Coasters: uniform resource provisioning and access for clouds and grids

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Big Picture: Deploy applications on resources

Application invocations:
- Applications
- Data
- Dependencies

Interfaces:
- Cluster
- Grid
- Cloud
- HPC

Resources:
- CPUs
- Storage
- Services

Coasters: uniform resource provisioning
Motivation: Queuing systems

- What we have (PBS, SGE)

- What we would like
Big Picture: Reusable service components

Application invocations
- Applications
- Data
- Dependencies

Resources
- CPUs
- Storage
- Services

Interfaces
- Cluster
- Grid
- Cloud
- HPC

Coaster Service

Coaster Pilot Job

Coasters: uniform resource provisioning
Big Picture: No hands operation

Client

Coaster Client

Coaster Service Code

Head Node

GRAM/SSH

Bootstrap

Cache

Coaster Service

Coasters: uniform resource provisioning
Big Picture: Manage scientific applications

Application invocations

Produce inputs
Compute
Analyze
Reduce

Interfaces
Coaster Service
Cluster
Grid
Cloud
HPC

Resources
CPUs
Storage
Services

Coasters: uniform resource provisioning
Motivation: File system use on Grids

- Typical file path when using GRAM
- For a stage-in, a file is read 3 times from disk, written 2 times to disk, and goes 4 times through some network
- Assumption: it’s more efficient to copy data to compute node local storage than running a job directly on a shared FS.
Motivation: ... can be made more efficient

- 2 disk reads, one write, and 2 times through network
- Assumption: compute node has no outside world access, otherwise the head node can be bypassed
Big Picture: Make these resources *uniform*

*Enable high portability*

- Application-level
  - Task execution
  - Data access and transfer
- Infrastructure-level
  - Pilot job management
  - Configuration management
- Enable automation of configuration
Big Picture: Create a live pathway between client side and compute nodes

Coasters: uniform resource provisioning
Outline

- Overview of scientific scripting with Swift
- Description of Coasters features
- Application use case: protein docking
- Data transfer methods in Coasters
- Deployment on Amazon EC2 with Globus Provisioning
Big Picture: Enable complex application logic

Not just MapReduce!

- Iteration
- Typed data
- Structures, arrays
- Automatic dataflow concurrency
- Functions, external applications
- External file data
- Site-specific configuration
Scientific scripting - SwiftScript

- Support file/task model directly in the language

```swift
app (file output) sim(file input) {
    namd2 @input @output
}
```

- Provide natural concurrency through automatic data flow analysis and task scheduling

```swift
file o11 = sim(input1);
file o12 = sim(input2);
file m = exchange(o11, o12);
file i21 = create(o11, m);
file o21 = sim(i21);
...
```

- Separate application script from site configuration details

- Support scientific data sets in the language through language constructs such as structs, arrays, mappers, etc.
Swift features

- Data types
  
  `string s = “hello world”;`
  
  `int i = 4;`
  
  `int A[];`

- Mapped data types
  
  `type image;`
  
  `image file1<“snapshot.jpg”>;`

- Conventional expressions
  
  `if (x == 3) {`
  
  `  y = x+2;`
  
  `  s = @strcat(“y: “, y);`
  
  `}`

- Structured data
  
  `image  A[]<array_mapper…>;`

- Loops
  
  `foreach f,i in A {`
  
  `  B[i] = convert(A[i]);`
  
  `}`

- Data flow
  
  `analyze(B[0], B[1]);`
  
  `analyze(B[2], B[3]);`

**Swift: A language for distributed parallel scripting, J. Parallel Computing, 2011**
Execution infrastructure - Coasters

- Coasters: a high task rate execution provider
  - Automatically deploys worker agents to resources with respect to user task queues and available resources
  - Implements the Java CoG provider interfaces for compatibility with Swift and other software
  - Currently runs on clusters, grids, and HPC systems
  - Can move data along with task submission
  - Contains a “block” abstraction to manage allocations containing large numbers of CPUs
We need to submit jobs and move data to/from various resources

