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NATIONAL INSTITUTE FOR COMPUTATIONAL SCIENCES
NICS

Overview of Kraken

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User Support

Joint Cray XT5 Workshop
Feb 1-3 2010, Berkeley, CA

Outline

1. Basics
2. How to
3. NICS Survival Kit
4. Important Policies
5. Docs & Reference & Help
6. Q&A

1. Basics

National Institute for Computational Sciences

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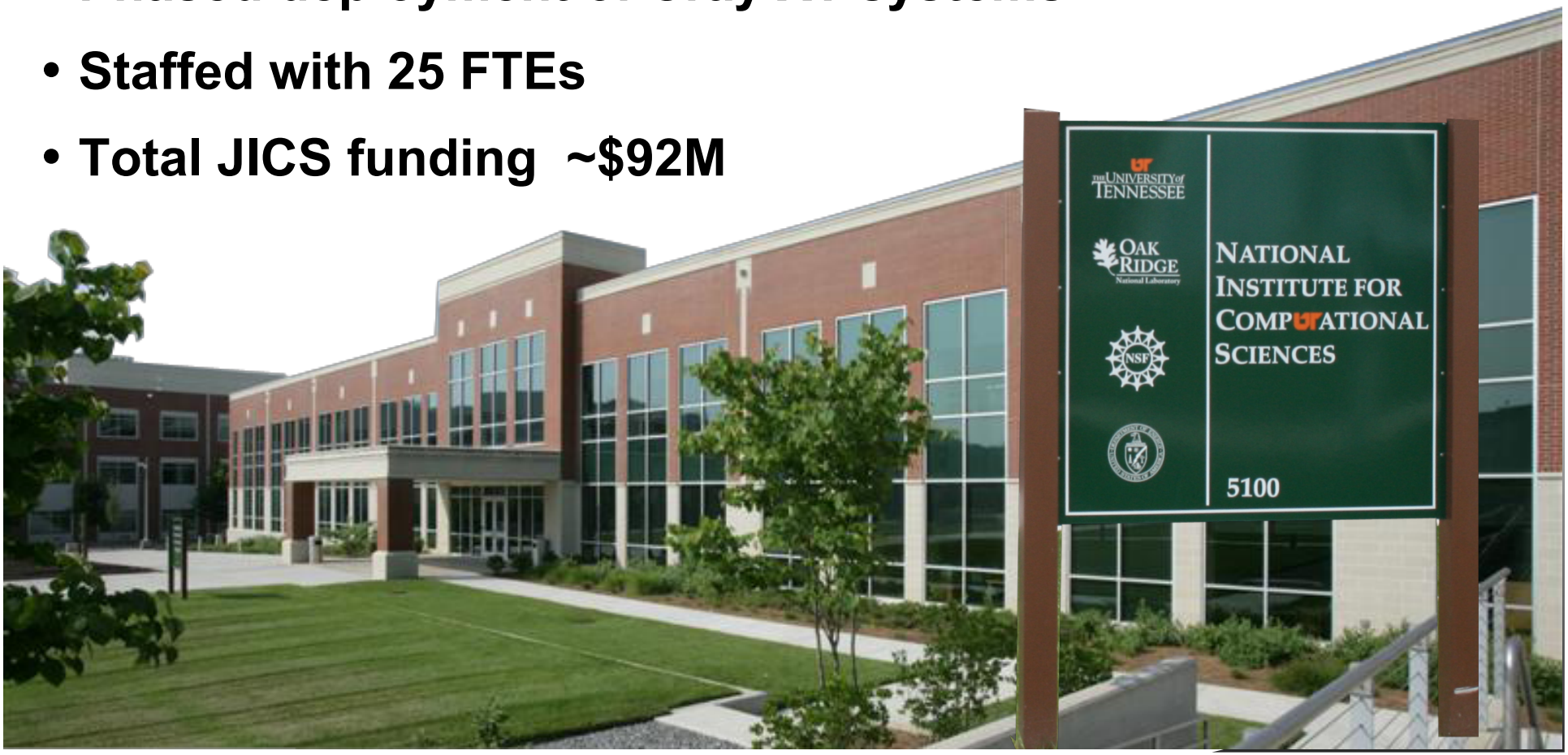
- NICS is a collaboration between UT and ORNL
- Awarded the NSF Track 2B ($65M)
- Phased deployment of Cray XT systems
- Staffed with 25 FTEs
- Total JICS funding ~$92M



Kraken's Timeline

NSF grant awarded in late '07

	XT3	XT4	Initial XT5	Final XT5
	April '08	July '08	Feb '09	Oct '09
Compute Cores	7,352	18,048	66,048	99,072
Compute Memory	7.4TB	17.6TB	100TB	129TB
# Cabinets	40	48	88	88
Peak FLOPS	38.6TF	166.5TF	608TF	1030TF
Top500 Ranking	#57	#15	#6	#3

3rd Most Powerful SuperComputer

TOP500 List - November 2009 (1-100)

R_{max} and R_{peak} values are in TFlops. For more details about other fields, check the TOP500 description.

