

Intelligent Workload Management Software for HPC and Cloud Environments

Broadening Moab/TORQUE for Expanding User Needs

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Agenda

- DataWarp
- Intel MIC "KNL"
- Viewpoint Web Portal
 - User Portal
 - Administrator Portal
 - Remote Visualization
 - Nitro HTC



Agenda

- DataWarp (fast I/O)
- Intel MIC "KNL"
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- Stage job data with fast SSD-based storage
 - Input data before job starts
 - Output data after job ends
- Fast persistent storage for job workflows
- Fast job checkpoint/restore



Cray DataWarp

- SSD-based storage system independent of parallel file system (PFS)
- Hosted on DataWarp (DW) service nodes
 - Contain actual SSDs
 - Nodes connect to Aries high-speed network
- DataWarp Service (DWS)
 - Organizes DW storage for jobs and persistent storage
 - Manages SSD storage across DW service nodes



Cray DataWarp Physical Architecture

- DW storage
 - 2-hop roundtrip
 - Aries HSN
 - Electronic access times
- PFS storage
 - 4-hop roundtrip
 - 2-hop Aries HSN
 - 2-hop InfiniBand
 - Electro-mechanical access times
- DWS not shown





Cray DataWarp Support

- DataWarp Storage Types
 - Job-based
 - Persistent
- Script-based integration with Moab/TORQUE
- DW-enabled jobs processed by Moab "job submit filter"
- Moab automatically creates DW job workflow



DataWarp Integration Project

- All DW storage scheduled by Moab
 - Job DW storage by job scheduling
 - Persistent DW storage by reservation scheduling
- Out-of-the-box functionality
 - Some site-specific information configuration required



Moab 3-Job DataWarp Model

- Follows Moab Data-staging Model
 - Uses Moab "system" jobs to create/destroy DW storage and stage data in/out
- Automatically creates 3-job workflow
 - DW creation/input data-staging system job
 - User job
 - Output data-staging/DW destruction system job



DataWarp-enabled Job Workflow

- User submits user job
- Job Submit Filter detects #DW directives
- Job Submit Filter creates
 3-job workflow
 - DW Creation / Input Datastaging System job
 - 2. User Job
 - 3. Output Data-staging / DW Destruction System Job





Allocated Resources



Automatic Job/DW Workflow Generation

- What if user submits multiple-job workflow
 - And some user jobs in job workflow use DataWarp storage?
- Job Submit Filter creates proper DW job dependencies, but not for entire user job workflow
- Example
 - Data validation
 - Compute (uses DataWarp)
 - Visualization

User Job A User Job B (DW) User Job C



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Automatic Job/DW Workflow Generation

- User Job Dependencies
 - Data validation
 User Job A
 - Compute User Job B (DataWarp-enabled job)
 - Visualization
 User Job C
 - Job A (ok) ← Job B (ok) ← Job C
- Job workflow generation script must work with Job Submit Filter to create proper job dependencies (solid lines below)





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Multi-Job Workflow Generation Script

Submit data validation job A
jobAid=`msub -1 nodes=1,walltime=10:00 myCheck.sh`



Persistent DataWarp Storage

- Moab schedules and tracks all DW storage capacity
- Moab persistent DW storage uses DW storage reservation
- Persistent DataWarp storage management
 - Created by reservation start trigger
 - Destroyed by reservation end trigger
- Jobs get mount point





Benefits

- Moab schedules and manages both job and persistent DataWarp storage
- Users have good user experience
 - No race conditions cause cancelled jobs!
- Jobs have fast I/O
- Jobs execute in less time



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- Intel introduces 2nd-gen Xeon Phi processor
- KNL supports
 - 3 different NUMA configurations with 5 modes
 - 3 different MCDRAM configurations with 4 modes
 - 20 possible NUMA/MCDRAM configurations
- Some applications execute fastest with specific NUMA/MCDRAM configuration



Intel MIC "Knights Landing" (KNL)

- 5 NUMA configurations for cores and DDR4 and MCDRAM memories
 - No NUMA (all2all, hemisphere, quadrant) and sub-NUMA cluster 2 and 4
 - a2a, hemi, quad, snc2, snc4
- 4 MCDRAM "mode" configurations
 - Cache, flat, 50/50 hybrid, 25/75 hybrid
 - cache, flat, equal, split



Moab Cray KNL Support

- 20 pre-defined combinations
 - Select combination as "OS" at job submission
 msub nodes=20, os=CLE_snc4_flat myJobScript
- Moab re-provisions Cray compute nodes when necessary
 - Uses Moab's built-in re-provisioning capability
 - Quickly re-provisions Cray KNL compute nodes for jobs requesting specific NUMA/MCDRAM modes



