more.

Try Swift! http://swift-lang.org (Swift/K) and www.mcs.anl.gov/exm (Swift/T)
Summary: Challenges of workflow at extreme scale

- Inter-resource coordination
- Hybrid programming tools
- The challenges of data motion
  - Data management strategies and system envelopes
- The challenges of task scheduling and dispatch
  - Task rates and task distribution
  - Resource utilization vs. time to solution
- Workflow expression and separation of concerns
- Provenance: tracking what was done
Workflow references

- Workflows for e-Science Book
- VderA patterns
- Pegasus patterns
- Paper on characterization (Lavana, Gannon et al)
- Bibliography ... ???
Swift: A language for distributed parallel scripting

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\textbf{Abstract}

Scientists, engineers, and statisticians must execute domain-specific application programs many times on large collections of file-based data. This activity requires complex orchestration and data management as data is passed to, from, and among application invocations. Distributed and parallel computing resources can accelerate such processing, but their use further increases programming complexity. The Swift parallel scripting language reduces these complexities by making file system structures accessible via language constructs and by allowing ordinary application programs to be composed into powerful parallel scripts that can efficiently utilize parallel and distributed resources. We present Swift’s implicitly parallel and deterministic programming model, which applies external applications to file collections using a functional style that abstracts and simplifies distributed parallel execution.
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- The Swift team:
  - Tim Armstrong, Ian Foster, Mihael Hategan, Dan Katz, David Kelly, Ketan Maheshwari, Justin Wozniak, Mike Wilde, Justin Wozniak, Zhao Zhang
- Swift/T:
  - Justin Wozniak and Tim Armstrong, with Yadu Nand and Scott Krieder
- GeMTC (IIT):
  - Ioan Raicu, Scott Krieder, Ben Grimmer
- ExM:
  - Tim Armstrong, Ian Foster, Rusty Lusk, Ketan Maheshwari, Todd Munson, Matei Ripeanu, Sameer Al-Kiswani, Hao, Mike Wilde
- Java CoG Kit used by Swift developed by:
  - Mihael Hategan, Gregor Von Laszewski, and many collaborators
- Scientific application collaborators and usage described in this talk:
  - U. Chicago Open Protein Simulator Group (Karl Freed, Tobin Sosnick, Glen Hocky, Joe Debartolo, Aashish Adhikari, Mark Parisien)
  - U.Chicago Radiology and Human Neuroscience Lab, (Dr. S. Small, Sarah Kenny, Uri Hasson)
  - RDCEP / CIM-EARTH: Joshua Elliott, David Kelly
  - ParVis and FOAM: Rob Jacob, Sheri Mickelson (Argonne); John Dennis, Matthew Woitaszek (NCAR)
  - UColumbia Chemistry, David Reichman, Glen Hocky
  - Argonne Power Grid Simulator, V. Zavala, K. Maheshwari, M. Hereld
Exercise views and supplemental slides
Exercise - MODIS satellite image processing

- **Input**: tiles of earth land cover (forest, ice, water, urban, etc)
  - Output: regions with maximal specific land types

![MODIS dataset](image)

![MODIS analysis script](image)

5 largest forest land-cover tiles in processed region
Goal: Run MODIS processing pipeline in cloud

MODIS script is automatically run in parallel:

Each loop level can process tens to thousands of image files.
Swift/T example: Part 11

- Overview: Find biggest parallelepiped volume via Python and R
  - Construct several matrices according to simple arithmetic
  - Compute determinants in parallel in Python (via Numpy)
  - Fix maximal determinant in R (reduction step)
  - Python reference code is included (dets.py == dets.swift)

- Construct matrices (in Swift arithmetic)
  - Matrices stored in distributed global store

- Determinant (Numpy/Python)
  - Cf. numpy.swift

- Find maximum (in R)

- Could call to C, C++, Fortran, instead

- Normally would call to application components, not numerical libraries
MODIS script in Swift: main data flow

```swift
foreach g, i in geos {
    land[i] = getLandUse(g, 1);
}

(topSelected, selectedTiles) =
    analyzeLandUse(land, landType, nSelect);

foreach g, i in geos {
    colorImage[i] = colorMODIS(g);
}

gridMap = markMap(topSelected);

montage =
    assemble(selectedTiles, colorImage, webDir);
```
Swift can send work to multiple sites

Diagram showing Swift interacting with remote campus clusters through GridFTP, scp, etc.

