CS 595 - Hot topics in database systems:
Data Provenance

II. Beyond Database Provenance
II.1 Workflow Provenance

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Workflow Provenance

- Track back the execution of workflows
- Usually developed for a specific workflow management system
- Mostly coarse-grained
  - Workflow "operations" as black boxes
- New challenges
  - Do not know provenance behaviour of atomic operations
  - Probably no fixed data model
  - Distributed storage and execution models with limited control

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Outline

Excursion Workflows

What is a Workflow?

- A collection of simple(r) tasks such as
  - Filter out certain wavelengths from an image
  - Remove duplicates from a data set
  - Compute the mean of a dataset
  - Plot some data as a graph
  - ...
- ...Combined to achieve a more complex task
  - Simulating the changes of ocean currents for the next 100 years and visualize the result
  - Analyze raw telescope input data to detect and classify stars
  - ...

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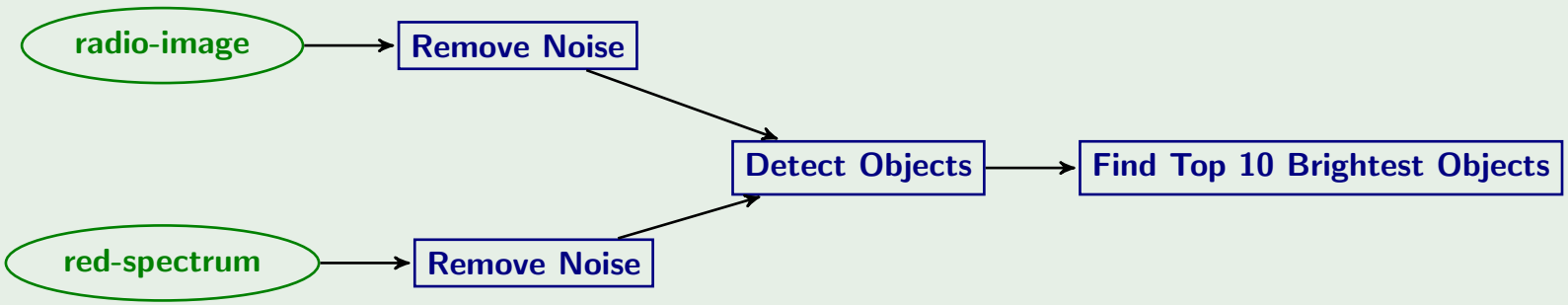
Excursion Workflows

How to model a Workflow?

- Usually a directed (acyclic?) graph (DAG)
- Nodes are tasks
- Edges denote data-flow
  - . . . sometimes also control flow

Example



Excursion Workflow Management Systems

What is a Workflow Management System (WMS)?

- "Supervised" execution environment for workflows
- Usually comes with **workflow** and **execution** model
  - maybe also **data** model
- Visual interface for constructing workflows

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Excursion Workflow Management Systems

Why are WMS needed?

- Reuse of components (tasks)
- Reuse of workflows
- Documentation of what happened and preservation of results
  - $\Rightarrow$provenance!
- Hide complexity
  - . . . of distributed processing
  - . . . of scheduling tasks
  - . . . of monitoring execution
  - . . . of data movement
  - . . . of fault tolerance

Excursion Workflow Management Systems

Some WMS

- Kepler
- Taverna
- Triana
- Pegasus
- GridNexus
- DiscoveryNet
- BioWBI
- GridBus
- ...

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Excursion Workflow Management Systems

Execution Models

- Grid-based: Tasks are Web-service calls
- MapReduce
- Traditional processes
- ...

Scheduling

- User-defined vs. automatic
- Strategies:
  - minimize execution time
  - minimize resource usage

Excursion Workflow Management Systems

Data Models

- No model: data stored in flat files
- XML-based: Kepler (one option)

Fault Tolerance

- Checkpoints
- Redundancy
- Replication

Data Movement

- User-defined
- Automatic

Excursion Workflow Management Systems

Example (Taverna)

- Workflows for Biologists
- Part of the *my*Grid project
- Tasks are services (mostly web-services)
- Taverna consists of
  - User-interface: design workflows, discover available tasks, browse provenance
  - Workflow enactor: engine to execute workflows using the web-services
  - Discovery of services (service registry and ontologies)
  - Resolving interface mismatches
    - Ontologies for semantics and structure of service input and outputs
    - "shams": components to convert data for structural mismatches

