Altair

Innovation Intelligence®

Driving More Efficient Workload Management on Cray Systems with PBS Professional

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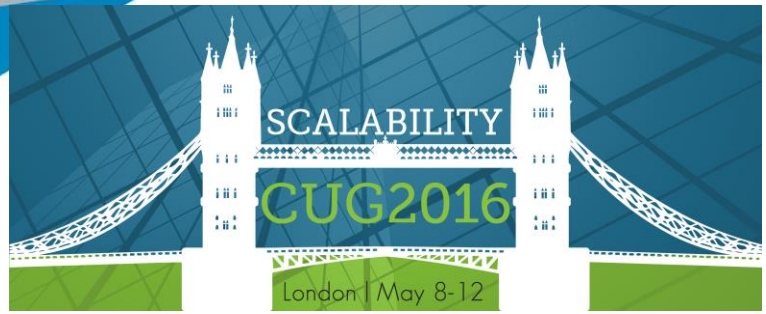

PBS Professional

Architected for Cray Systems

Re-architected Cray Support

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Flexible PBS Server/Scheduler

- **PBS Server/Scheduler can exist outside the Cray environment**
- **Utilize PBS Professional High Availability**
- **Impose per-named user/group/project limits**
- **Manage Cray compute nodes & Repurposed Compute/MAMU Nodes**
- **Manage Cray XC & Cray CS systems**

Re-architected Cray Support

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Full “PBS vnode” features supported for Cray

- **MPI task selection and placement – seamless transition between Cray and clusters with select & place language**
- **See which compute nodes the job is running on via qstat**
- **See each compute node in via pbsnodes**
- **Topology-aware scheduling**
  Grouping & placement set framework
- **More robust reservations**
- **Plus numerous speed improvements**

Topology-aware Scheduling

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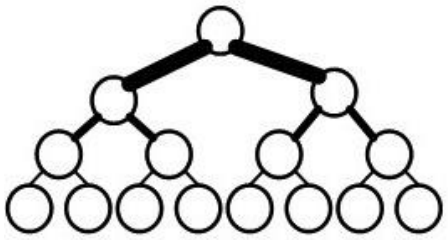
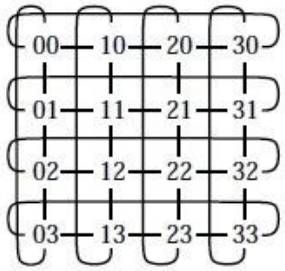
Speeds Application Performance and Boosts Utilization

Topology represented by “placement sets”

- Both inter (clusters, switches, grids) and intra (NUMA) node topology
- Infiniband, Ethernet, custom networks -- tree, torus, hypercube, dragonfly, anything
- Easily updated without the need to restart PBS

PBS Professional





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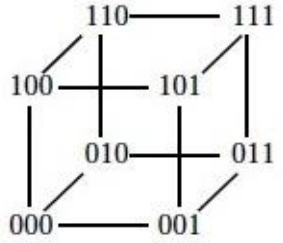

$M(2,3)$

*illustrations from HPC-Opinion.blogspot.com

Tunable Scheduling Formula

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Define any policy – including on-the-fly "exceptions"

Simple formulas are very simple (big jobs go first)

```
ncpus * (walltime/3600.0)
```

Complex formulas are pretty simple too… (adds priority accrual for smaller jobs, high-priority queue, deferred queue, "run this job next")

```
(ncpus * (walltime/3600.0)) * Wsize +

(eligible_time/3600.0) * Wwait +

special_p
```

Estimated Job Start Times

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Plan Your Workflow & Meet Your Deadlines

```
% qstat -T

                                                                Req'd Req'd     Est
Job ID  Username Queue  Jobname   SessID NDS TSK Memory Time  S Start
------- -------- -----  --------  ------ --- --- ------ ----- - -----
5.quark  bill    workq  foo       12345  1   1   128mb 00:10 R   -
9.quark  bill    workq  bar         --   1   1   128mb 00:10 Q 11:30
10.quark bill    workq  gril        --   1   1   128mb 00:10 Q 11:40
7.quark  bill    workq  baz         --   1   1   128mb 00:10 Q Tu 18


% qstat -f
    . . .
    estimated.exec_vnode = (pepsi:ncpus=1)
    estimated.start_time = Fri Apr 26 11:52:44 2013
```

PBS Professional

Recent Enhancements for Cray

EXCLUSIVE vs non-EXCLUSIVE Reservation Mode

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- **EXCLUSIVE mode has been used**
  - Only one ALPS reservation can be made on nodes; special privileges
  - Previously, PBS created all ALPS reservations as EXCLUSIVE
- **non-EXCLUSIVE mode does not mean "shared”**
  - Refer to Cray documentation for more information on EXCLUSIVE ALPS reservations.
  - Allows PBS Pro to suspend/resume jobs
- **PBS allows EXCLUSIVE or non-EXCLUSIVE to be user selectable**
  - non-EXCLUSIVE is default
- **To request an EXCLUSIVE ALPS reservation, submit a job with "-l place=excl”**
  - EXCLUSIVE on the Cray is not the same as the PBS place=excl
- **Examples of when jobs may require EXCLUSIVE reservations**
  - aprun -sl/-sn/-S
  - aprun -F exclusive
  - requesting network performance counters

Suspend & Resume w/ CLE 5.2 and later

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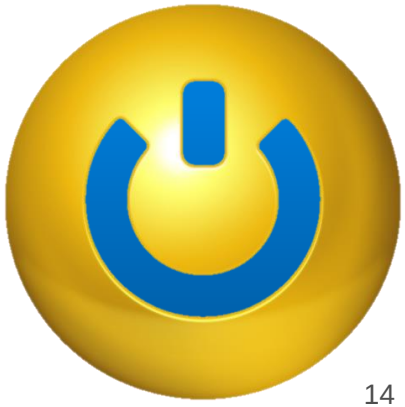
- **Preemption - Suspend and Resume**
  - PBS releases only the CPUs when a job is suspended
  - *Cray compute nodes do not have swap space, thus memory is not released*
- **Requires jobs to request non-EXCLUSIVE reservations**
  - Non-EXCLUSIVE reservations are default
  - Cray does not allow ALPS "EXCLUSIVE" reservations to be suspended
- **Configuring PBS Scheduler (PBS_HOME/sched_priv/sched_config)**
  - preemptive_sched: True All
  - preempt_order: SR
    - Don't want to requeue jobs? Remove the 'R'
  - kill -HUP <pbs_sched_pid>

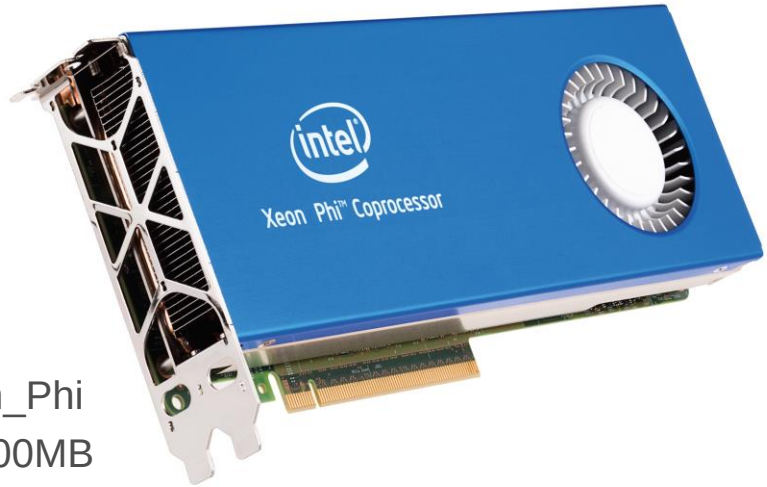


Xeon Phi Co-Processor Support

- **Automatically detects a Xeon Phi in the ALPS inventory**

- **PBS vnode attributes**
  - accelerator_model
  - accelerator_memory

- **pbsnodes output**
  - resources_available.accelerator_model=Xeon_Phi
  - resources_available.accelerator_memory=4000MB