Simple campus Swift usage: running locally on a cluster login host
User first tests a new script on a local login host

Swift script is location-independent – debug locally then run distributed
$ cat modis.swift

type imagefile;
type landuse;
type perlscript;

perlscript getlanduse_pl <"getlanduse.pl">;

app (landuse output) getLandUse (imagefile input, perlscript ps)
{
  perl @ps @filename(input) stdout=@filename(output);
}

# Constants and command line arguments
string MODISdir = @arg("modisdir", ".../data/modis/2002");

# Input Dataset
imagefile geos[] <filesys_mapper; location=MODISdir, suffix=".rgb">;

# Compute the land use summary of each MODIS tile
landuse land[] <structured_regexp_mapper; source=geos, match="(h..v)",
  transform=@strcat("landuse/\1.landuse.byfreq")>;

foreach g,i in geos {
  land[i] = getLandUse(g, getlanduse_pl);
}
User runs on a campus or department cluster

Single-node script scales easily to local cluster

Cluster

Compute Nodes

Applications

Input

Swift script

config files

Cluster file server

Cluster node

... Cluster node

Cluster interactive node

swift

Output

Logs
User runs on a campus cluster: what’s inside

Cluster file server
- Applications
- Input
  - Swift script
  - config files

Cluster interactive node
- Logs
- swift
- Output

Cluster Compute Nodes
- Input
- Swift worker
- logs
- application
- Output

Multiple data streams of data moved from client to worker local FS

www.ci.uchicago.edu/swift
Campus or XSEDE supercomputer access is same

Same script runs unchanged between campus research cluster and Cray XE systems
Simple script runs 300+ apps in under a minute
Swift moves user’s dataset from campus server direct to Cray compute nodes

...and passes Cray-specific PBS parameters

...but most of the site spec is the same as for the campus cluster

$ cat beagle-ssh.cf

wrapperlog.always.transfer=true
sitedir.keep=true
execution.retries=0
status.mode=provider
use.provider.staging=true
provider.staging.pin.swiftfiles=false

#site beagle-ssh WALLTIME=00:55:00
#app perl=/usr/bin/perl
midway001$
$
$
$ cat sites.xml
<config>
<pool handle="beagle">
  <execution provider="coaster" jobmanager="ssh-cl:pbs" url="login4.beagle.ci.uchicago.edu">
    <profile namespace="globus" key="jobsPerNode">24</profile>
    <profile namespace="globus" key="lowOverAllocation">100</profile>
    <profile namespace="globus" key="highOverAllocation">100</profile>
    <profile namespace="globus" key="providerAttributes">pbs.aprun;pbs.mpp;depth=24</profile>
    <profile namespace="globus" key="maxtime">3600</profile>
    <profile namespace="globus" key="maxWalltime">00:55:00</profile>
    <profile namespace="globus" key="userHomeOverride">/lustre/beagle/{env.USER}/swiMwork</profile>
    <profile namespace="globus" key="slots">2</profile>
    <profile namespace="globus" key="maxnodes">1</profile>
    <profile namespace="globus" key="nodeGranularity">1</profile>
    <profile namespace="karajan" key="jobThrottle">.47</profile>
    <profile namespace="karajan" key="initialScore">10000</profile>
    <filesystem provider="local"/>
  </execution>
  <workdirectory>/tmp/{env.USER}/swiMwork</workdirectory>
</pool>
</config>
$
Example

```
midway001$ ls landuse
h00v08.landuse.byfreq  h11v10.landuse.byfreq  h17v06.landuse.byfreq  h21v10.landuse.byfreq  h27v10.landuse.byfreq
h00v09.landuse.byfreq  h11v11.landuse.byfreq  h17v07.landuse.byfreq  h21v11.landuse.byfreq  h27v11.landuse.byfreq
...
h11v06.landuse.byfreq  h17v02.landuse.byfreq  h21v06.landuse.byfreq  h27v06.landuse.byfreq  h35v10.landuse.byfreq
h11v07.landuse.byfreq  h17v03.landuse.byfreq  h21v07.landuse.byfreq  h27v07.landuse.byfreq
h11v08.landuse.byfreq  h17v04.landuse.byfreq  h21v08.landuse.byfreq  h27v08.landuse.byfreq
h11v09.landuse.byfreq  h17v05.landuse.byfreq  h21v09.landuse.byfreq  h27v09.landuse.byfreq
```

```
midway001$ cat landuse/h03v07.landuse.byfreq
211094 0 00
5348 1 01
4376 2 02
3236 3 03
3196 4 04
1242 5 05
731 6 06
405 7 07
292 8 08
225 9 09
83 10 0a
61 11 0b
43 12 0c
39 13 0d
25 14 0e
4 15 0f
```