Outline

Overview

Approaches

- WMS are very diverse
- ⇒Almost one approach per system
- Open Provenance Model
  - A graph model for provenance
  - Community design
  - Should enable interoperability between systems
- Most provenance models are coarse-grained
  - ⇒tasks are black-boxes
  - Or provenance behaviour has to be supplied as part of task descriptions
- WMS as supervised execution environment that tracks provenance

Kepler - Efficient Provenance Storage and Querying

Kepler

- Data model and Execution model:
  - Tasks create and consume XML data
  - Input of a task is a stream (sequence) of XML elements (tokens)
    - Tokens are either data or collections
    - Each token has a unique identifier
  - A task can
    - Pass on input tokens unmodified
    - Add new tokens
    - Delete tokens
    - Modify tokens
- Tasks expected to output dependency information (provenance)
  - A token x depends on a token y through task a

Kepler cont.

Provenance storage

- Dependencies are stored in central DB
- Rules to derive additional annotations
- Compression schemes for provenance
  - Store overlapping provenance only once
  - Do not materialize provenance that can be derived through rules

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Taverna

- Tasks are web-services
- Ontologies describe services and their interfaces
- Automatic discovery of services and semantic and structural mismatches
- Provenance is represented using RDF (resource description framework) and ontologies RDFS (RDF schema)
  - RDF: A graph spanned by triples (`object`, `predicate`, `subject`)
  - Nodes are entities
  - A triple is an labelled edge from `object` to `subject` labelled with `predicate`
- Querying using RDF query languages like SPARQL

Taverna

Different views on provenance

- Process view: Event log (Process provenance)
- Data view: Data provenance
- Organizational view: Track the who (which machine, user, ...)
- Knowledge view: Using the ontologies to provide abstraction
  - e.g., `instanceOf` for data products
- Connection between provenance graphs for workflows
  - Using URIs to identify data, processes, and invocations

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PigLatin with Provenance for Workflows

PigLatin

- SQL-like data flow language
- Compiled into MapReduce tasks

Provenance for PigLatin Workflows

- Tasks = Modules
  - Written as PigLatin scripts
- Limit to subset of language
- Use provenance polynomials (the graph representation)
  - Plus aggregation extensions
- ⇒fine-grained provenance but tasks have to be expressed in Pig

Generalized MapReduce Workflows (GMRW)

- Presented by Jiawei
- Workflows tasks are map and reducer functions
- plus union and split to deal with multiple outputs or inputs
  - MapReduce only supports single output and input data sets
- Store provenance using the `(key,value)` model of MapReduce
  - Add provenance information to the `value` part
- Replace the original mapper and reducer functions of the workflow with Wrappers
  - A wrapper strips of the provenance information
  - Calls the original function
  - Attaches provenance information to the output of the function
  - $\Rightarrow$Provenance of these functions derived from generic mapper/reducer semantics

Open Provenance Model (OPM)

- Approach to standardize provenance models
  - . . . a bit tailored towards workflow mindset
- Abstract graph based model
- Provenance graph models past execution of a workflow execution and interdependencies

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Open Provenance Model (OPM)

Node Types

- Artifact: Piece of data or physical state
  - E.g., a blood sample, an image file
- Process: Transformation producing and/or consuming artifacts
  - E.g., image transformation, a clustering algorithm, a weather sensor measurement process
- Agent: An entity controlling or triggering a process
  - E.g., a user starting the workflow, the workflow enactment engine,

Open Provenance Model (OPM)

Edges

- Denote causal dependencies
- Edge Types
  - Process → Artifact: Process created artifact
    - ⇒Outputs
  - Artifact → Process: Artifact was used by process
    - ⇒Inputs
  - Artifact → Artifact: Artifact was derived from artifact
    - data provenance as we covered in this class
  - Agent → Process: Agent controlled process
    - E.g., user started the process, workflow engine executed process
  - Process → Process: Process was trigged by process
    - E.g., process starts several subprocesses, .e.g., divide-and-conquer algorithm

Open Provenance Model (OPM)