- **Example: You want 30 PEs and a Xeon Phi accelerator on each host, and the accelerator should have at least 4000MB, and you don't care how many hosts the job uses**

-l select=30:ncpus=1:accelerator_model="Xeon_Phi”:accelerator_memory=4000MB

Hyper-Threading Support

- **PBS fully supports Cray hyper-threading**
  - Requires some additional configuration by sys admin
- **Automatic detection w/ BASIL 1.3 and later**
  - nppus
    - Total number of Physical Processing Units per vnode
  - vps_per_ppu
    - Number of virtual processors per physical processing unit
    - vps_per_ppu='1' indicates 1 virtual processor per PPU; hyperthreading off
    - vps_per_ppu='2' indicates 2 virtual processors per PPU; hyperthreading on
- **Interaction w/ batchCPCU (alps.conf)**
  - Desire hyperthreading on by default, then set batchCPCU to 0
  - Desire hyperthreading off by default, then
    - Set batchCPCU to 1
    - Set the server's default_chunk.nppus to the number of compute units per node (# of CPUS per node / # of Threads per CPU
      - qmgr -c "set server default_chunk.nppus=N"

Hyper-Threading Support, cont.

- **nppcu**
  - Number of Processors Per Compute Unit - Cray BASIL 1.3 attribute in the RESERVE XML for specifying how many processors of a compute unit should be used.
  - Value of ncpus / nppus

- **If nppus is requested and nppcu is not an integer**
  - PBS does not set nppcu in the ALPS reservation request.
  - PBS logs a message in the MoM log at level DEBUG3:
  - “The ratio of ncpus/nppus is not an integer; therefore it is not known how many processors per compute unit to request, so none were requested.”

Power-aware Scheduling

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Green Provisioning™ – Save Power, Save Money, Save the Earth

Power capping, e.g., power_budget = 0.5 MW

- Implemented via Cray's capmc
- Fit more hardware into your datacenter

Per-job power profiles, e.g., power = 600 W

- Implemented via Cray's capmc
- Run at optimal power for your workload

Energy accounting, e.g., energy = 64.2kWh

- Integrated with Cray's capmc & RUR
- Viewable in qstat and PBS accounting log
- Visualize via PBS Analytics

Power idle nodes on/off

- Coming soon

Power-aware Scheduling Demo

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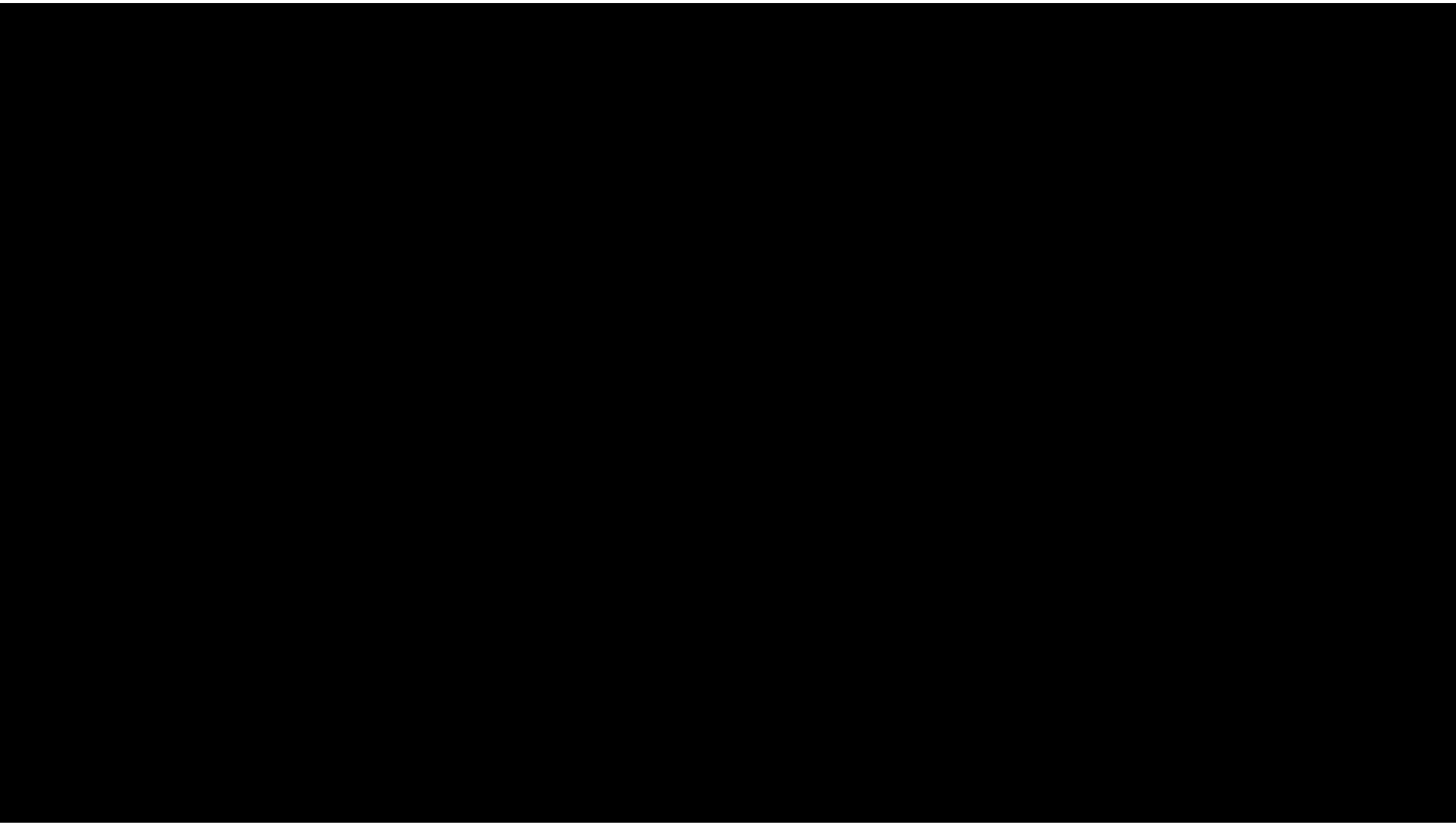

http://www.pbsworks.com/PBSSolution.aspx?v=1&i=6&n=Green-Computing

Other notable enhancements

- **Allow periodic mom hook to modify job resources on "this node”**
- **Support config file for hooks**
- **Support for cgroups on Login nodes & Repurposed Compute Nodes (MAMU nodes)**
- **New qsub -f option keeps qsub from daemonizing itself after executing**
- **Improve server/MoM inventory performance; vnode_pool, which can be used to reduce the communication traffic between server and MoMs**
  - Typically create all MoM nodes in same vnode_pool so only 1 node in pool reports inventory
- **Periodically re-query the ALPS inventory and update PBS**

PBS 13.0.401 Release

- **Merge of Cray capabilities with PBS 13.0 branch**
- **Includes all the Cray specific functionality from 12.2.404**

- **Highlights**
  - Increased job submission rates
  - Significantly shorter scheduling cycles
  - Reduced time to results

PBS Pro 13.0 – Architected for Exascale

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Speed	• 10x faster throughput
Scale	• 5x larger system sizes
Resilience	• 100% health check infrastructure
Power	• Profiles, caps, accounting
Scheduling	• Expanded priority formula, fairshare formula, and preemption targets
Plugins	• New hook events and extensions
More	• Usability, platforms, Windows, . . .

