HTPC - High Throughput Parallel Computing (on the OSG)

> Dan Fraser, UChicago OSG Production Coordinator Horst Severini, OU (Greg Thain, Uwisc)

OU Supercomputing Symposium Oct 6, 2010

## Rough Outline

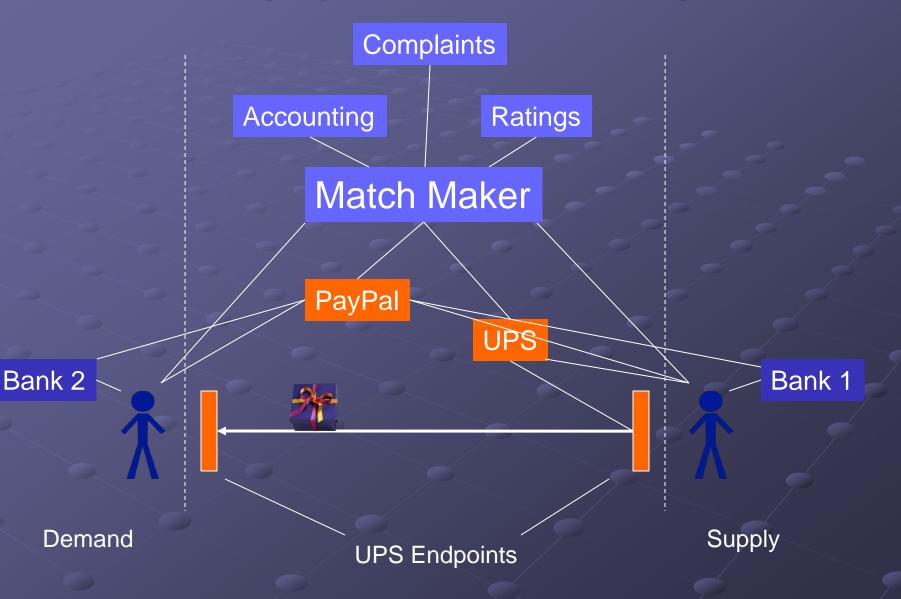
What is the OSG? (think ebay) HTPC as a new paradigm Advantages of HTPC for parallel jobs How does HTPC work? Who is using it? The Future Conclusions

Making sense of the OSG OSG = Technology + Process + Sociology 70+ sites (& growing) -- Supply contribute resources to the OSG Virtual Organizations -- Demand VO's are Multidisciplinary Research Groups Sites and VOs often overlap OSG Delivers: ~1M CPU hours every day I Pbyte of data transferred every day

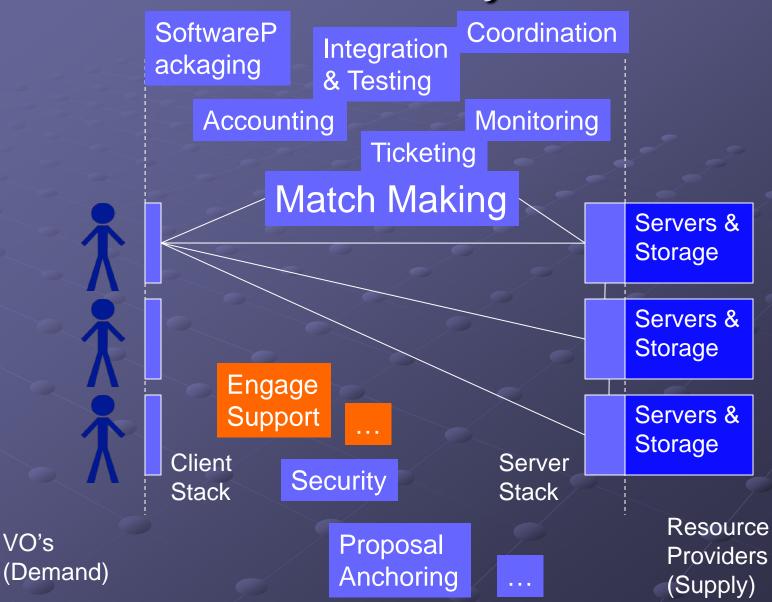




## eBay (more realistic)







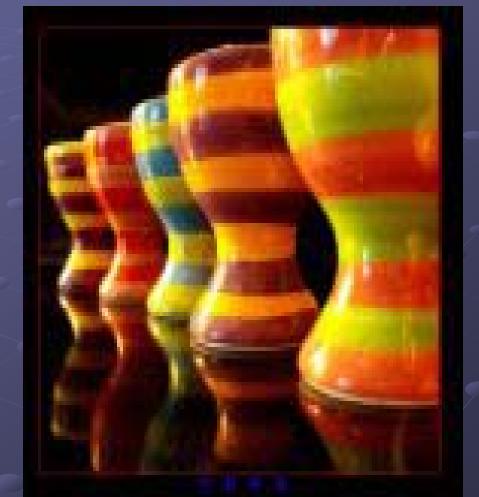
# Where does HTPC fit?