Reasoning Rules

- Generic inference rules applicable to all OPM graphs
- Transitive closure of, e.g., artifact-artifact edges
  - E.g., $\exists(A_1, A_2) \wedge (A_2, A_3) \Rightarrow (A_1, A_3)$
- Derive new process-artifact and artifact-process edges based on sub-processes (process-process) edges
  - E.g., $\exists(P_1, P_2), (P_2, A) \Rightarrow (P_1, A)$

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Karma 3

- Grid-model (workflow steps are services)
- Application Factory Toolkit: wraps programs as seb services
- Services used in workflows can be workflows (hierarchical composition)
- Variation of Business Process Execution Language (BPEL) to describe workflows
- A provenance service collects provenance data (messages)
- Both services and the workflow enactment engine are instrumented to generate provenance messages
  - Two types of models: notification model (asynchronous) and direct API service calls (synchronous)
- The provenance service stores incoming messages in a relational DB

Karma 3

Querying provenance

- provenance service API calls
- SQL over the backend DB
- Hardcoded client-side queries (e.g., Java)

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PReServ: Provenance Recording for Services

- General service-oriented system (SOA)
- Provenance service that records p-assertions
  - messages send by services about their (provenance) behaviour
- Provenance store: Service that records and persists p-assertions
- Developers have three options for creating p-assertions
  - Web-service calls (SOAP, Simple Object Access Protocol)
  - Java API (Java library generates SOAP calls)
  - Instrumentation
    - Automatic generation of p-assertions by wrapping services
    - Only for services implemented using Apache Axis Web Services libraries

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A Graph Model of Data and Workflow Provenance

- Transformations expressed in DFL (data flow language)
- DFL is an extension of NRC (nested relational calculus)
- Define a graph model for execution of DFL expressions
- Using Haskell (functional programming language)
- Haskell implementation that generates a provenance graph as a side-effect of computation
  - Executes DFL expression
  - Generates provenance graph
  - Provenance graph is Haskell program (executable)
- Very detailed and precise (maybe too detailed?)
- Datalog queries for extracting Where- and Why-provenance from provenance graphs

Outline

Recap

Workflow Management Systems

- Design of Workflows
- Execution Engine for Workflows
- Atomic tasks
  - Services (Web-services)
  - Processes
  - ...

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Recap

Provenance for Workflows

- Often coarse-grained
- Some fine-grained approaches
  - Kepler (UC Davis)
  - Using Pig (UPenn)
  - Provenance for Generalized MapReduce Workflows GMRW (Stanford)
- Many different models
- Standard approach
  - Workflow enactment engine serves as supervised execution environment
  - Tracks provenance during workflow execution

Recap

Covered Approaches

- Kepler (UC Davis)
- Using Pig (UPenn)
- Provenance for Generalized MapReduce Workflows GMRW (Stanford)
- The Open Provenance Model (OPM)
- Karma 3 (Indiana University)
- PReServ (University of Southampton)
- A graph model of data and workflow provenance (University of Edinburgh and others)

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Outline

OS Provenance Challenges

- Different Use Cases
  - Detect Errors in Execution at much lower level
  - Detect Security Breaches
- Very fine-granular and detailed provenance
  - System calls, reading/writing files/pipes
  - IPC (Inter process communication): shared memory,
  - Network communication: socket communication
  - Transformations are executable programs
  - Environment
    - Environment variables
    - Users
    - Library and OS version
    - ...

Excursion Operating Systems

- Disclaimer: A very very brief overview of some concepts
- Take of CS450, CS550, CS551 for in-depth coverage

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Excursion Operating Systems

Virtual Memory

- Multitasking operating system
  - Multiple processes share the physical memory of a machine
  - ⇒Memory regions of these processes may be interleaved
  - ⇒Complicates application programming
- Approach: Each process has its own virtual memory address space
  - Hides fragmentation of physical memory of a process
  - ⇒Programmer does not need to worry about fragmentation
- Virtual memory can be larger than available physical memory
  - OS takes care of swapping: storing/retrieving pages from disk
    - Pages are organizational unit of memory for swapping
  - ⇒From the applications point of view memory is almost unlimited
  - ⇒No need to implement swapping in each application

Excursion Operating Systems

Processes and Threads

- Process
  - Heavy-weight construct
    - Process are associated with large state
    - Switching between processes is expensive (context-switch)
  - Usually execution of program
    - . . . but, process can start child processes
  - Each process has its own memory space
  - OS provides support for communication between processes
- Thread
  - Light-weight construct
    - Context-switch is faster than for processes
    - Less resources needed for each operating system thread state
  - Threads of the same process share memory space