Big benefits for all PBS users – big and small

PBS Pro 13.0.400: Cray Specific Features

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Vnode Per NUMA Node Option

- Create vnode per compute node – improves scheduler performance

- This feature is available only for systems without accelerators e.g. GPUs and co-processors

PBS Pro 13.0.401: Cray Specific Features

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Adjust Reservations	• pbs_ralter – Adjust Start & End Time. Can change the end time for a running reservation with running jobs
ASAP Reservations	• Fix For Server Crash
ALPS Sync Hook	• Update Inventory Sync Hook

Roadmap: PBS Pro 13.0.402: Cray Specific Features

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Power Management

- Phase 2: Nodes On/Off

Release Expected: May 2016

Roadmap: PBS Pro 13.0.403: Cray Specific Features

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IMPS Installer	• Including support for CLE 6.0
Xeon Phi	• LA support for KNL

Released Expected: June 2016

DataWarp Preview

New Storage Aware Scheduling Capability

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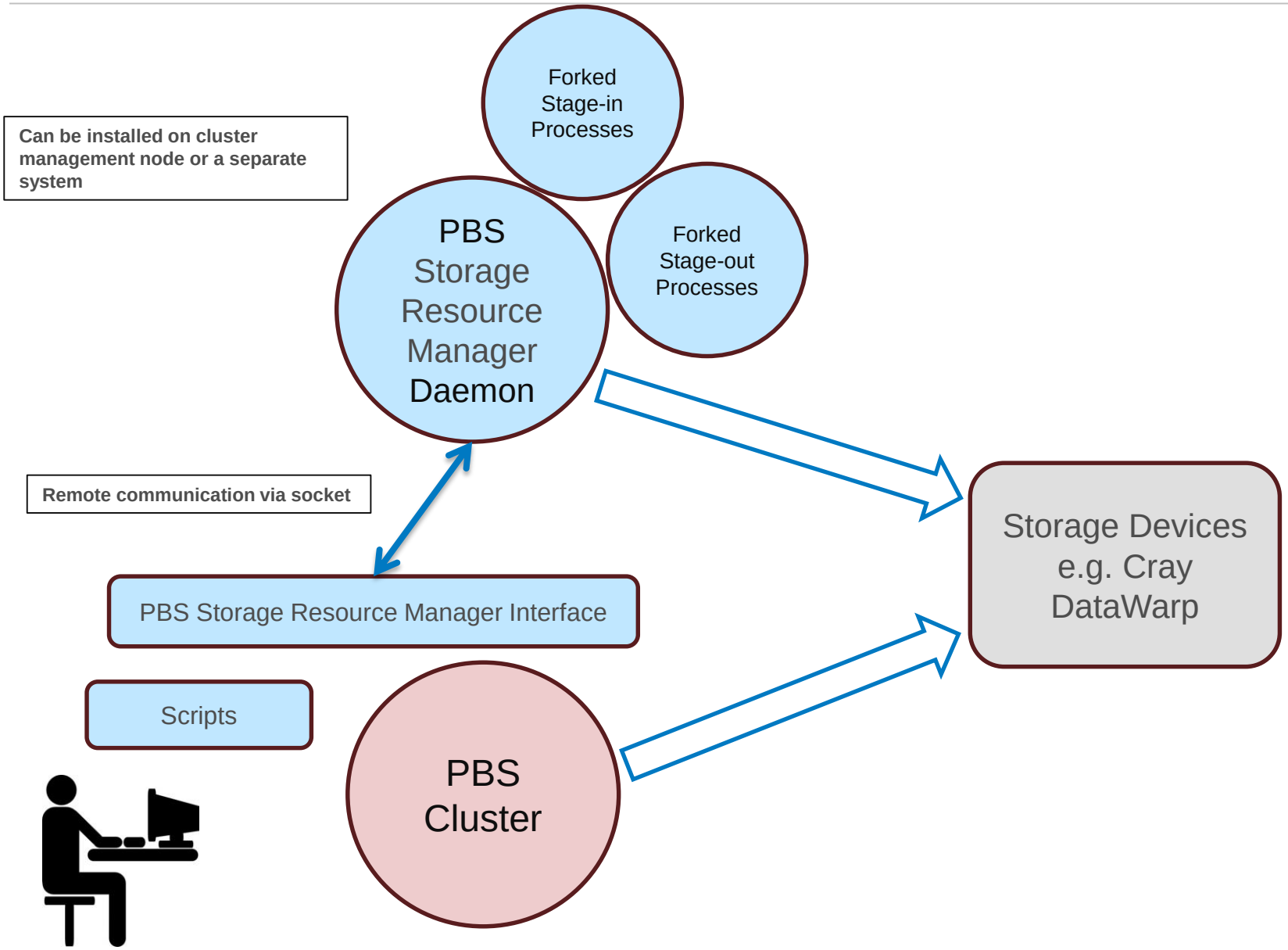
- **PBS Storage Resource Manager**
- **Centralised data management**
- **Integrated with PBS Professional to allow storage and data to influence *when* and *where* PBS runs jobs**
  - Jobs are only dispatched when associated storage and data are ready
    - E.g. enough free capacity, storage device load within limits for CPU load, network load etc
    - Optimises job throughput and execution times
- **Designed to support heterogeneous storage devices**
  - Islands of storage
  - Burst buffers
  - Multiple storage devices per jobs
- **PBS no longer responsible for data staging**
  - Avoids idle compute nodes while copying data
  - Utilisation of compute nodes is increased
- **Autonomous management and monitoring of storage devices and data entities**
  - Decouples scheduling from data management
  - Monitoring of storage device resources and limits

Benefits of PBS Storage Resource Manager

- **2 data staging models**
  - Just-in-time data staging to avoid filling up local storage
  - Immediate data staging, when jobs are submitted
- **Job dependencies are data aware**
  - Dependent jobs not dispatched until data is ready, instead of when previous job is completed
    - Support afterok, afternotok and afterany
- **Enhanced user experience**
  - User monitors job and data progress using enhanced version of qstat

Architecture



Job Submission

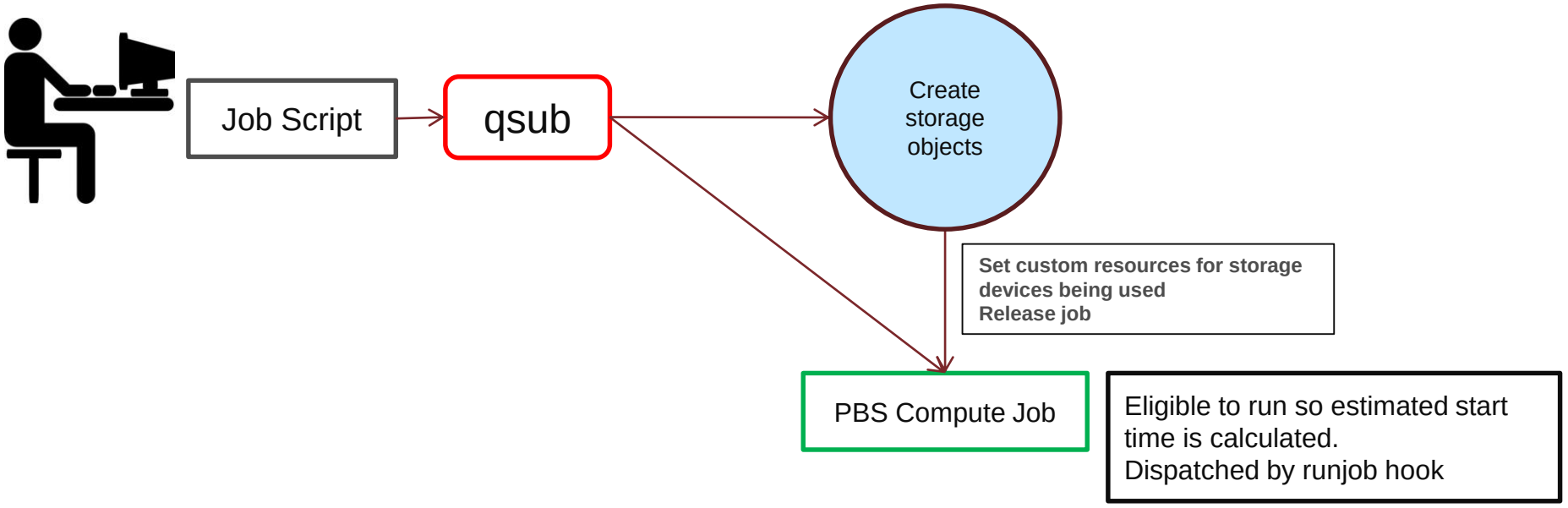
Example Cray DataWarp job script

```
#!/bin/bash

#PBS -l ncpus=128
#PBS -N test_dw_job

#DW jobdw type=scratch capacity=10GB access_mode=striped,private pfs=/scratch
#DW stage_in type=directory source=/pfs/dir1 destination=$DW_JOB_STRIPED/dir1
#DW stage_in type=list source=/pfs/inlist
#DW stage_in type=file source=/pfs/file1 destination=$DW_JOB_STRIPED/file1
#DW stage_out type=directory destination=/pfs/dir1 source=$DW_JOB_STRIPED/dir1
#DW stage_out type=list source=/pfs/inlist
#DW stage_out type=file destination=/pfs/file1 source=$DW_JOB_STRIPED/file1

aprun -n 128 -N 32 $BB_JOB_PRIVATE/abc $BB_JOB_STRIPED/abc an_app
```



