Workflow Systems

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Swift and e-Science

• Swift is a system for the rapid and reliable specification, execution, and management of large-scale science and engineering workflows. It supports applications that execute many tasks coupled by disk-resident datasets - as is common, for example, when analyzing large quantities of data or performing parameter studies or ensemble simulations.

• For example:
  – Cancer research: looking for previously unknown protein changes by comparing mass spectrum data with data known about proteome.
  – A monte-carlo simulation of protein folding, 10 proteins, 1000 simulations for each configuration, inside simulated annealing algorithm with 2x5=10 different parameter values. Each simulation component takes ~ 5 CPU-minutes, so about ~ 1 CPU-year for a whole run; producing 10...100Gb of data.
Other Work

- **Coordination language**
  - Linda [Ahuja, Carriero86], Strand [Foster, Taylor90], PCN [Foster92]
  - Durra [Barbacci, Wing86], MANIFOLD [Papadopoulos98]
  - Components programmed in specific language (C, FORTRAN) and linked with system

- **“Workflow” languages and systems**
  - Taverna [Oinn, Addis04], Kepler [Ludäscher, Altintas05],
    Triana [Churches, Gombas05], Vistrail [Callahan, Freire06], DAGMan, Star-P
  - XPDL [WfMC02], BPEL [Andrews, Curbera03], and BPML [BPML02],
    YAWL [van de Aalst, Hofstede05], Windows Workflow Foundation
    [Microsoft05]
A 4x200 flow leads to a 5 MB BPEL file … chemists were not able to write in BPEL”
[Emmerich,Buchart06]
A brief history of SwiftScript

• ~2003: VDL - the Virtual Data Language. express directed acyclic graphs of unix processes processes take input and produce output through files 'virtual data' - when needed, materialise data either by copying from elsewhere or by deriving it from other data that is available

Lots of thinking about "graph transformations"

• ~2006: VDL2 (which became SwiftScript)
  – key features:
    • iterating over collections of files in the language
    • accidentally became Turing-complete

• ~2010: still going - language tweaks, scaling improvements
Scientific programmers use some science-domain specific language to write the "science" bit of their application (eg R for statistics, Root for particle physics).

They aren't "high performance" or "distributed system" programmers.

Want to help them use "big" systems to run their application - eg machines with $10^5$ CPU cores.

Traditional MPI (Message Passing Interface) is hard to think about.

Swift tries to provide an easier model that still allows many applications to be expressed, and performed with reasonable efficiency.

SwiftScript is the language for programming in that model.
file output <"output.txt">; Declares output to be a variable whose value is stored in the file system rather than in-core.

"output.txt" means that the value is stored in a file output.txt (this can be a URL)

This is a simple example with a literal single filename.
- More complex syntax allows mapping arrays of files, with more dynamic behaviour (eg generating filename patterns at runtime)

We can omit the <...> mapping expression in which case Swift will make up a filename - useful for intermediate files.
app procedures

- app (file o) count(file i) { uniq "-c" stdin=@i stdout=@o; }
This is how the real work gets done - by getting some other science-domain specific program to do it.

- app procedures execute unix processes, but not like system() or runProcess

- The environment in which an app procedure runs is constrained:
  Application will start in "some directory, somewhere". There, it will find its input files, and there it should leave its output files.

- Applications need to be referentially transparent (but SwiftScript doesn't clearly define what equivalence is)
• Pick an execution site
• Transfer input files there (if they are not already cached there)
• Put the job in an execution queue at the execution site
• Wait for execution to finish
• Transfer output files back
• Check everything worked ok
Online repository of neuroimaging data

A typical study comprises
  3 groups,
  20 subjects/group,
  5 runs/subject,
  300 volumes/run
→ 90,000 volumes, 60 GB raw →
1.2 million files processed

100s of such studies in total

http://www.fmridc.org
Large user base
- World wide collaboration
- Thousands of requests

Wide range of analyses
- Testing, production runs
- Data mining
- Ensemble, Parameter studies
Three Obstacles to Creating a Community Resource

• Accessing messy data
  – Idiosyncratic layouts & formats
  – Data integration a prerequisite to analysis

