Toward Improved Support for Loosely Coupled Large Scale Simulation Workflows

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Motivation & Challenges

• Bigger machines (e.g., TITAN, upcoming Exascale systems)
  – Environment targets coarse-grain, massively parallel executions
    • Relatively “heavy weight” tools for program startup, execution, and shutdown
    • “Few” active program dispatch instances on service nodes

• Growing use of large scale many-task computing:
  – Ensemble computing for Leadership class allocation
  – Genomics, bioinformatics, data analytics ...
  – Parameter sweep and optimizations (Industrial use)

• Runtime environment (RTE) is a crucial software component
  – Not supportive of this kind of workload

Can we provide user-level run-time environment to better support large scale loosely coupled workloads?
Key Requirements

• Minimal (no?) incremental impact on service nodes as number of executing instances scales up.

• Low overhead for execution initiation, monitoring, and termination.

• Efficient resource utilization
  – Number of cores/node will only increase

• Current ALPS/aprun environment
  – Limits on number of concurrent aprun instances on service node
  – Relatively long startup/shutdown times per aprun invocation
  – Policy limits on node sharing.
Other tools

• Serial Tasks:
  – Relatively easy - rely on `system()` calls from compute nodes
  – BigJob, Parallel Command Processor (PCP) ..etc.
  – Cannot be extended to parallel tasks

• Parallel Tasks
  – Integrated Plasma Simulator (IPS)
  – Still uses `aprun/mpirun` under the hood
  – Need different runtime to use anything else
Scalable RunTime Component Infrastructure – STCI

• Goals
  – Scalable start-up and management of scientific simulations
  – Resilience/fault tolerance
  – *Ease the study and development of new system tools and/or applications for HPC*

• Key characteristics
  – User space modular architecture
  – Provide reusable components

• Lightweight front end tools
  – Task instantiation, monitoring, and termination
  – Better fit for handling many concurrent executing tasks.
STCI Architecture

- Agents
  - Instantiate both the STCI infrastructure and applications/tools
  - Different “types” of agents
    - *Frontend*: user frontend running on user’s terminal
    - *Controller*: logical agent representing the job from a control point of view
    - *Root agent*: privileged agent for resource allocation; one per node; non-specific to a job
    - *Session agent*: local management of users’ job; one per user and per node
    - *Tool agent*: instantiation of an application or a tool

- Topologies
  - Represent connections between agents
  - Examples: trees, meshes, binomial graphs
STCI Architecture (2)

• Launcher
  – Deploy a job by creating the necessary agents across the HPC platform
  – Two challenges
    • Scalable deployment method: by default, a tree-based topology
    • Method to create the required agents
      – Example: fork, ssh, ALPS
      – On Cray:
        » Torque gives the list of target compute nodes
        » ALPS is used to create the RAs
        » then RAs create other agents

• Event system
  – Support for asynchronous execution model
  – Various progress models available: implicit or explicit progress
Alternate Runtime for MPI tasks on Crays

• Based on Open-MPI
  – Replace the default runtime (ORTE)
  – Benefit the RTE abstraction in Open-MPI
    • Out-of-band communications
    • Naming service
  – RTE mainly used for the deployment of MPI ranks
    • STCl communication substrates used during bootstrapping
    • Open-MPI high-performance communication substrates once bootstrapping completed

• Front end tools for task management
  – stcistart, stciexec, stciwait, stcikill, stcistop
STCI For Many Task Computing

• Original STCI supports a single startup-execute-shutdown cycle, for a single app invocation.