Job/Data Monitoring with enhanced qstat

```
$ qstat -x

Job id                    Name             User             Time Use S Queue
----------------          ---------------- ---------------- -------- - ---
19959.server{DataComplete}  test_dw_job      graham           00:00:00 F workq
19961.server{StagingOut}    test_dw_job      graham           00:00:00 F workq
19963.server{Ready}         test_dw_job      graham           00:00:00 R workq
19970.server{StagingIn}     test_dw_job      graham                 0 Q workq
19977.server{Created}       test_dw_job      graham                 0 Q workq
```

Closing

Altair Knows HPC

Altair is the only company that

***makes* HPC tools…**

Altair | PBS Works™

***AND develops* HPC applications…**

Altair | HyperWorks®

***AND uses* these to solve real problems**

Altair | ProductDesign

700+ Altair engineers worldwide

use HPC every day

to design, simulate, and optimize highly-engineered products

For More Information

- **Stop by Altair's table**
  - Discuss Altair HyperWorks, PBS Works and other offerings
- **Visit Altair online**
  - www.altair.com
  - www.pbsworks.com
- **Contact Altair**
  - Graham Russell
  - graham.Russell@uk.altair.com

Supporting Slides

CRAY PORT: ADMINISTRATOR'S POINT OF VIEW

New PBS Resources

- **vntype**
  - Differentiate between vnode types, two are defined by default
    - cray_login – login nodes where the MOM resides
    - cray_compute – Cray execution nodes where the computational work is done
  - Admins can define new types!!
  - Users can request the vnode type during submission

- **nchunk**
  - Number of chunks; replaces default_chunk.mppwidth
  - Only for specifying default number of chunks at server and queue level (default_chunk.nchunk)
  - Can NOT be requested by a job/reservation

New PBS Resources (cont.)

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- **naccelerators**
  - Specifies the number of accelerators on a host
    - On a Cray: number of “UP” accelerators
    - Visible in pbsnodes output

- **accelerator**
  - Specifies whether an accelerator is associated with the vnode
  - Boolean Resource

    set node <nodename> resources_available.accelerator=True
  - Users can request accelerator w/ compute nodes

    qsub -l select=1:ncpus=2:accelerator=true myscript

New PBS Resources (cont.)

- **accelerator_model**
  - Automatically detected in ALPS inventory
  - Specifies the model of the accelerator
    - Example: Tesla_x2090
  - Users can request specific accelerator models

    qsub -l select=3:ncpus=2:acclerators=True:accelerator_model=”Tesla_x2090” :accelerator_memory=4000MB myscript

- **accelerator_memory**
  - Automatically detected in ALPS inventory
  - Specifies the amount of memory associated with the accelerator
  - Users can request accelerator memory

    qsub -l select=3:ncpus=2:acclerators=True:accelerator_model=”Tesla_x2090” :accelerator_memory=4000MB myscript

New Cray Custom Resources

- **PBScrayhost**
  - Used to differentiate the Cray systems
  - Enabling one instance of PBS Professional to manage multiple Cray systems
    - Requires CLE >2.2
    - If managing multiple Crays, qmgr -c “set sched do_not_span_psets=True”
  - CLE 2.2 Cray systems; PBScrayhost=default
    - **WARNING:** Do not use one instance of PBS to manage more than one Cray CLE 2.2 system because it cannot differentiate between systems
  - Users can request the PBScrayhost during submission

    qsub -l select=3:ncpus=2:PBScrayhost=examplehost

New Cray Custom Resources (cont.)

- **PBScraynid**
  - Set to the ALPS node ID
  - Visual cue for associating the PBS vnode to the Cray compute node
- **PBScrayseg**
  - Set to the ALPS NUMA node
  - Useful for the user if aprun -S, -sl, or -sn are used
- **PBScrayorder**
  - Order in which the nodes are returned in ALPS inventory (AKA NID Ordering)
  - Use node_sort_key: “PBScrayorder LOW” to match the order of the ALPS inventory

New Cray Custom Resources (cont.)

- **PBScraylabel_<label name>**
  - ALPS inventory w/ labels get automatically created!
  - Boolean Resource

    resources_available.PBScraylabel_interlagos=True

  - Users can then request or avoid this resource using True or False

    qsub -l select=3:ncpus=2:PBScraylabel_interlagos=true myscript

NOTE: It is NOT required to have labels defined via xtprocadmin.

Admins can create a custom string resource and associate a ‘label’ …

All within PBS!

Hosts and vnodes

```
george_80_0
     Mom = login1
     state = free
     pcpus = 4
     resources_available.arch = XT
     resources_available.host = george_80
     resources_available.mem = 8192000kb
     resources_available.ncpus = 4
     resources_available.PBScrayhost = george
     resources_available.PBScraynid = 80
     resources_available.PBScrayorder = 1
     resources_available.PBScrayseg = 0
     resources_available.vnode = george_80_0
     resources_available.vntype = cray_compute
     sharing = force_exclhost

george_80_1
     Mom = login1
     state = free
     pcpus = 4
     resources_available.arch = XT
     resources_available.host = george_80
     resources_available.mem = 8192000kb
     resources_available.ncpus = 4
     resources_available.PBScrayhost = george
     resources_available.PBScraynid = 80
     resources_available.PBScrayorder = 1
     resources_available.PBScrayseg = 1
     resources_available.vnode = george_80_1
     resources_available.vntype = cray_compute
     sharing = force_exclhost
```

pbsnodes -av output

1 Compute Node with 2 NUMA Nodes

pbsnodes -av: vnode name

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```
george_80_0
     Mom = login1
     state = free
     pcpus = 4
     resources_available.arch = XT
     resources_available.host = george_80
     resources_available.mem = 8192000kb
     resources_available.ncpus = 4
     resources_available.PBScrayhost = george
     resources_available.PBScraynid = 80
     resources_available.PBScrayorder = 1
     resources_available.PBScrayseg = 0
     resources_available.vnode = george_80_0
     resources_available.vntype = cray_compute
     sharing = force_exclhost
```

vnode name
- Cray Host
- ALPS Node ID
- ALPS NUMA Node #

Hosts and vnodes: state

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```
george_80_0
     Mom = login1
     state = free
     pcpus = 4
     resources_available.arch = XT
     resources_available.host = george_80
     resources_available.mem = 8192000kb
     resources_available.ncpus = 4
     resources_available.PBScrayhost = george
     resources_available.PBScraynid = 80
     resources_available.PBScrayorder = 1
     resources_available.PBScrayseg = 0
     resources_available.vnode = george_80_0
     resources_available.vntype = cray_compute
     sharing = force_exclhost
```