• Describing & executing complex computations
  – Expression, discovery, reuse of analyses
  – Scaling to large data, complex analyses

• Making analysis a community process
  – Collaboration on both data & programs
  – Provenance: tracking, query, application
The Swift Solution

• Accessing messy data
  – Idiosyncratic layouts & formats
  – Data integration a prerequisite to analysis

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• Making analysis a community process
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Scientific data is often logically structured

- E.g., hierarchical structure
- Common to map functions over dataset members
- Nested map operations can scale to millions of objects
The Messy Data Problem (2)

- Heterogeneous storage format & access protocols
  - Same dataset can be stored in text file, spreadsheet, database, ...
  - Access via filesystem, DBMS, HTTP, WebDAV, ...
- Metadata encoded in directory and file names
- Hinders program development, composition, execution
SwiftScript

• Typed parallel programming notation
  – XDTM as data model and type system
  – Typed dataset and procedure definitions

• Scripting language
  – Implicit data parallelism
  – Program composition from procedures
  – Control constructs (foreach, if, while, …)

Clean application logic
Type checking
Dataset selection, iteration
Discovery by types
Type conversion

A Notation and System for Expressing and Executing Cleanly Typed Workflows on Messy Scientific Data [SIGMOD05]
Swift Runtime System

- Runtime system for SwiftScript
  - Translate programs into task graphs
  - Schedule, monitor, execute task graphs on local clusters and/or distributed Grid resources
  - Annotate data products with provenance metadata

- Grid scheduling and optimization
  - Lightweight execution engine: **Karajan**
  - **Falkon**: lightweight dispatch, dynamic provisioning
  - Grid execution: site selection, data movement
  - Caching, pipelining, clustering, load balancing
  - Fault tolerance, exception handling
There are many different execution resources in the world: clusters on your campus, supercomputers, your own laptop.

It is useful to be able to choose and switch between sites, and choose between different mechanisms for accessing a site, because:

• your usual site is broken today

• someone is developing a better mechanism (higher performance) for submitting to your usual site (ongoing r&d there)

• you want to use the combined power of several sites at once (research question: if many sites available, which is best to use?)
Failure happens a lot in our target environments (integer percentages in some environments) so reliability is not "a nice feature to have" - it is essential.

• Retries: if an application execution fails, we try it 2 more times
• Restarts: if retries fail, then the whole script fails (eventually). Maybe want to restart manually where we left off. Assume that app blocks are expensive and everything else is cheap, so start the script from beginning again, skipped apps that we've already run (using a log file)
• Replication: deals with a softer class of failure. Sometimes an app goes into a queue and sits "forever" (really forever, or perhaps much longer than most other apps). We can launch a new attempt to run the app, without killing the original. When one starts, we kill the other(s)
• Fast, scalable lightweight threading model
• Suitable constructs for control flow
• Flexible task dependency model
  – “Futures” enable pipelining
• Flexible provider model allows for use of different run time environments
  – Desktop, clusters, Grids
  – Flow controlled to avoid resource overload
• Workflow client runs from a Java container

Java CoG Workflow, Gv Laszewski, M. Hatigan, Workflows for e-Sciences 2007
Falkon dynamic provisioner:
- Monitors demand (incoming user requests)
- Manages supply: selects resources; creates executors (via Globus GRAM+LRM)
- Various decision strategies for acquisition and release

Falkon executor:
- 440 tasks/sec max
- 54,000 executors
- millions of tasks

Falkon: Fast and Light-weight Task Execution Framework, I. Raicu, Y. Zhao et al. SC07
Figure 3. Swift scripts execute using the Falkon distributed resource manager on the BG/P architecture.
Swift running on BlueGene/P

Figure 2. Architecture for petascale scripting.

- **Swift scripts**: Swift: scripting language, task coordination, throttling, data management, restart
- **Datasets**: Collective data management: broadcast of large common datasets, scatter and gather of small files
- **Command lists**: Falkon: ultrafast task dispatch and load balancing over processor sets
- **Shell scripts**: ZeptoOS: full Linux with fork/exec, dynamic linking and torus/collective net access
The other key area of interest is...