• Explicit STCI shutdown command
  – Keep STCI agents alive after tasks complete

• Add support for new frontend tools
STCI Many Task Overview

Frontend Commands

stcistart, stcistop

stciexec, stciwait

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Service Node

Compute Node

Compute Node

Persistent Management infrastructure

Task 1

Task 2

F Front-end Agent
C Controller Agent
R Root Agent
S Session Agent
T Tool Agent

stciexec

stcistart, stcistop

stciwait

stciexec
STCI Front End Commands

- Execute within a single batch allocation
- Targeting streamlined many-task management.
- Minimize impact on service node resources.
- Could be used directly, or as the backend for a smart workflow management interface.
STCI commands: stcistart

- Syntax `stcistart -N #NNODES`
  - `#NNODES`: Number of STCI managed nodes (e.g. `$PBS_NUM_NODES`)

- Only call to `aprun` in a STCI session

- Start STCI agents to support tasks on `#NNODES` compute nodes

- Returns: session id (`sid`) for use in future STCI commands
  - Returned as stdout string

- Blocking command
  - return after all STCI infrastructure agents have been initiated
STCI commands : stciexec

- Syntax: `stciexec -S sid -np nprocs <prog> [args]`
  - `sid`: session id returned from stcistart.
  - `nprocs`: number of ranks in MPI task

- Start `<prog>` on `nprocs` free cores,
  - Fail if not enough free cores are available

- Non-blocking:
  - Returns **STCI** task id `-tid` immediately upon successful launch.
  - Task id returned as stdout
STCI commands: stciwait

- Syntax: stciwait -S sid [-any] tid[,,tid]*
  - sid: session id returned from stcistart
  - tid: task id returned from a prior call to stciexec
- Wait for one or more STCi tasks to finish
- Default: blocking wait for all tid’s to terminate
- -any causes return after one or more tasks finish
- Return immediately if all tasks have finished.
- Print list of taskid:retval on stdout
Other STCI Commands

• `stcikill -S sid tid`  
  Kill task `tid` started under session `sid`

• `stcilist -S sid`  
  List status of all tasks for session `sid`

• `stcistop -S sid`  
  Terminate session `sid` and all its remaining tasks
(Very) Preliminary Results using STCI

• Tests run on Chester
  – development Cray XK7 at ORNL
  – 80 compute nodes * 16 cores/node

• Using a single core user task
  – Support for user tasks with np > 1 currently in testing

• Three tests:
  – Impact on service node
  – Task initiation/shutdown overhead
  – Node sharing between distinct MPI tasks
Impact on service node memory

- 32 concurrent mpisleep tasks, launched 10 sec apart.
- Using background aprun (red) and stcistart/stciwait (blue)
- Sleep time chosen to have all tasks concurrently active
Task Initiation/Termination overhead

- 100 `mpisleep` 0 tasks executed sequentially
- Repeated 10 times
- STCI time include `stcistart`, `stcistop`, and 10 sec delay between `stcistart` and 1st task
End-to-End Execution time

- Repeated 12 times on 2 Chester nodes (16 cores/node)
- Total **STCI** time includes `stcistart`, `stcistop`, and 10 sec delay.
- Node sharing among separate MPI tasks
- Ongoing tests using `n > 1` MPI tasks

Average time for 12 runs
Task Output Management

• Controller logs output from tasks launched via ‘stciexec’
  – STDOUT -> stci-stdout-sid-<SID>.log
  – STDERR -> stci-stderr-sid-<SID>.log

• The individual task output can be extracted using a post-processing script, pyramid-chopjob.pl

```bash
$ ./pyramid-chopjob.pl < stci-stdout-sid-31683.log
Created: /tmp/stdout-stcijob-1.log
Created: /tmp/stdout-stcijob-2.log
...
Created: /tmp/stdout-stcijob-14.log
$ cat stdout-stcijob-14.log
( 0) My rank is: 0 sleeping 3 sec. (host=nid00078)
```
Combined output file from all tasks

```
$ head /tmp/stci-stdout-sid-31683.log
==14-start==
(    0) My rank is: 0  sleeping 3 sec. (host=nid00078)
==14-end==
==28-start==
(    0) My rank is: 0  sleeping 2 sec. (host=nid00079)
==28-end==
...
```
Conclusion

• STCI enables lightweight, fast task management infrastructure for ALPS based Cray systems.

• Open MPI-based flexible runtime environment.

• Future work
  – Complete support for n>1 MPI tasks
  – User-controlled placement of tasks
  – Fault tolerance and recovery
  – Explore in-memory caching of binary image on compute nodes
  – Integration with more sophisticated front-end tools (e.g. the IPS).
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Thank You

Questions?

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