Excursion Operating Systems

Inter Process Communication (IPC)

- Methods for communication between processes
- Filesystem
  - One process writes to a file and another reads from the file
- Signals
  - Stop, kill, or continue a process
  - Informs process of errors: e.g., SIGSEGV is send by POSIX OS if process accesses invalid virtual memory address
- Sockets
  - Network communication
  - Can also be used in one machine
    - E.g., DBMS server and client running on the same machine communicating via TCP

Excursion Operating Systems

IPC cont.

- Message Queues
  - Asynchronous communication:
    - One process submits messages to the queue
    - Other process reads message from queue
- Pipes
  - Connects processes stdin and stdout
- Semaphores
  - Control access to limited resources by multiple processes
- Shared memory
  - Memory that can be accessed by more than one process

Excursion Operating Systems

File-systems (UNIX)

- Organize content on disk
- Some linux supported file-systems: ext2/3/4, ReiserFS
- Store file data and meta-data
  - e.g., creation-time
- Meta-data stored in inodes

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Excursion Operating Systems

Kernel vs. User space

- Kernel monopolizes (abstracts from) access to hardware
  - Memory
  - File-systems
  - Graphics
- Kernel realizes scheduling of processes
- Kernel space vs. user space
  - Applications (user space) access hardware indirectly through kernel interface (system calls)

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Approaches

- Provenance-aware file systems
  - Lineage File System
  - PASS
  - Praana: A Personalized Desktop Filesystem
- Kernel-extensions (instrumented kernels)
  - Hi-Fi
  - PASS
- Provenance support in virtualization layers
  - Provenance support via the Xen Hypervisor
- Instrumenting Executable Programs to track provenance
  - Extend Valgrind for provenance collection

Outline

PASS

- File- and process-level provenance
- Modified Linux Kernel
  - Provenance capturing is automatic and transparent to applications
- Provenance model
  - Graph
  - Nodes are files and processes (and sockets)
  - Edges between processes and files indicate
    - Process reads file
    - Process writes to file

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PASS

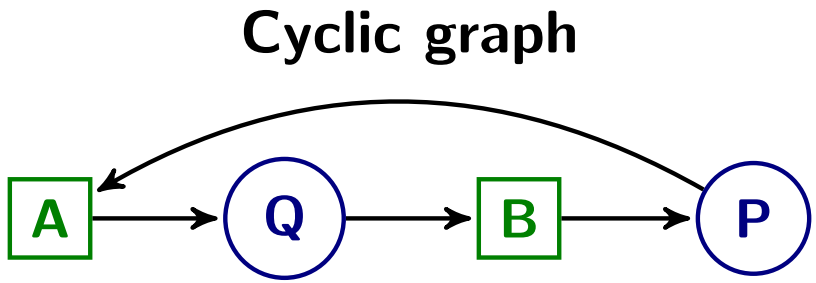
Architecture

- Pasta: The provenance and storage layer
  - File-system that tracks provenance
  - Old-versions are not persisted ⇒no versioning
  - Provenance records (p-nodes) are never deleted
  - KBDB: Kernel implementation of Berkley DB
    - stores provenance information
- Provenance Collector
  - Provenance Data Recording
  - Breaking Cycles
    - Avoid generating a new object version on each change
    - Merging nodes during cross-referencing
- Query tool

PASS

Example

	Process P	Process Q
1		read A
2		write B
3	read B	
4	write A	



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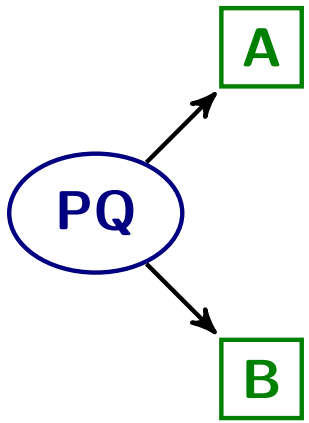
PASS

Example

	Process P	Process Q
1		read A
2		write B
3	read B	
4	write A	

After Merging



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Lineage File System

- Modified Linux kernel
- System calls for process creation and file manipulation instrumented
  - create provenance records in kernel buffer (`printk`)
- User daemon collects provenance
  - Wakes up regularly
  - Writes provenance to MySQL database