**Massive implicit parallelism**

We can declare a mapped array of files: (eg

```
mydata.*.img
```

```c
file inp[] <simple_mapper; prefix="mydata.",
suffix=".img">; and iterate over it:
```

```c
foreach s,i in inp { out[i] = f(s); // same as out[i] = f(inp[i]);
} All iterations can happen in parallel (subject to runtime
limits, but could be many thousands of CPUs)
```

In real use, f might be an app procedure taking 30s, with

```
10^5 loop iterations.
```
• Execution order is data dependency order
• Everything can be executed in parallel, except where there are dataflow dependencies.
• Dataflow dependencies are expressed by single assignment variables:
  int a; int b; int c; a = f(c); b = g(6); c = h(7); Execution of f will be after h. Execution of g will be unordered wrt f and h.
• Extends into (non-app) procedures. Only concurrency control in SwiftScript - no locks, etc. Assignment can be "in memory" or giving a file its content.
• **Arrays are not single-assignment**
  - int a[]; int b; a[0] = 128; a[1] = 129; b = sum(a); // pass in the whole array a is not single assignment. But the elements of a are.
• Static analysis of code to see which statements might write to a. When all potential writers are finished, then the array is "closed" for writing. Cannot modify an element once it has been assigned.
• Arrays are "monotonic" - we know more over time, and once we know something, it is true forever. A weaker form of single assignment.
• But there are deadlocks (in practice, and maybe in theory?):

```c
int a[];
foreach i in [1:10] {
    if (i < 9)
        a[i] = 5;
    else // i==10
        int b;
        b = f(a);
}
```

`a` will be closed when the whole `foreach` is finished... but the `foreach` will never finish because `f(a)` is waiting for `a` to close.

• Leads to programmer confusion when overly conservative

• More static+runtime analysis? Better structures/iterators? (map-like?)
Metrics are related to scientific computing focus.

Mostly, what was done with app procedures by an application:

- How many CPU-hours in total? (eg 208763 CPU-hours)
- How many CPUs in use simultaneously? (eg 2000 CPUs)

In terms of language execution, interested in raw SwiftScript speed where it impedes the above: can we sustain 100 app block launches per second?

- How short can you make your SwiftScript program? (so interesting to see how *few* lines of code are written in SwiftScript...)
Less concrete idea (1): Provenance

- provenance = record of the history of an artifact to help convince you that it is genuine/valuable
- In Swift: record what output files were generated - which input files, which programs, where programs were run
- Which datafiles used this site? (because we must discard any results from it)
- Regenerate interesting results because we've damaged our copy
- Functional/dataflow style helps there but many other issues.
- Prototype implementation
Processing datasets that grow over time - e.g., a database of fMRI images that is added to as new patients are seen.

Represent the database as a mapped array that is never closed. We can iterate with `foreach` over that array, and leave the SwiftScript program running "forever".

Maybe no need to change the language definition much / at all.

No implementation, only some mailinglist chatter.
Q: why did you implement this as a new language rather than embedding?
A: An accident of history - we started off making a glorified DAG description language, not a "real programming language"
But we can still wonder whether it would be a better or worse idea...
How would we implement:
Out-of-core data and applications
Massive (10^5) multithreading and everything-is-a-future style
for example: in Haskell or Java
In the beginning we were expecting people to make things that looked almost like DAGs of programs but "a bit more interesting."

Now people want to do sin and cos and in-memory matrix multiplication.

It's a hassle to add wire in existing libraries in other languages for every new feature.

The implementation is not really suited to in-core data processing - even a single integer has a very large footprint (because originally our 'values' were mostly many-megabyte files, where overhead mattered less).

Areas that I've seen: parsing/printing data files; matrix operations; sin/cos

Would be great to easily import some other languages library collection.
Optimizations:
fMRI Workflow Execution without Pipelining

(reorientRun/1) → (reorientRun/2) → (alignlinearRun/3) → (resliceRun/4)

(Dispatch is performed here via GRAM+PBS)
Optimizations: Karajan Futures Enable Pipelining

(Dispatch is performed here via GRAM+PBS)
Optimizations: Load Balancing

fMRI pipeline on two sites

reorientRun/1

reorientRun/2

alignlinearRun/3

resliceRun/4

UC: 218
TP: 262
### Table 1. Example parallel scripting applications.