Cray KNL Re-provisioning Process

User submits job requiring specific KNL NUMA / MCDRAM configuration

msub -1 nodes=20,os=CLE_snc4_flat myJob

- Moab schedules KNL job to nodes
- Moab runs NodeModifyURL script to modify compute node configurations and reboot them
- Script executes Cray capmc to set KNL NUMA node and MCDRAM configurations and to reboot nodes
- Cray's capmc modifies nodes' BIOS settings and reboots nodes
- Cray reports new NUMA node / MCDRAM configurations
- pbs_reporter maps NUMA node/MCDRAM configuration to OS name and reports OS name to pbs_server
- TORQUE pbs_server passes new OS name to Moab, which starts the KNL job





Benefits

- Users can run applications with KNL NUMA and MCDRAM configuration for optimal job execution.
- Easy to request specific KNL configuration with job submission



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Use Case

- Many HPC sites asked to expand user base
- Non-technical users
 - "What is a command line?"
- Non-traditional users
 - Non-research Engineers and Scientists
 - Humanities
 - Local or regional industries with no HPC experience



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- Someone said I need to use "xyz" program
- I have data
 - Someone gave me my data
 - Someone mentored/trained me and I created my own data
 - I taught myself and created my own data
- How do I use "xyz" with my data?



Log in as user to Viewpoint Web Portal

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Click Workload to check on your "xyz" job

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Benefits

- Allows non-technical users to submit jobs using pre-defined application templates
- Application templates contain
 - Job script for running application
 - Web form design with pre-defined and/or custom widgets and their variables
 - Job submission replaces variables within job script with form's widget values



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Use Case

- Administrator needs to support many nontechnical users and their applications
- Define application templates using editor
 - Define and customize application template form using pre-defined "widget" types
 - Define widgets' variable name, default value, and other characteristics to build form
 - Create job script



Log in as admin to Viewpoint Web Portal

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EXPORT TEMPLATE

SAVE TEMPLATE

SAVE AND CLOSE

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EXPORT TEMPLATE SAVE TEMPLATE SAVE AND CLOSE

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Create/import job script with Script Builder

Dasic settings		Script	t Builder	e* ×	Published O Unpublished
Basic Job Settings Label Variable Name Default Value	Name NAME ansys	1 2 3 4 5 6 7 8 9 10 11 12 13 14 15	<pre>module load ansys/%VERSION% cd \$PBS_0_WORKDIR # Copy input files to TMPDIR and then # change working directory cp %INPUT% \$TMPDIR cd \$TMPDIR /usr/bin/ansys%VERSION%0 -np %NUMOFCORES% -i # Copy output files back to your working # directory and clean up \$TMPDIR cp -r \$TMPDIR \$PBS_0_WORKDIR</pre>	Variables Moab Inputs ACCOUNT ARCHITECTURE DESTINATIONQUEUE DURATION ELIGIBLEDATE EMAILOPTIONS ENDINDEX ERRORPATH EXECUTIONDIRECTORY	Published O Unpublished
Label Variable Name Default Value	Submission Scri SCRIPT Customize Script	16	rm -rf \$TMPDIR	FEATURETAGS GENERICRESOURCES HOLD JOIN MAILLIST MEMORYPERNODE MOABENVIRONMENTVA MOABTEMPLATE NAME NODEACCESSPOLICY	

Add widget variables to job script

		Script	t Builder		2	● × ● ● ● ● ● ● ● ● ● ● ● ● ● ● ● ● ● ●
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Benefits

- Application templates let an administrator create application templates for nontechnical users.
- Non-technical users have a simple way to submit jobs for specific applications.



Agenda

- DataWarp
- Intel MIC "KNL"
- Viewpoint Web Portal (non-technical users)
 - User Portal
 - Administrator Portal
 - Remote Visualization (graphical interfaces)
 - Nitro HTC





- Users need to visualize their data to gain insights from it.
- Desktops or workstations with decent visualization hardware can be expensive.
- Data can be too large to move to another location.
- Non-technical users need a way to easily set up a remote visualization session.



Choose Remote Visualization Templates

HOME	WORKLOAD	TEMPLATES	FILE MANAGER	SESSIONS	
Search		Select Application Te	mplate		× load Summary
Workloa	ad 😰	Template Type All	*	Q	OBS IN A COMPLETED STATE
Job ID 🕴 Jo	ob Name 🕴 Submit	ANSYS All		Desktop	• COMPLETED
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Moab.105 an	nsys hpotter	2016-04-12 2016-0 11:52:04 11:51:5	4-12 COMPLETED 1	1 00:00:01:00	
Show 10	entries		← prev	1 2 next →	

Choose Remote Desktop App Template

Search	10 10 10 10 10 10 10 10 10 10 10 10 10 1	Select Application Tem	plate		× load Summary
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Choose Graphical Desktop Type