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Praana: A Personalized Desktop Filesystem

- File-system with support for annotations
  - extends ext3
- Metadata Repository
  - Relational Database
  - Relation Graphs
    - Each file is a node
    - Edges between files in same directory
    - New edges based on provenance
- Inference Learning Engine (ILE)
  - "Learns" edge weights in graph based on user feedback and provenance

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Provenance using Xen Hypervisor

- Xen Hypervisor
  - Virtual machine engine
- Adapt the PASS approach for instrumenting the Xen Hypervisor
- $\Rightarrow$Enables provenance collection for virtual machines

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Instrumenting Programs using Valgrind

- Use program instrumentation framework Valgrind
- Instrument programs using dataflow analysis
- Dynamic dataflow analysis
  - For a variable and a given part of a program
  - Determine which variable assignments (memory values) influence the variable at this position
  - Do that for a given input (execution)
- Use slicing to determine which input reads influence an output statement (write)
- $\Rightarrow$get very fine-grained provenance for arbitrary executable programs

Instrumenting Programs using Valgrind

Valgrind

- Program instrumentation framework
- Used mainly for debugging memory errors
  - detects access beyond array boundaries
  - detects access to previously free'd memory
  - detects memory holes: memory that is not referenced from anywhere but was not free'd
  - ...
- Functionality is achieved by instrumenting programs
  - $\Rightarrow$Modify the program's (machine) code

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Instrumenting Programs using Valgrind

Dataflow Analysis

- Track on which variables the value of a variable at a certain point in the program depends on
- Using dependency relations
  - $DEP(x, i)$: variables the value of variable x at line i depends on
- Computed recursively for static analysis
- Computed by forward construction for dynamic analysis

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Instrumenting Programs using Valgrind

Example

```
 1  read(x,y);
 2  total = 0;
 3  sum = 0
 4  if (x <=1) {
 5     sum = y;
 6  }
 7  else {
 8     read(z);
 9     total = x * y * z;
10  }
11  write(total, sum);
```

Example

Input: $x = 1,\ y = 5$

$DEP(sum, 11) = \{y\}$

Input: $x = 2,\ y = 3,\ z = 2$

$DEP(total, 11) = \{x, y, z\}$

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Outline

Recap

OS Provenance Challenges

- Different use cases that need very fine-granular provenance
  - Detecting Security Breaches
  - Detecting Execution Anomalies
  - Repeatability
  - Auditing
- Very low-level provenance
- Many approaches work for arbitrary programs

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Recap

Covered Approaches

- PASS
- Lineage File System
- Praana
- Xen Hypervisor provenance
- Provenance using program instrumentation with Valgrind

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Outline

Distributed Systems

- Disclaimer: Very limited discussion needed to understand the presented approaches
- Take classes for in-depth discussion: one of the many distributed systems classes including cloud computing ...
- HPC-clusters or Grids:
  - Distributed processing of expensive computations
    - e.g., physics simulations
  - on a large number of machines
- Overlap with workflow systems:
  - many of the discussed workflow systems are actually distributed systems

GY

Scripting Languages for Distributed Computation

- Makes distribution to some degree transparent
  - Translates script into a bunch of jobs
  - These jobs are executed distributively using a job submission system
  - Determine when to move load and/or data from one host to another
  - Failover
- Chimera: VDL
- Swift
- JSDL
- ...

Outline

Chimera

- VDL (Virtual Data Langage)
  - Describe data set properties
  - "Script" large-scale distributed executions
- Catalog that stores
  - Transformation descriptions
  - Execution descriptions
  - Data set descriptions
  - Provenance