<table>
<thead>
<tr>
<th>Field</th>
<th>Description</th>
<th>Characteristics</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>Astronomy</td>
<td>Creation of montages from many digital images</td>
<td>Many 1-core tasks, much communication, complex dependencies</td>
<td>Experimental</td>
</tr>
<tr>
<td>Astronomy</td>
<td>Stacking of cutouts from digital sky surveys</td>
<td>Many 1-core tasks, much communication</td>
<td>Experimental</td>
</tr>
<tr>
<td>Biochemistry*</td>
<td>Analysis of mass-spectrometer data for post-translational protein modifications</td>
<td>10,000-100 million jobs for proteomic searches using custom serial codes</td>
<td>In development</td>
</tr>
<tr>
<td>Biochemistry*</td>
<td>Protein structure prediction using iterative fixing algorithm; exploring other biomolecular interactions</td>
<td>Hundreds to thousands of 1- to 1,000-core simulations and data analysis</td>
<td>Operational</td>
</tr>
<tr>
<td>Biochemistry*</td>
<td>Identification of drug targets via computational docking/screening</td>
<td>Up to 1 million 1-core docking operations</td>
<td>Operational</td>
</tr>
<tr>
<td>Bioinformatics*</td>
<td>Metagenome modeling</td>
<td>Thousands of 1-core integer programming problems</td>
<td>In development</td>
</tr>
<tr>
<td>Business economics</td>
<td>Mining of large text corpora to study media bias</td>
<td>Analysis and comparison of over 70 million text files of news articles</td>
<td>In development</td>
</tr>
<tr>
<td>Climate science</td>
<td>Ensemble climate model runs and analysis of output data</td>
<td>Tens to hundreds of 100- to 1,000-core simulations</td>
<td>Experimental</td>
</tr>
<tr>
<td>Economics*</td>
<td>Generation of response surfaces for various economic models</td>
<td>1,000 to 1 million 1-core runs (10,000 typical), then data analysis</td>
<td>Operational</td>
</tr>
<tr>
<td>Neuroscience*</td>
<td>Analysis of functional MRI datasets</td>
<td>Comparison of images; connectivity analysis with structural equation modeling, 100,000+ tasks</td>
<td>Operational</td>
</tr>
<tr>
<td>Radiology</td>
<td>Training of computer-aided diagnosis algorithms</td>
<td>Comparison of images; many tasks, much communication</td>
<td>In development</td>
</tr>
<tr>
<td>Radiology</td>
<td>Image processing and brain mapping for neurosurgical planning research</td>
<td>Execution of MPI application in parallel</td>
<td>In development</td>
</tr>
</tbody>
</table>

Note: Asterisks indicate applications being run on Argonne National Laboratory’s Blue Gene/P (Intrepid) and/or the TeraGrid Sun Constellation at the University of Texas at Austin (Ranger).
Medical Imaging: fMRI

- Wide range of analyses
  - Testing, interactive analysis, production runs
  - Data mining
  - Parameter studies

[SC07] “Falkon: a Fast and Light-weight task execution framework”
[SWF07] “Swift: Fast, Reliable, Loosely Coupled Parallel Computation”
Applications
Medical Imaging: fMRI

- GRAM vs. Falkon: 85%~90% lower run time
- GRAM/Clustering vs. Falkon: 40%~74% lower run time

[SC07] “Falkon: a Fast and Light-weight task execution framework”
[SWF07] “Swift: Fast, Reliable, Loosely-Coupled Parallel Computation”
Applications
Astronomy: Montage

B. Berriman, J. Good (Caltech)
J. Jacob, D. Katz (JPL)

[SC07] “Falkon: a Fast and Light-weight task execution framework”
[SWF07] “Swift: Fast, Reliable, Loosely Coupled Parallel Computation”
Applications
Astronomy: Montage

- GRAM/Clustering vs. Falkon: **57%** lower application run time
- MPI* vs. Falkon: **4%** higher application run time
- * MPI should be **lower bound**