Coasters is implemented to use the Java CoG Kit providers

Coasters implements the Java CoG abstractions

**Java CoG supports:** Local execution, PBS, SGE, SSH, Condor, GT, Cobalt

**Thus, it runs on:** Cray, Blue Gene, OSG, TeraGrid, clusters, Bionimbus, FutureGrid, EC2, etc.

Coasters can automatically allocate blocks of computation time for use in response to user load: “block queue processing”

Runs as a service or bundled with Swift execution
Implementation: The job packing problem (I)

- We need to pack small jobs into larger jobs (blocks)

- Resources have restrictions:
  - Limit on total number of LRM jobs
  - Limit on job times
  - Non-unity granularity (e.g. CPUs can only be allocated in multiples of 16)

- We don’t generally know where empty spots in the scheduling are

- We want to fit Coasters pilot jobs into the queue however we can
Implementation: The job packing problem (II) (not to scale)

- Sort incoming jobs based on walltime
- Partition required space into blocks
Implementation: The job packing problem (II) (also not to scale)

- Commit jobs to blocks and adjust as necessary based on actual walltime

- The actual packing problem is NP-complete
- Solved using a greedy algorithm: always pick the largest job that will fit in a block first
Coasters settings

- “Block” or “Passive” queue processor
- Wall time inputs and customization (overallocation)
- General queue settings
  - Node count specification
  - Spread
- Scheduler-specific queue settings
  - PBS, SGE, Globus settings, etc.
- Swift settings
  - Throttles on job submission, data transfer
  - Allows user to conform to site rules
Application case - ModFTDock

- modFTDock: Novel application to perform protein docking using large batches of sequential tasks
- SwiftScript was rapidly built and deployed on Beagle, the new Cray XE6, and the Bionimbus cloud system
- Bionimbus: easily scaled to 100,000 tasks on 20 nodes, 80 cores in preliminary testing
- Production runs will require similar task quantities, longer tasks, more cores
ModFTDock

```
string str_roots[] = readData( @arg( "list" ) );
int n = @toint(@arg("n","1"));

foreach str_root in str_roots
{
    string str_file_static = @strcat( @arg("in", "input"), str_root, ".pdb" );
    string str_file_mobile = "input/4TRA.pdb";

    file_pdb file_static<single_file_mapper;file=str_file_static >;
    file_pdb file_mobile<single_file_mapper;file=str_file_mobile >;
    file_dat dat_files[]<simple_mapper;
padding = 3,
    location=@arg("out", "output"),
    prefix=@strcat(str_root, "_"),
    suffix=".dat">;

    foreach mod_index in [0:n-1]
    {
        string str_modulo = @strcat(mod_index, ":", modulus);
        dat_files[mod_index] =
            do_one_dock(str_root, str_modulo, file_static, file_mobile);
    }
}
```

Coasters: uniform resource provisioning
Many tasks: many small files

fMRI image analysis
Coasters provider staging

Shared file system
Coasters provider staging

Proxy file transfer
Coasters provider staging

Service file transfer
Use on commercial clouds

- Swift/Coasters is easy to deploy on Globus Provisioning (GP)
- GP provides simple start-up scripts and several other features we may use in the future (NFS, VM image, CHEF)
- Usage:
  0. Authenticate to AWS
  1. `start-coaster-service`  
     `gp-instance-create`  
     `gp-instance-start`
  2. `swift` `myscript.swift` ...
     Repeat as necessary
  3. `stop-coaster-service`  
     `gp-instance-terminate`
Related Swift/Coasters work...

- **Collective Data Management (CDM)**
  - Improve support for shared filesystems on distributed resources
  - Make use of specialized, site-specific data movement features
  - Employ caching through the deployment of distributed storage resources on the computation sites
  - Aggregate small file operations into operations on archives, etc.
    *Case studies in storage access by loosely coupled petascale applications, Proc. Workshop PDSW at SC, 2009*

- **Many Parallel-Task Computing (MPTC)**
  - Support large batches of small MPI or Global Arrays jobs
  - Multiple scheduler modes - JETS project
    *JETS: Language and system support for many-parallel-task computing, Proc. Workshop P2S2 at ICPP, 2011*

- **ExM: Many-task computing on extreme-scale systems**
  - Deploy SwiftScript applications on exascale-generation systems
  - Developing new compiler, new distributed progress management infrastructure, and new global data store
Thanks

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Questions