Basic Settings					
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				Cancel	CREATE

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Submit Remote Desktop Job

asic Settings					Job with ID "Moab.115" has be submitted
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Resources					
Number of Cores	Total Amount of Cores	· ·			
Total Cores	1	~			
esktop Settings					
Desktop Interface	Gnome	·			
				Cancel	CREAT

Remote Desktop Job's Compute Node

Data Management			Other Information
Execution Path	/home/hpotter	•	Partition Access List None
Output Path	/home/hpotter	•	Start Count 1
Error Path	/home/hpotter	•	
Resource Requirement Summa	ry/		
Total Processors Requested	1		Total Nodes Requested 0
Total Memory Requested	1.0 GB		Allocated Node List quadro
Total Swap Requested	N/A		Allocated Node Count 1
Total Disk	N/A		Allocated Partition demo
Features	gpu		Operating System N/A
			Architecture N/A
			Total Generic Resources N/A
Requirement Details			

Remote Desktop Session Screen

👬 Applications Places System 😔 🔗

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											=

Tue Apr 19, 10:43 AM hpotter

Remote Visualization Session Controls





Resized Remote Viz Session Desktop

👫 Applications Places System 🌏 💮 🗾





hpotter's Home







Terminal





hpotter

Job Detail with Remote Viz Session



-

Canceling the Remote Desktop Session



Choose ParaView Application Template

HOME	WORKLOA	D	TEMPLATE	S	FILE MANAGER		SE	SSIONS		
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Moab.103 pa	araview h	potter	2016-04-12	2016-04-12	COMPLETED	4	1	00:12:00:00		

ParaView Input Data file selection

	Open File	×	welcome, inporter <u>orginolor</u> o
HOME WORKLOAD	Remote File System / home / hpotter / paraview		
Create Job	↑ Name	Date	
Paraview	blood cells.pvsm	2016/03/15	
✤ Basic Settings	rectorid.pvsm	2016/03/15	
Basic Job Settings Name para	*		٢
Resources Total Memory (GB) 4.00			
✓ Paraview Settings	Show 10 • entries		
Data File		Close SELECT	
		Car	CREATE

Submitting ParaView Remote Viz Job

Moab VI	EWPOIN	Г					Welcome, hpotter	Job with ID "Moab.116" has b
HOME	WORKLO	DAD	TEMPLATES	FILE MANAGER	SESSIONS			submitted
reate Job								
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 Basic Setting 	S							
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✓ Paraview Set	tings							
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						Cancel		CREATE

ParaView Remote Viz Session



Adjusting Session Image Quality

Settinas

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Remote Desktop / ParaView Session

Applications Places System

👫 Applications Places System 😔 👩 🗾		🚔 📣 🖺	Tue Apr 19, 10:47 AM	hpotte
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// ParaView 4.4.0 64-bit				

Benefits

 Technical and non-technical users can easily create remote visualization sessions with their applications and data.


Agenda

- DataWarp
- Intel MIC "KNL"
- Viewpoint Web Portal (non-technical users)
 - User Portal
 - Administrator Portal
 - Remote Visualization
 - Nitro (HTC job scheduling)



Use Cases

- A user can have thousands or millions of single-core to single-node jobs.
 - Parameter sweeps
 - Monte Carlo simulations
 - Regression tests
 - Other
- Large job queues
- Long scheduling cycles



Nitro HTC Scheduler Application

- Scheduler-agnostic HTC scheduler application
 - TORQUE
 - Slurm
 - Platform LSF
 - Cray ALPS
- Submitted as HPC job to scheduler



Nitro Job

- User converts HTC jobs to Nitro "tasks"
 - Tasks defined in Nitro Task file
- Submit 1 Nitro job with Task file
 - Schedule 1 parallel HPC job
 - Execute millions of HTC tasks

• What about HTC for non-technical users?



Choose Nitro Application Template

HOME	WORKLOAD	TEMPLA	TES FILE MANAGE	R SESSIONS
Search	-	Select Applic	cation Template	ad Summary
vorkioa	a 😇	Template Type	All	
Job ID + Job Moab.117 para Moab.116 para Moab.115 des Moab.114 ans	 Name Sub raview_desktop hpo raview hpo sktop hpo sys hpo 	ter 2016/4/19 moab-admin ter Cocker App ter 2016/3/2	All Definition Definit	 ▶ Desktop 2016/3/15 moab-admin ▶ Nitro Application 2016/4/8
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Moab.111 ope	endtect hpo	ter		
Moab.110 para	raview hpo	ter		Close
Moab.109 Nite	ro_job hpo	ter 12-25-34	10-05-07	

