Workflow Systems

Part 1 of 3

Ioan Raicu
Center for Ultra-scale Computing and Information Security
Department of Electrical Engineering & Computer Science
Northwestern University

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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]

Other Work

	SwiftScript	BPEL	XPDL	MW Wflow	DAGMan	Tavena	Triana	Kepler	Vistrail	Star-P
Scales to Grids	++	-	-	-	++	-	-	-	-	+
Typing	++	++	++	++	-	-	-	+	-	+
Iteration	++	-/+	-	+	-	-	-	+	-	+
Scripting	++	-	-	+	+	+	-	-	+	++
Dataset Mapping	+	-	-	-	-	-	-	-	-	-
Service Interop	+	-	+	-	-	-	-	+	-	-
Subflow/comp.	+	-	+	+	-	-	+	+	-	+
Provenance	+	-	-	+	-	+	-	+	+	-
Open source	+	+	+	-	+	+	+	+	+	-

"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

Target programmers

- 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.

Mappers and file types

- 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 constrainted:
  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)

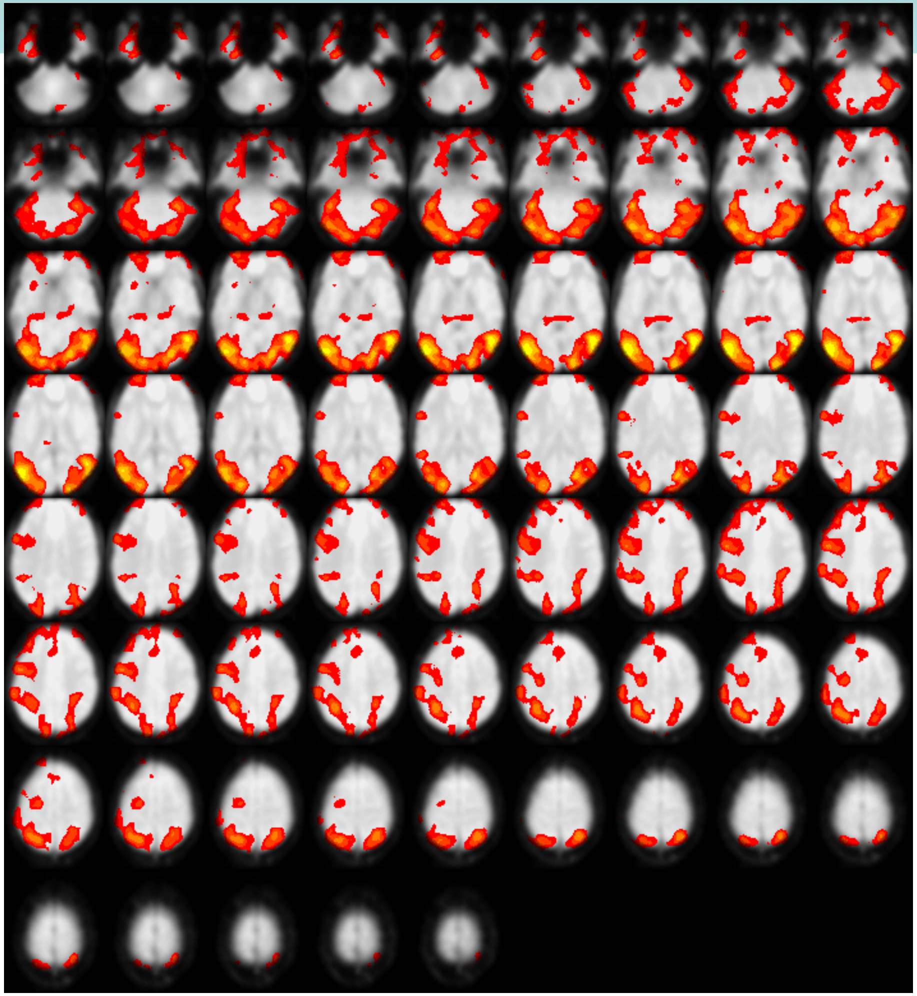
Executing an app {} procedure

- 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

Case Study
Functional MRI (fMRI) Data Center

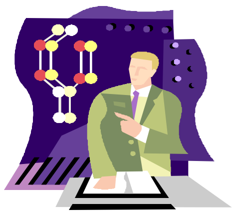
- Online repository of neuroimaging data
- A typical study comprises
  - 3 groups,
  - 20 subjects/group,
  - 5 runs/subject,
  - 300 volumes/run