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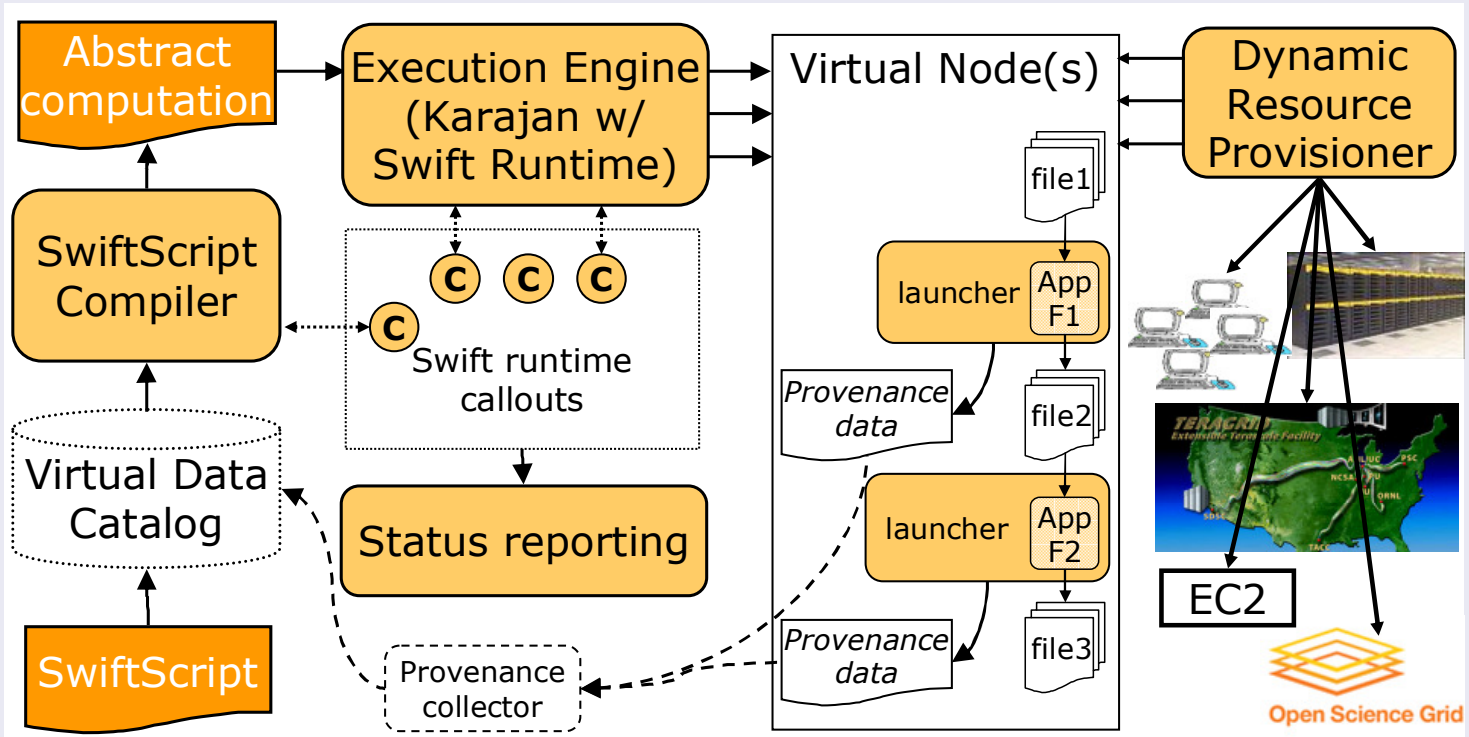
Swift

- Extension of Chimera
- Concise specification and efficient execution of large loosely coupled computations
- Scripting Langauge **SwiftScript**
  - Describes Data
    - **logical** and **physical** structure of the dataset to be processed
    - Mappers to map data from and to XML
  - Task to execute
- **Karajan** and **Falkon**: job submission system and compiler
- Provenance generator: **Kickstart**
  - wraps the executables
  - tracks their behaviour

Architecture



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Tracking and Sketching Distributed Provenance

- Extends ideas of PASS and other OS approaches
- For distributed computations
- Provenance model includes location and references to provenance on other hosts
- Less centralized storage model
  - each host stores its own provenance
- Track network traffic to detect inter-host dependencies
  - e.g., ssh
- Provenance Sketches
  - Compressed approximate representation of provenance
  - using bloom filters

Outline

Recap

Provenance for distributed systems

- Scripting languages for distributed computation
  - Chimera
  - Swift
  - ...
- Tracking and Sketching Distributed Data Provenance
  - Similar to OS-based approaches
  - but tailored for distribution
    - by considering inter-host dependencies
    - distributed storage of provenance
  - Provenance Sketches
    - compact approximate representation of provenance
    - uses Bloom filters

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