[SWF07] “Swift: Fast, Reliable, Loosely Coupled Parallel Computation”
• Determination of free energies in aqueous solution
  – Antechamber – coordinates
  – Charmm – solution
  – Charmm - free energy
Applications

Molecular Dynamics: MoLDyn

- 244 molecules $\rightarrow$ 20497 jobs
- 15091 seconds on 216 CPUs $\rightarrow$ 867.1 CPU hours
- Efficiency: 99.8%
- Speedup: 206.9x $\rightarrow$ 8.2x faster than GRAM/PBS
- 50 molecules w/ GRAM (4201 jobs) $\rightarrow$ 25.3 speedup

[NOVA08] "Realizing Fast, Scalable and Reliable Scientific Computations in Grid Environments"
Applications
Word Count and Sort

- Classic benchmarks for MapReduce
  - Word Count
  - Sort
- Swift and Falkon performs similar or better than Hadoop (on 32 processors)
Applications Economic Modeling: MARS

- CPU Cores: 130816
- Tasks: 1048576
- Elapsed time: 2483 secs
- CPU Years: 9.3

Applications

Pharmaceuticals

ZINC 3-D structures

PDB protein descriptions

protein (1MB)

DOCK6 receptor

(1 per protein: defines pocket to bind to)

FRED receptor

(1 per protein: defines pocket to bind to)

NAB Script template

NAB script parameters (defines flexible residues, #MDsteps)

BuildNABScript

Amber prep:

1. AmberizeLigand

2. AmberizeReceptor

4. perl: gen nabscript

NAB Script

Amber Score:

1. AmberizeLigand

3. AmberizeComplex

5. RunNABScript

For 1 target:

4 million tasks

500,000 cpu-hrs

(50 cpu-years)

Applications
Pharmaceuticals: DOCK

CPU cores: 118784
Tasks: 934803
Elapsed time: 2.01 hours
Compute time: 21.43 CPU years
Average task time: 667 sec
Relative Efficiency: 99.7%
(from 16 to 32 racks)
Utilization:
• Sustained: 99.6%
• Overall: 78.3%

Applications
Astronomy: AstroPortal

- **Purpose**
  - On-demand “stacks” of random locations within ~10TB dataset

- **Challenge**
  - Processing Costs:
    - O(100ms) per object
  - Data Intensive:
    - 40MB:1sec
  - Rapid access to 10-10K “random” files
  - Time-varying load

<table>
<thead>
<tr>
<th>Locality</th>
<th>Number of Objects</th>
<th>Number of Files</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>111700</td>
<td>111700</td>
</tr>
<tr>
<td>1.38</td>
<td>154345</td>
<td>111699</td>
</tr>
<tr>
<td>2</td>
<td>97999</td>
<td>49000</td>
</tr>
<tr>
<td>3</td>
<td>88857</td>
<td>29620</td>
</tr>
<tr>
<td>4</td>
<td>76575</td>
<td>19145</td>
</tr>
<tr>
<td>5</td>
<td>60590</td>
<td>12120</td>
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<td>10</td>
<td>46480</td>
<td>4650</td>
</tr>
<tr>
<td>20</td>
<td>40460</td>
<td>2025</td>
</tr>
<tr>
<td>30</td>
<td>23695</td>
<td>790</td>
</tr>
</tbody>
</table>

[DADC08] “Accelerating Large-scale Data Exploration through Data Diffusion”
[TG06] “AstroPortal: A Science Gateway for Large-scale Astronomy Data Analysis”
Applications
Astronomy: AstroPortal

• AstroPortal
  – Makes it really easy for astronomers to create stackings of objects from the Sloan Digital Sky Survey (SDSS) dataset

• Throughput
  – 10X higher than GPFS

• Reduced load
  – 1/10 of the original GPFS load

• Increased scalability
  – 8X

Many-Task Computing
Swift: Summary

- Clean separation of logical/physical concerns
- Concise specification of parallel programs
  - SwiftScript, with iteration, etc.
- Efficient execution (on distributed resources)
  - Karajan+Falkon: Grid interface, lightweight dispatch, pipelining, clustering, provisioning
- Rigorous provenance tracking and query
  - Virtual data schema & automated recording

→ Improved usability and productivity
  - Demonstrated in numerous applications
Questions