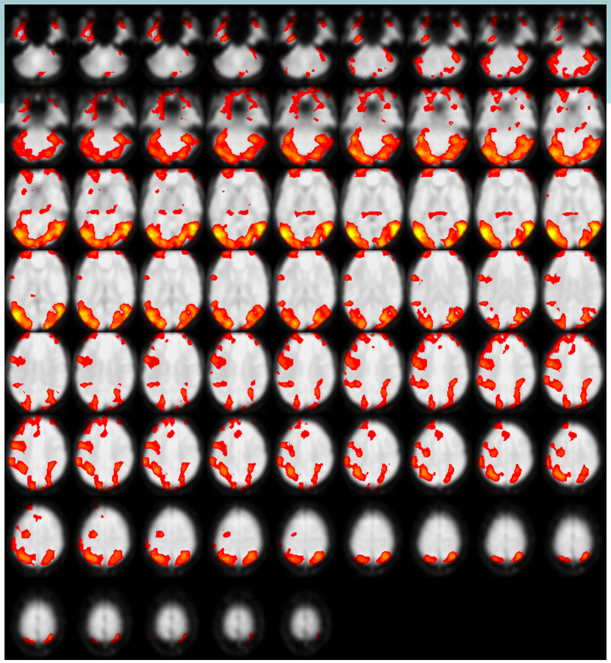
  → 90,000 volumes, 60 GB raw → 1.2 million files processed
- 100s of such studies in total

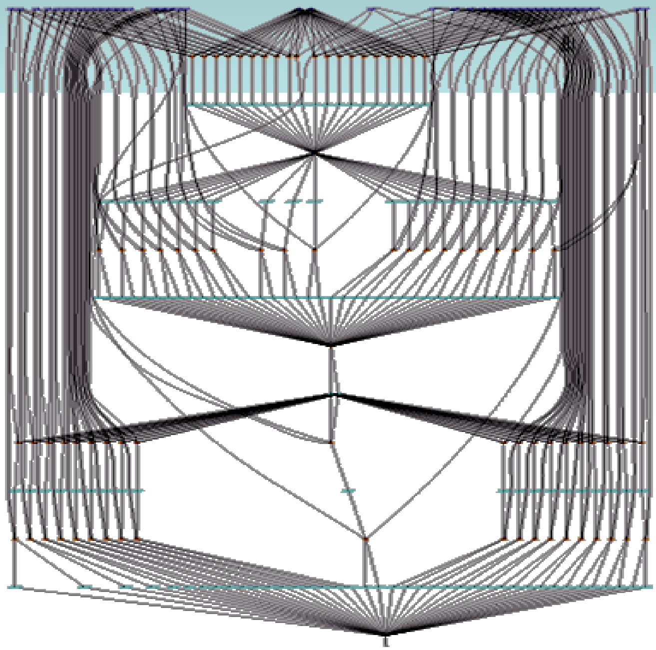


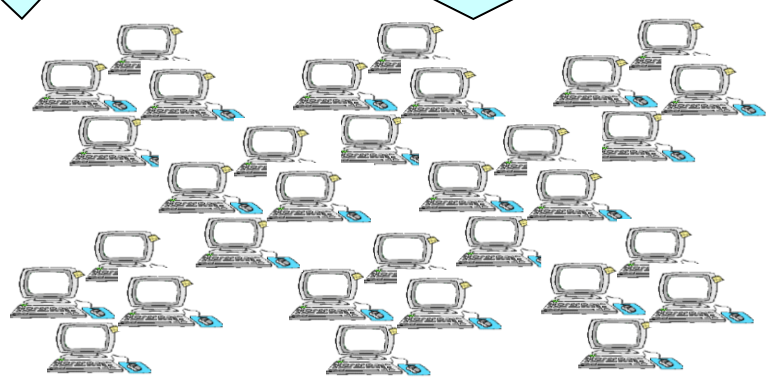
http://www.fmridc.org

fMRI Data Analysis









- 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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XDTM