# The two familiar HPC Models High Throughput Computing (e.g. OSG) Run ensembles of single core jobs Capability Computing (e.g. TeraGrid) A few jobs parallelized over the whole system Use whatever parallel s/w is on the system

#### HTPC – an emerging model

Ensembles of smallway parallel jobs (10's – 1000's)

Use whatever parallel s/w you want © (It ships with the job)



#### **Tackling Four Problems**

Parallel job portability

Effective use of multi-core technologies

Identify suitable resources & submit jobs

Job Management, tracking, accounting, …

#### Current plan of attack

Force jobs to consume an entire processor Today 4-8+ cores, tomorrow 32+ cores, … Package jobs with a parallel library HTPC jobs as portable as any other job • MPI, OpenMP, your own scripts, ... Parallel libraries can be optimized for on-board memory access All memory is available for efficient utilization Submit the jobs via OSG (or Condor-G)

#### Problem areas

Advertising HTPC capability on OSG
 Adapting OSG job submission/mgmt tools
 GlideinWMS

 Ensure that Gratia accounting can identify jobs and apply the correct multiplier
 Support more HTPC scientists
 HTPC enable more sites

#### What's the magic RSL?

Site Specific We're working on documents/standards PBS (host\_xcount=1)(xcount=8)(queue=?) LSF (queue=?)(exclusive=1) Condor (condorsubmit=('+WholeMachine' true))

## Examples of HTPC users:

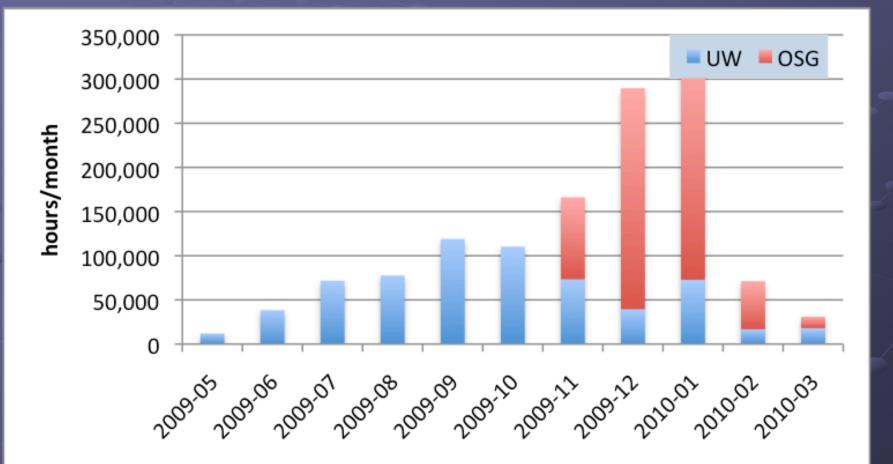
Oceanographers: Brian Blanton, Howard Lander (RENCI) Redrawing flood map boundaries ADCIRC Coastal circulation and storm surge model Runs on 256+ cores, several days Parameter sensitivity studies Determine best settings for large runs 220 jobs to determine optimal mesh size Each job takes 8 processors, several hours

## Examples of HTPC users:

Chemists
UW Chemistry group
Gromacs
Jobs take 24 hours on 8 cores
Steady stream of 20-40 jobs/day

Peak usage is 320,000 hours per month
 Written 9 papers in 10 months based on this

# Chemistry Usage of HTPC



# OSG sites that allow HTPC OU The first site to run HTPC jobs on the OSG! Purdue Clemson Nebraska San Diego, CMS Tier-2

Your site can be on this list!

#### Future Directions

More Sites, more cycles!

More users
 Working with Atlas (AthenaMP)
 Working with Amber 9
 There is room for you...

• Use glide-in to homogenize access

#### Conclusions

• HTPC adds a new dimension to HPC computing – ensembles of parallel jobs This approach minimizes portability issues with parallel codes Keep same job submission model Not hypothetical – we're already running HTPC jobs Thanks to many helping hands

#### **Additional Slides**

#### Some of these are from Greg Thain (UWisc)

#### The players

Dan Fraser Computation Inst. University of Chicago **Miron Livny U** Wisconsin John McGee RENCI Greg Thain **U** Wisconsin **Key Developer** 

Funded by NSF-STCI



## **Configuring Condor for HTPC**

Two strategies:
Suspend/drain jobs to open HTPC slots
Hold empty cores until HTPC slot is open

http://condor-wiki.cs.wisc.edu

#### How to submit

```
universe = vanilla
requirements = (CAN_RUN_WHOLE_MACHINE =?= TRUE)
+RequiresWholeMachine=true
executable = some job
arguments = arguments
should_transfer_files = yes
when_to_transfer_output = on_exit
transfer_input_files = inputs
queue
```

#### MPI on Whole machine jobs

#### Whole machine mpi submit file

universe = vanilla requirements = (CAN\_RUN\_WHOLE\_MACHINE =?= TRUE) +RequiresWholeMachine=true

# executable = mpiexec arguments = -np 8 real\_exe should\_transfer\_files = yes when\_to\_transfer\_output = on\_exit

#### transfer\_input\_files = real\_exe

queue

#### How to submit to OSG

universe = grid GridResource = some\_grid\_host GlobusRSL = MagicRSL executable = wrapper.sh

arguments = arguments

should\_transfer\_files = yes

when\_to\_transfer\_output = on\_exit

transfer\_input\_files = inputs

transfer\_output\_files = output

queue