Input is MODIS satellite raster image dataset

Output is histogram of land use codes
UChicago campus “collective” adds OSG resources

UC3 architecture abstracts all the Condor resource flocking issues; Swift accesses local, MWT2, and OSG as a unified Condor facility using campus user identity

www.ci.uchicago.edu/swift
midway001$ pwd
/home/wilde/osgdemo/modis/svn/run051
midway001$ cat sites.xml
<config>
<pool handle="uc3">
  <execution provider="coaster" url="uc3-sub.uchicago.edu" jobmanager="ssh-cl:condor"/>
  <profile namespace="karajan" key="jobThrottle">3.99</profile>
  <profile namespace="karajan" key="initialScore">10000</profile>
  <profile namespace="globus" key="jobsPerNode">1</profile>
  <profile namespace="globus" key="maxWalltime">3600</profile>
  <profile namespace="globus" key="highOverAllocation">100</profile>
  <profile namespace="globus" key="lowOverAllocation">100</profile>
  <profile namespace="globus" key="slots">400</profile>
  <profile namespace="globus" key="maxNodes">1</profile>
  <profile namespace="globus" key="nodeGranularity">1</profile>
  <profile namespace="globus" key="condor.+AccountingGroup">"group_friends.(env.USER)"</profile>
  <profile namespace="globus" key="jobType">nonshared</profile>
  <filesystem provider="local" url="none" />
  <workdirectory>.
</workdirectory>
</pool>
</config>
midway001$

# Example of running 1,000 MODIS jobs on just the UC3 collective: local UC3 resources full but work routed to Midwest Tier 2 and OSG

$ showsites

midway  0
beagle  0
uc3   0
mwt2  256
OSG   744
Total 1000

When local UC3 “seeder” resource full, UC3 flocks to other resources

Swift forwards Condor parameters
Now user runs on multiple resources:

Same script runs on broad range of resources; separate throttles can be set for each site.
<config>
  <pool handle="uc3">
    <execution provider="coaster" url="uc3-sub.uchicago.edu" jobmanager="ssh-cl:condor"/>
    <profile namespace="karajan" key="jobThrottle">10.00</profile>
    <profile namespace="karajan" key="initialScore">10000</profile>
    <profile namespace="globus" key="JobsPerNode">1</profile>
    ...
    <profile namespace="globus" key="jobType">nonshared</profile>
    <!-- <profile namespace="globus" key="condor+Requirements">isUndefined(GLIDECLIENT_Name) == FALSE</profile> -->
    <workdirectory>.</workdirectory>
  </pool>

  <pool handle="beagle">
    <execution provider="coaster" jobmanager="ssh-cl:pbs" url="login4.beagle.ci.uchicago.edu"/>
    <profile namespace="globus" key="JobsPerNode">24</profile>
    <profile namespace="globus" key="lowOverAllocation">100</profile>
    <profile namespace="globus" key="highOverAllocation">100</profile>
    <profile namespace="globus" key="providerAttributes">pbs.aprun;pbs.mpp;depth=24;pbs.resource_list=advres=wilde.1768</profile>
    ...
    <workdirectory>/tmp/{env.USER}/swiftwork</workdirectory>
  </pool>

  <pool handle="sandyb">
    <execution provider="coaster" jobmanager="local:slurm"/>
    ...
    <workdirectory>/tmp/{env.USER}</workdirectory>
  </pool>

  <pool handle="westmere">
    <execution provider="coaster" jobmanager="local:slurm"/>
    ...
    <workdirectory>/tmp/{env.USER}</workdirectory>
  </pool>

  <workdirectory>/tmp/{env.USER}</workdirectory>
</config>

Multiple site definitions, managed by support staff

User can specify custom parameters

App list selects where app() run

$ cat tc
uc3 perl /usr/bin/perl null null null
beagle perl /usr/bin/perl null null null
sandyb perl /usr/bin/perl null null null
westmere perl /usr/bin/perl null null null
Swift’s location-independent scripting lets the user focus on science

- Example of running 3,000 jobs to 3 hosts including the UC3 campus collective:
  
  ```
  $ ./showsites
  midway  289
  beagle   1070
  uc3      1011
  mwt2     295
  OSG      335
  Total    3000
  ```

- The user started on a basic login host processing 10 files and moved up to a 3,000 file dataset, changing only the dataset name and a site-specification list to get to the resources above.

- Expanded the scope of their computations from one node to hundreds or thousands of cores.

- **User didn’t need to look at what sites were busy, or adjust arcane scripts, to get to these resources.**