State of the vnode
apstat -n UP & B[ATCH]

Hosts and vnodes: Cray Custom Resources

```
george_80_0
     Mom = login1
     state = free
     pcpus = 4
     resources_available.arch = XT
     resources_available.host = george_80
     resources_available.mem = 8192000kb
     resources_available.ncpus = 4
     resources_available.PBScrayhost = george
     resources_available.PBScraynid = 80
     resources_available.PBScrayorder = 1
     resources_available.PBScrayseg = 0
     resources_available.vnode = george_80_0
     resources_available.vntype = cray_compute
     sharing = force_exclhost
```

Cray Host

ALPS Node ID

ALPS NID Ordering

ALPS NUMA Node

Hosts and vnodes: vntype

```
george_80_0
     Mom = login1
     state = free
     pcpus = 4
     resources_available.arch = XT
     resources_available.host = george_80
     resources_available.mem = 8192000kb
     resources_available.ncpus = 4
     resources_available.PBScrayhost = george
     resources_available.PBScraynid = 80
     resources_available.PBScrayorder = 1
     resources_available.PBScrayseg = 0
     resources_available.vnode = george_80_0
     resources_available.vntype = cray_compute
     sharing = force_exclhost
```

vntype

Distinguish between login, compute, etc

Hosts and vnodes: vntype

```
george_80_0
     Mom = login1
     state = free
     pcpus = 4
     resources_available.arch = XT
     resources_available.host = george_80
     resources_available.mem = 8192000kb
     resources_available.ncpus = 4
     resources_available.PBScrayhost = george
     resources_available.PBScraynid = 80
     resources_available.PBScrayorder = 1
     resources_available.PBScrayseg = 0
     resources_available.vnode = george_80_0
     resources_available.vntype = cray_compute
     sharing = force_exclhost
```

Example: Serial Workload (non-MPP resources)

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Objective: You do not want users reserving Cray MPP nodes for pre- or post-computational work, but would rather them use dedicated service nodes for this task. Which could be a mixture of external and internal login (service) nodes.

Admin Tasks:

1. Use qmgr to set the value for vntype on the vnodes representing external login nodes:

   qmgr -c “set node eslogin1 resources_available.vntype+=“cray_serial””

2. Use qmgr to add cray_serial to the vnodes representing internal login nodes:

   qmgr -c “set node login1 resources_available.vntype+=“cray_serial””

User Task:

- Submit the job

  qsub -l select=2:ncpus=2:vntype=cray_serial myscript

Example: Gating Queues Based on PEs (min/max limits)

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Objective: You are trying to gate your queues based on the total number of processing elements requested by a job.

Solution:

- Instead of: resources_min.mppwidth=8
- Use: resources_min.mpiprocs=8
- Make sure that mpiprocs can be counted for each job chunk, thus remember to set:

  qmgr –c “set server default_chunk.mpiprocs=1”

“Old” queue:

```
create queue workq
set queue workq queue_type=Execution
set queue workq resources_min.mppwidth=1
set queue workq resources_max.mppwidth=24
```

“New” queue:

```
create queue workq
set queue workq queue_type=Execution
set queue workq resources_min.mpiprocs=1
set queue workq
    resources_max.mpiprocs=24
```

CRAY PORT:
USER'S POINT OF VIEW

Requesting Job Resources – Chunks & Select

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- **A chunk is the ‘smallest’ unit of a job which can be placed on the host(s)/vnode(s)**

  Syntax: qsub -l select=[N:]chunk

- **Job requesting 3 chunks, each with 2 CPUs**

  qsub -l select=3:ncpus=2

- **Job requesting 3 chunks, each with 2 CPUs, PLUS 12 chunks, each with 1 CPU and have an accelerator**

  qsub -l select=3:ncpus=2+12:ncpus=1:accelerator=true

Requesting Job Resources – mpiprocs

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- **mpiprocs**
  - Defines the number of MPI processes for a job
  - Controls the content of the PBS_NODEFILE

- **User requesting 3 chunks, each with 2 CPUs and running 2 MPI process**

  qsub -l select=3:ncpus=2:mpiprocs=2

- **PBS_NODEFILE:**

  VnodeA
  VnodeA
  VnodeB
  VnodeB
  VnodeC
  VnodeC

Requesting Job Resources – ompthreads

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- **ompthreads**
  - pseudo-resource defining OMP_NUM_THREADS, per chunk
  - If ompthreads is not used, then OMP_NUM_THREADS is set to the value of the ncpus resource of that chunk

qsub -l select=3:ncpus=2:mpiprocs=2:ompthreads=1

PBS_NODEFILE:
VnodeA
VnodeA
VnodeB
VnodeB
VnodeC
VnodeC

The OpenMP environment variables:
For PBS task #1 on VnodeA: OMP_NUM_THREADS=1 NCPUS=1
For PBS task #2 on VnodeA: OMP_NUM_THREADS=1 NCPUS=1
For PBS task #3 on VnodeB: OMP_NUM_THREADS=1 NCPUS=1
For PBS task #4 on VnodeB: OMP_NUM_THREADS=1 NCPUS=1
For PBS task #5 on VnodeC: OMP_NUM_THREADS=1 NCPUS=1
For PBS task #6 on VnodeC: OMP_NUM_THREADS=1 NCPUS=1

Requesting Job Resources – Job Wide Resources

- **Job Wide Resources**
  - Resources that are requested outside a select statement
    - Examples: walltime, cput, …
  - Resources that are not associated to host(s)/vnode(s)

- **Job requesting 1 hour of walltime:**

  qsub -l select=3:ncpus=2 -l walltime=01:00:00 myscript

Requesting Job Resources – Job Placement

- **Users can specify how chunks are placed on vnodes using the "place" statement**

  Syntax: qsub -l select=<…> -l place= <type>| <sharing> | group=<res>

  qsub -l select=3:ncpus=2 -l place=pack myscript

Arrangement	Value	Description
type	free	place job on any vnode(s)
	pack	all chunks will be taken from one host
	scatter	only one chunk is taken from any host
	vscatter	only one chunk is take from any vnode
sharing	excl	only this job uses the vnodes chosen
	exclhost	the entire host is allocated to the job
	shared	this job can share the vnodes chosen
group	<resource>	chunks will be grouped according to a resource

Requesting Job Resources – Job Placement “Free”

- **Request:** 3 chunks, each with 2 CPUs and running 2 MPI process, and place it ‘freely’. Each host has 8 CPUs and 2 GB memory

  qsub -l select=3:ncpus=2:mpiprocs=2 -l place=free myscript

- **Variable $PBS_NODEFILE contains list of vnodes**

  vnodeA
  vnodeA
  vnodeA
  vnodeA
  vnodeA
  vnodeA

Requesting Job Resources – Job Placement “Scatter”