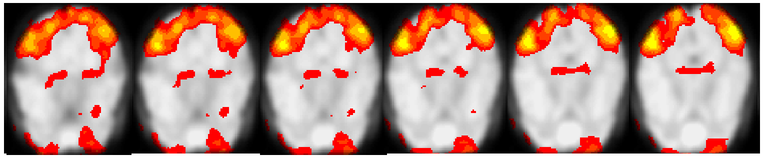
SwiftScript

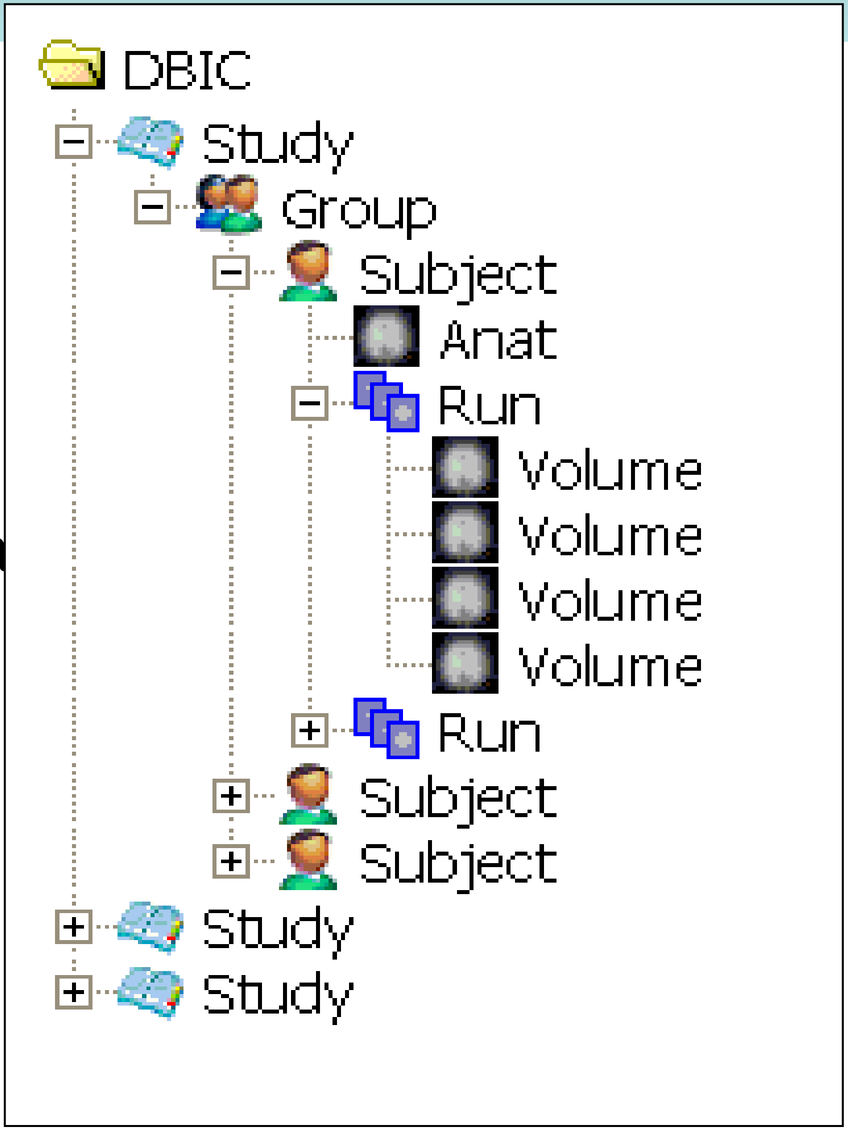
Karajan +Falkon

VDC

The Messy Data Problem (1)

- Scientific data is often logically structured
  - E.g., hierarchical structure
  - Common to map functions over dataset members
  - Nested map operations can sca 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

```
./knottastic
drwxr-xr-x  4 yongzh users 2048 Nov 12 14:15 AA
drwxr-xr-x  4 yongzh users 2048 Nov 11 21:13 CH
drwxr-xr-x  4 yongzh users 2048 Nov 11 16:32 EC

./knottastic/AA:
drwxr-xr-x  5 yongzh users 2048 Nov  5 12:41 04nov06aa
drwxr-xr-x  4 yongzh users 2048 Dec  6 12:24 11nov06aa

. /knottastic//AA/04nov06aa:
drwxr-xr-x  2 yongzh users  2048 Nov  5 12:52 ANATOMY
drwxr-xr-x  2 yongzh users 49152 Dec  5 11:40 FUNCTIONAL

. /knottastic/AA/04nov06aa/ANATOMY:
-rw-r--r--  1 yongzh users      348 Nov  5 12:29 coplanar.hdr
-rw-r--r--  1 yongzh users 16777216 Nov  5 12:29 coplanar.img

. /knottastic/AA/04nov06aa/FUNCTIONAL:
-rw-r--r--  1 yongzh users     348 Nov  5 12:32 bold1_0001.hdr
-rw-r--r--  1 yongzh users  409600 Nov  5 12:32 bold1_0001.img
-rw-r--r--  1 yongzh users     348 Nov  5 12:32 bold1_0002.hdr
-rw-r--r--  1 yongzh users  409600 Nov  5 12:32 bold1_0002.img
-rw-r--r--  1 yongzh users     496 Nov 15 20:44 bold1_0002.mat
-rw-r--r--  1 yongzh users     348 Nov  5 12:32 bold1_0003.hdr
-rw-r--r--  1 yongzh users  409600 Nov  5 12:32 bold1_0003.img
```

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

Questions

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