Nitro Task File selection

ites Dropbox All My Files nick	 January ANSYS (1).template Calculator.template Desktop.template 	C Search sleep 0 sleep 0 sleep 0 sleep 0	n	÷
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iCloud Drive	Job Array Clator.template nitro.task.txt Opendtect (as).template	sleep 0 sleep 0 sleep 0		
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templates Untitled		text - 900 F Created Jan 12, 201 Modified Jan 12, 201	KB 16, 10:01 AM 16, 10:01 AM 2016 at 9:59 AM	
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CREATE

Nitro Task file upload and job submission

Number of Cores Nodes with Core Count Total Nodes 1 1 * Cores Per Node 8 Data Management Output Path Nitro Inputs	ces					File has been successfully uploade
Total Nodes 1 Cores Per Node 8 Data Management Output Path /home/hpotter Nitro Inputs	umber of Cores	Nodes with Core Count	-	Total Memory (GB)	1.00	•
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Output Path /home/hpotter Nitro Inputs	lanagement					
vitro Inputs	Output Path	/home/hpotter				
	uts					
Task File /home/hpotter/nitro.task.txt Change	uts					

Nitro job progress and statistics

✤ Nitro Statistics				\$
Progre	55			
8%				
State	Running	Task File	/home/hpotter/nitro.task.txt	•
Coordinator Host	toi-901.vapor2.ac.localdomain	Task Log	/home/hpotter/nitro/Moab.118/nitro_Moab.118.tasklog.txt	•
	Job Log /home/hpotter/nitro/Moab.118/nitro_Moab.118.joblog		/home/hpotter/nitro/Moab.118/nitro_Moab.118.joblog.txt	•
Tasks		Worker S	ummary	

Pending	In Progress	Completed	Tasks / Sec
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User hpotte	er Group	hpotter Accou	unt engineeri

Workers Task Threads Avg Asgmt Duration Avg Task Duration 1 2 1.097 0.003



1

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Nitro job progress

Reservation Name: N/A

Template: Nitro Application (v.6 CURRENT)

Job Messa	ages									
✤ Nitro Stat	tistics							1		
	Progress									
		38%		•						
	State Running			Task File /	/home/hpotter/nitro.task.txt					
Coordina	Coordinator Host toi-901.vapor2.ac.localdomain				Task Log /home/hpotter/nitro/Moab.118/nitro_Moab.118.tasklog.t					
				Job Log /home/hpotter/nitro/Moab.118/nitro_Moab.118.joblog.txt						
Tasks				Worker Sum	nmary					
Pending	In Progress	Completed	Tasks / Sec	Workers	Task Threads	Avg Asgmt Duration	Avg Task Dura	tion		
1,250	500	38,000 -	513.51	1 -	2	0.915	0.002			
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Credentials	Credentials			CPU Statistics						
User hpotter Group hpotter Account engineeri			Nitro an	nlications track the	ir own usage statistic	Dianco				

Nitro Task Log file display during job

10.2.184.78:8081/file-manager/?path=/home/hpotter/nitro/Moab.118/nitro_Moab.118	.tasklog.txt	C	Q Search		☆ 🖻		+	A B
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iogs						5		
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		Moab.1183 3	Success 0 toi	i-901.vapor2.a	ac.loc			
		Moab.1184 4	Success 0 toi	i-901.vapor2.a i-901.vapor2 :	ac.loc ac.l&c			
	S	ize: 2.67 MB Mod	ified: 2016/04/19		\$			
					-			
		• • •		-0-	前			

Benefits

- Remove thousands-to-millions of HTC jobs from HPC scheduler queue(s)
- Execute HTC jobs faster
- Non-technical users can
 - Submit Nitro jobs
 - Monitor Nitro job progress
 - Examine Nitro Task results





Intelligent Workload Management Software for HPC and Cloud Environments

Questions?

PMIx Support

- Process Management Interface for eXascale
 - Open-source Project on github
 - Intel, Mellanox, IBM, Adaptive Computing, SchedMD
- Benefits
 - "Instant On" very fast job start (10 minutes → 2 seconds)
 - Asynchronous, non-blocking operations
 - Blob-based data transfers
 - Fast broadcasts/collectives
 - Interfaces with RMs (e.g., TORQUE)
 - Will work with malleable/evolving jobs in future



Malleable and Evolving Jobs

- Next-generation application/RTE support
 - Malleable jobs (scheduler → application/RTE)
 - Evolvable jobs (application/RTE → scheduler)
 - Need standard API to negotiate resources
 - Like MPI for parallel communications
 - Gathering use cases for PMIx API definition
- Benefits
 - Standard application API for scheduler/app dialog
 - Scheduler and Malleable/Evolving Application Dialog (SMEAD) API definition
 - Allows applications to ask for and return resources
 - Allows scheduler to give and take resources to and from a job





Intelligent Workload Management Software for HPC and Cloud Environments

Backup Slides