- **Request:** 3 chunks, each with 2 CPUs and running 2 MPI process, but evenly distribute the chunks across the vnodes (scatter). Each host has 8 CPUs and 2 GB memory

  qsub -l select=3:ncpus=2:mpiprocs=2 -l place=scatter myscript

- **Variable $PBS_NODEFILE contains list of vnodes**

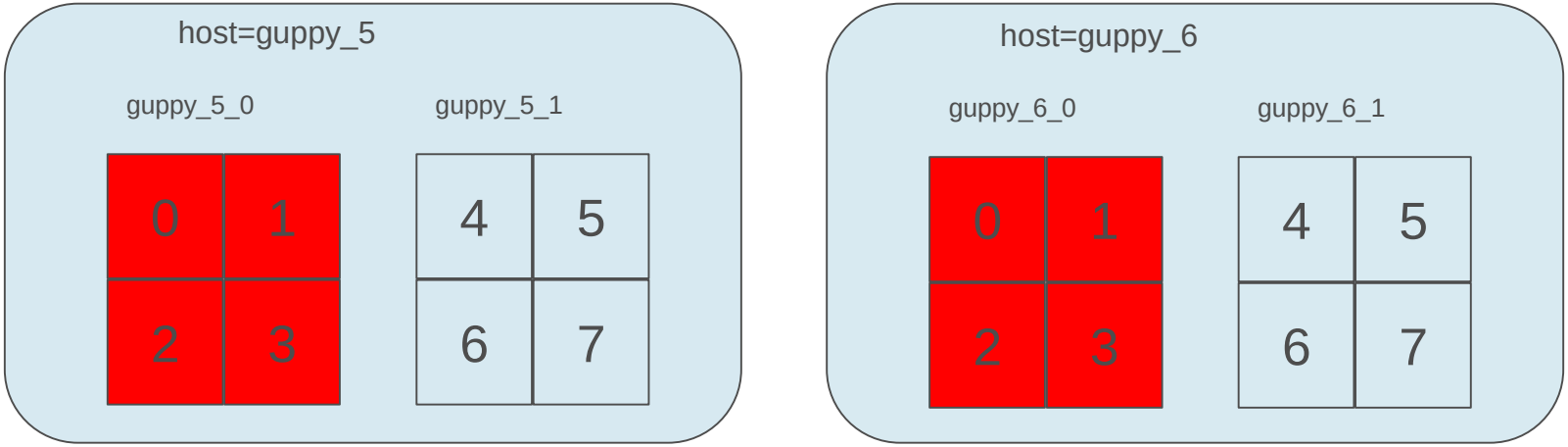
  vnodeA
  vnodeA
  vnodeB
  vnodeB
  vnodeC
  vnodeC

Job Submission & Placement: aprun -sn

Altair

Use a given number of segments

- **qsub -l select=2:ncpus=4:mpiprocs=4 –l place=scatter**



- **Corresponding aprun statement:**

  aprun -sn 1 -n 8 a.out

Job Submission & Placement: aprun -S

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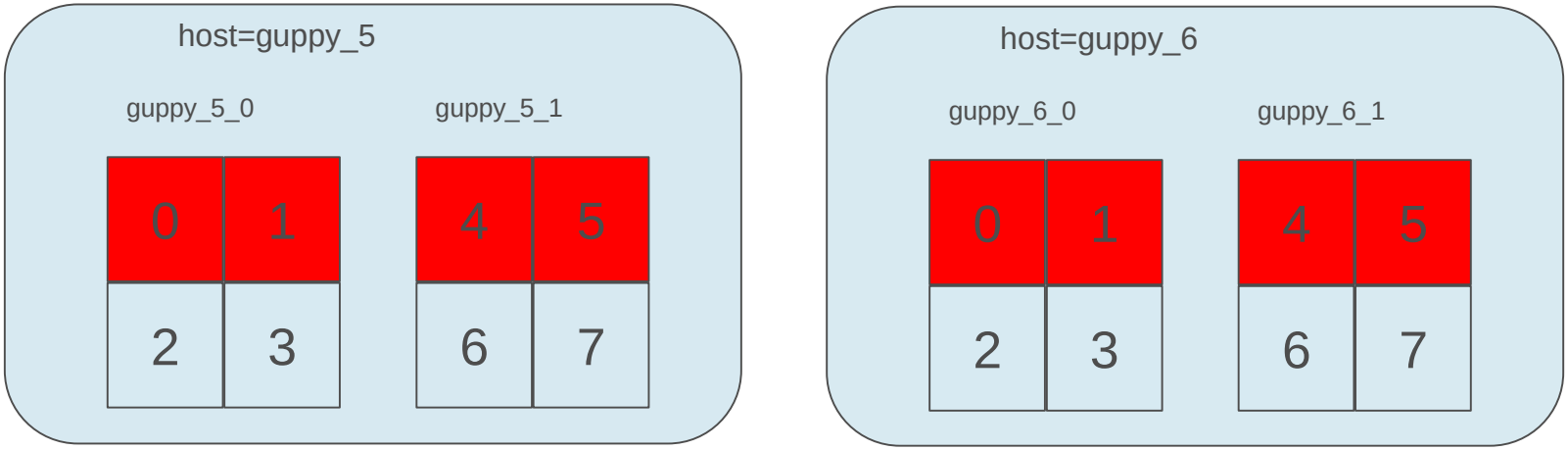
Specify the number of PEs per segment

- **qsub -l select=4:ncpus=2:mpiprocs=2 –l place=vscatter**



- **Corresponding aprun statement:**

  aprun -S 2 -n 8 a.out

Job Submission & Placement: mpp* translation

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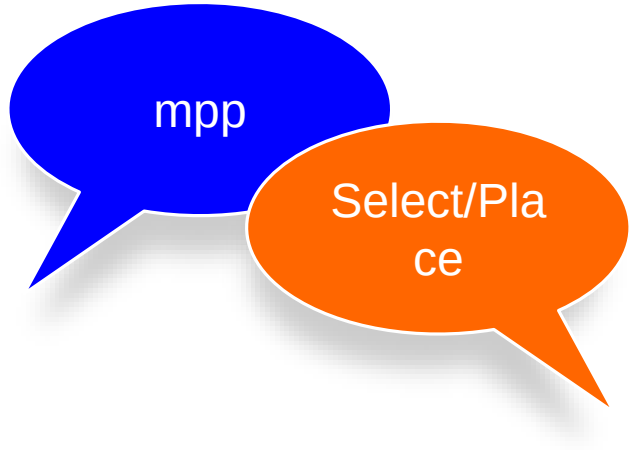
```
Job Id: 43.login1
    Job_Name = job
    [...]
    Resource_List.mppwidth = 8
    Resource_List.ncpus = 8
    [...]
    Resource_List.place = free
    Resource_List.select = 8:vntype=cray_compute
    schedselect = 8:vntype=cray_compute:ncpus=1
    [...]
    Submit_arguments = -lmppwidth=8 job
```

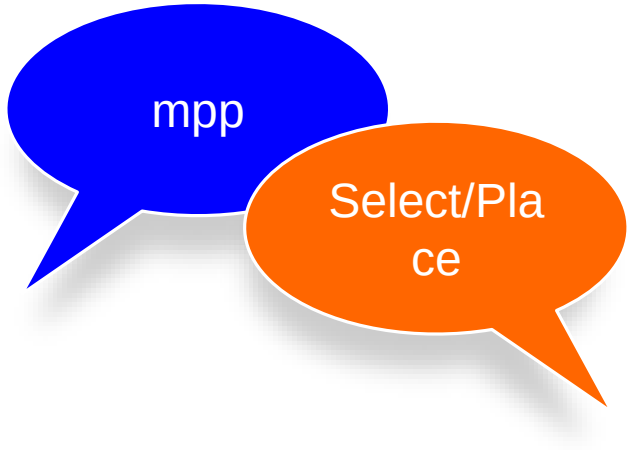


Old syntax still works;
qsub -l mppwidth=8

We also show what the command line arguments were when submitting (Submit_arguments).

Job Submission & Placement: mpp* translation

```
Job Id: 43.login1
    Job_Name = job
    [...]
    Resource_List.mppwidth = 8
    Resource_List.ncpus = 8
    [...]
    Resource_List.place = free
    Resource_List.select = 8:vntype=cray_compute
    schedselect = 8:vntype=cray_compute:ncpus=1
    [...]
    Submit_arguments = -lmppwidth=8 job
```



Automatically translated to select language

For managers, to see what the scheduler is trying to solve.
The schedselect parameter entails the union of the select specification of the job, and the queue and server defaults for resources in a chunk.

Where is my job running?

```
Job Id: 43.login1
    Job_Name = job
    Job_Owner = nishiya@login1
    [...]
    job_state = R
    queue = workq
    server = sdb
    Checkpoint = u
    ctime = Thu Jan 20 15:27:21 2011
    Error_Path = login1:/home/nishiya/test/job.e43
    exec_host = login1/0+login1/1+login1/2+login1/3+login1/4+login1/5+login1/6+login1/7+
    login1/8+login1/9+login1/10*0
    exec_vnode =
    (george_80_0:ncpus=1)+(george_80_0:ncpus=1)+(george_80_0:ncpus=1)+(george_80_0:ncpus=1)+(geo
    rge_80_1:ncpus=1)+(george_80_1:ncpus=1)+(george_80_1:ncpus=1)+(george_80_1:ncpus=1)+(george_
    81_0:ncpus=1)+(george_81_0:ncpus=1)+(george_81_1)
    [...]
    Resource_List.place = free
    Resource_List.select = 10:vntype=cray_compute
    schedselect = 10:vntype=cray_compute:ncpus=1
    [...]
    Submit_arguments = -lmppwidth=10 job
```

exec_host = Login Node, where jobscript is executed

Where is my job running? (cont.)

```
Job Id: 43.login1
    Job_Name = job
    Job_Owner = nishiya@login1
    [...]
    job_state = R
    queue = workq
    server = sdb
    Checkpoint = u
    ctime = Thu Jan 20 15:27:21 2011
    Error_Path = login1:/home/nishiya/test/job.e43
    exec_host = login1/0+login1/1+login1/2+login1/3+login1/4+login1/5+login1/6+login1/7+
    login1/8+login1/9+login1/10*0
    exec_vnode =
    (george_80_0:ncpus=1)+(george_80_0:ncpus=1)+(george_80_0:ncpus=1)+(george_80_0:ncpus=1)+(geo
    rge_80_1:ncpus=1)+(george_80_1:ncpus=1)+(george_80_1:ncpus=1)+(george_80_1:ncpus=1)+(george_
    81_0:ncpus=1)+(george_81_0:ncpus=1)+(george_81_1)
    [...]
    Resource_List.place = free
    Resource_List.select = 10:vntype=cray_compute
    schedselect = 10:vntype=cray_compute:ncpus=1
    [...]
    Submit_arguments = -lmppwidth=10 job
```

exec_vnode = NUMA Nodes, where application runs

You can see the NIDS!!

CRAY PORT: TROUBLESHOOTING

Don’t Do That!

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Do NOT use vnode configuration files to configure nodes

- This overrides the ALPS inventory node information
- Use qmgr instead

Do NOT use resources_default.mpp*

- Not translated to select/place
- See PBS Admin Guide for new defaults

Users can NOT use –lselect/place with mpp* resources

- Example: -l mppwidth=6 -l select=mem=1GB

Useful to Know for Admins

No longer have to set ncpus=128 on the login nodes (read the new install/config instructions in the Install Guide/Admin Guide)

If you use min/max, set both mpp* min/max and select/place resource min/max on systems where users submit both types of jobs

resources_max.mppwidth=8
resources_max.mpiprocs=8*
*assumes default_chunk.mpiprocs=1 is set at the server level

Remember to add any new resources to the sched_config file "resources:" line if you want the scheduler to schedule based on it

- PBScrayhost, PBScrayseg, etc.

ALPS inventory is only read at:

- MOM startup
- MOM HUP
- When an ALPS reservation is rejected by ALPS

Useful to Know for Users

Compute Node ONLY Jobs

- Using the select/place language users no longer have to request a resource on the login node

Login & Compute Node Jobs

- ***If*** you actually want a resource on a login node, please list the login node first in your resource request in order to reduce inter-MOM communication
- Example:

Qsub -l select=1:ncpus=1:vntype=cray_login+2:ncpus=2:vntype=cray_compute

Useful to Know for Users (cont.)

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Select Statement Order Matters!

qsub -l select=1:ncpus=1:vntype=cray_login+2:ncpus=2:vntype=cray_compute

qsub -l select=2:ncpus=2:vntype=cray_compute+1:ncpus=1:vntype=cray_login

PBS assigns resources left to right

- Useful for applications (e.g., CFD) which require decomposition node; make it first
- On Cray, the login node may or may NOT be the same login node where aprun is launched!
- In other words, introduce more inter-communication between PBS daemons

Admin Troubleshooting on a Cray

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Transient ALPS reservation error preparing request:

- **Look in the mom_logs:**
  - “vnode <vnode name> does not exist”
  - “vnode <vnode name> has no arch value”
  - verify the reservation PBS makes in ALPS
- **HUP the MOM to re-read ALPS inventory**

Custom resource not showing up?

- **Look in the server_logs:**
  - “error: resource <name> for vnode <name> cannot be defined”

Admin Troubleshooting on a Cray (cont.)

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Pbsnodes -av doesn't show my compute nodes:

- **Did you add the MOM vnode (i.e. login nodes) using**

  qmgr -c "c n <login node>"
- **Are the compute nodes in "batch" mode?**
  - Use xtprocadmin to verify mode

The login node shows up as "stale"

- **Does PBS list more than one vnode for the same login node?**
  - PBS will use the hostname returned by the DNS
  - Although PBS will create a vnode for aliases, those vnodes will be marked stale because the PBS server does not talk to that vnode name

User Troubleshooting on a Cray

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The job is not running on a compute node

- Did the job request vntype=cray_compute?
- Admin may want to set a default_chunk.vntype=cray_compute to help users out

The job is not running on the login node I want it to

- Did you list that login node first in the select/place request?
- Or did you use -l host with mpp* to tell it which login node to use?

The login node has some available resources but the job won't run on it

- If the job running on the login node requested -l place=excl or -l place=exclhost then the job has the login node exclusively

Supplemental Slides

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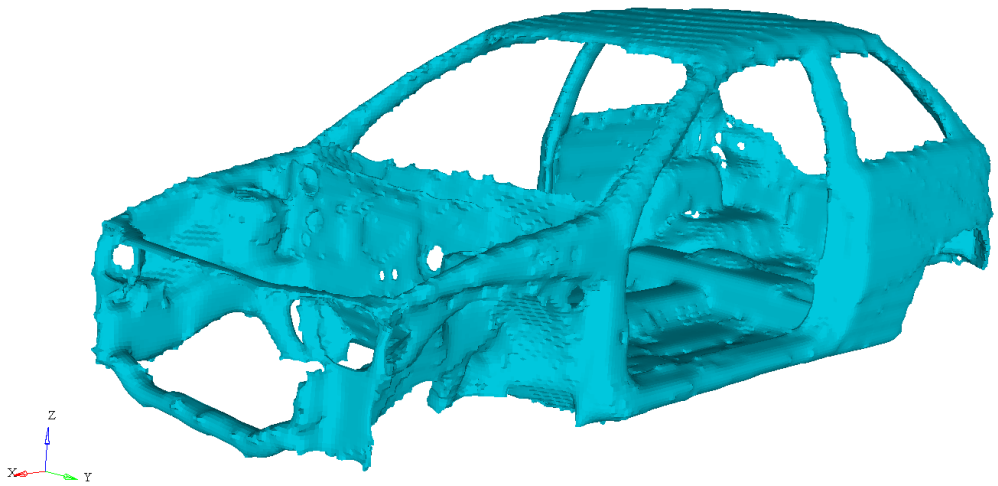

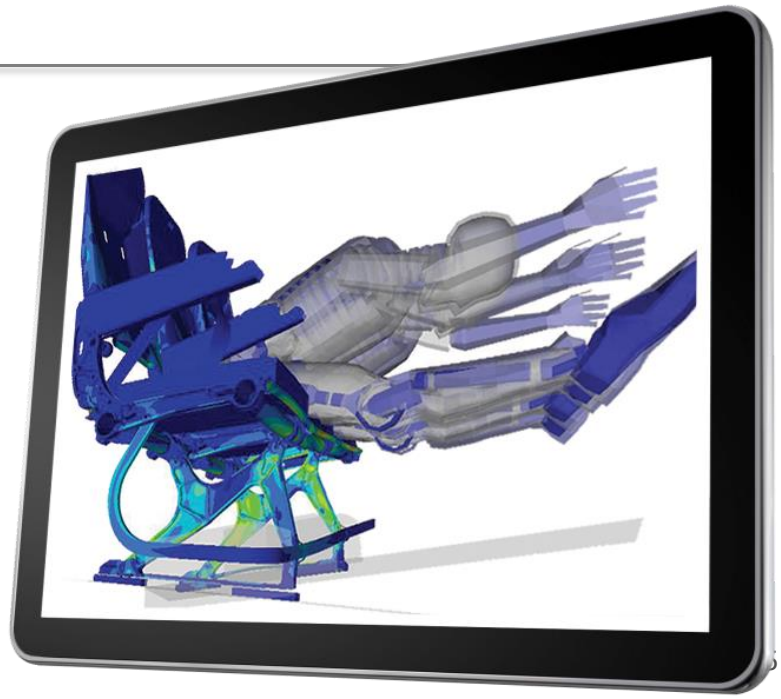

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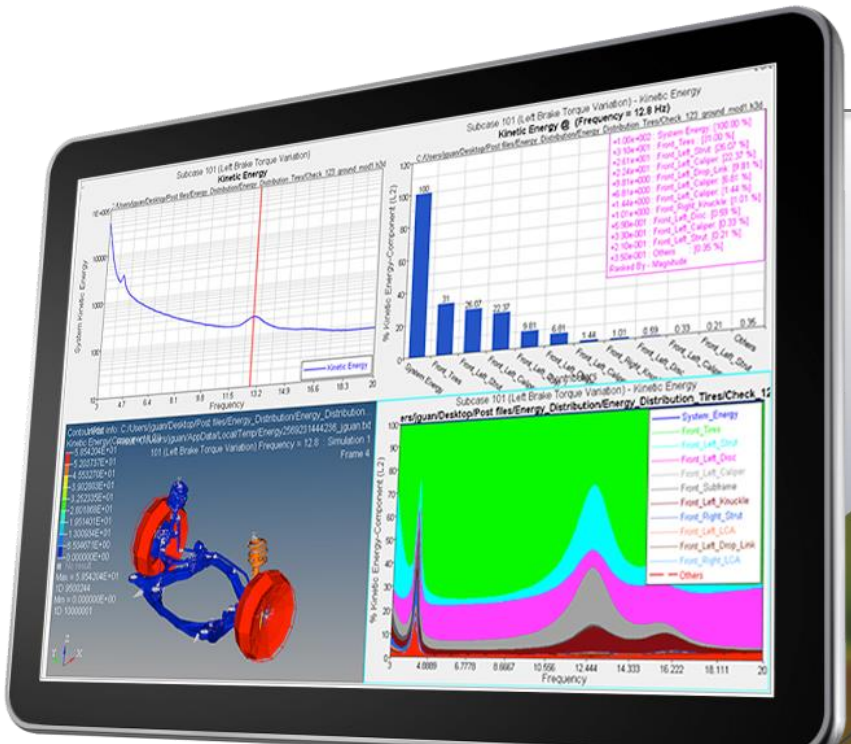

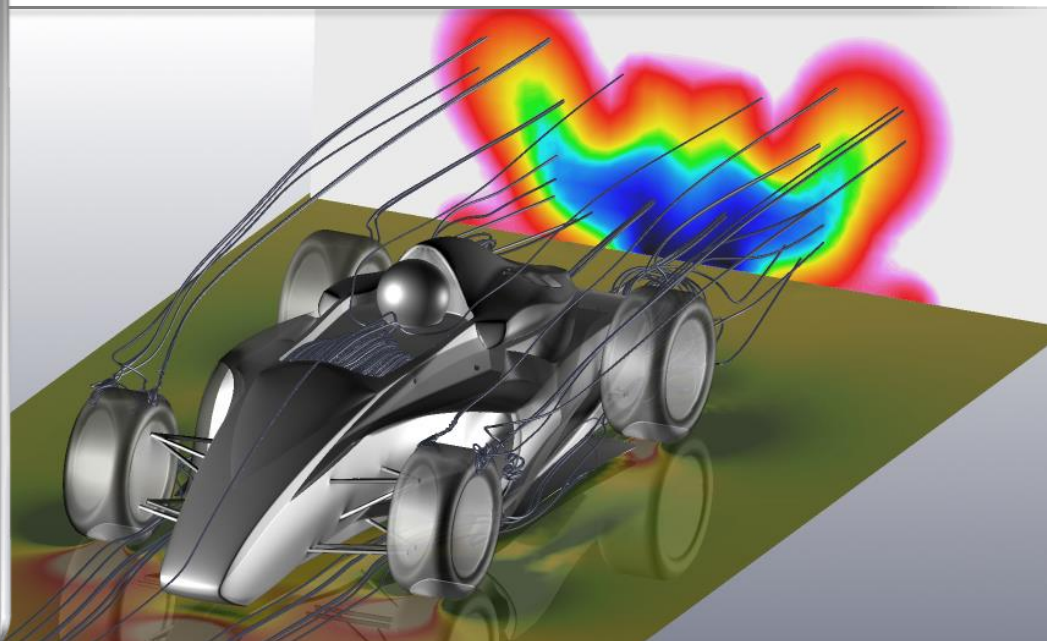

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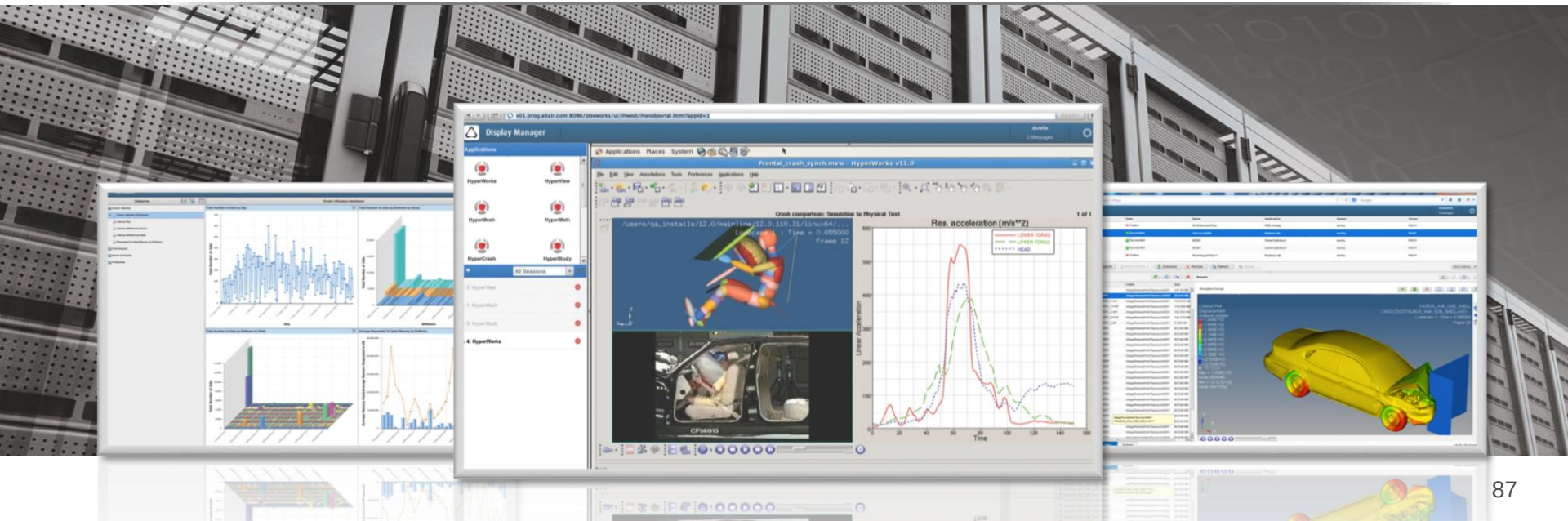

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