Power data in KW for entire system

nex

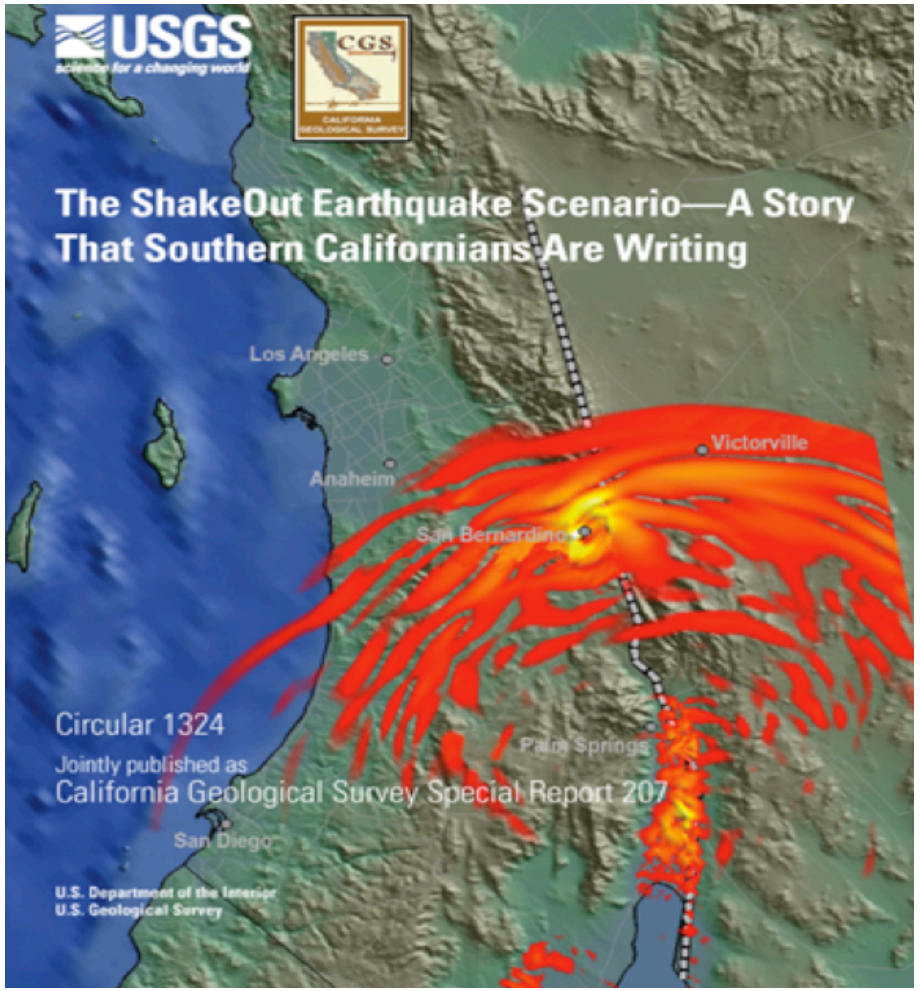
Rank	Site	Computer/Year Vendor	Cores	R_{max}	R_{peak}	Power
1	Oak Ridge National Laboratory United States	Jaguar - Cray XT5-HE Opteron Six Core 2.6 GHz / 2009 Cray Inc.	224162	1759.00	2331.00	6950.60
2	DOE/NNSA/LANL United States	Roadrunner - BladeCenter QS22/LS21 Cluster, PowerXCell 8i 3.2 Ghz / Opteron DC 1.8 GHz, Voltaire Infiniband / 2009	122400	1042.00	1375.78	2345.50
3	National Institute for Computational Sciences/University of Tennessee United States	Kraken XT5 - Cray XT5-HE Opteron Six Core 2.6 GHz / 2009 Cray Inc.	98928	831.70	1028.85	
4	Germany	IBM	294912	825.50	1002.70	2268.00
5	National SuperComputer Center in Tianjin/NUDT China	Tianhe-1 - NUDT TH-1 Cluster, Xeon E5540/E5450, ATI Radeon HD 4870 2, Infiniband / 2009 NUDT	71680	563.10	1206.19	

Largest Teragrid resource

High Performance Systems				
Name	**Institution**	**System**	***Peak TFlops***	**Memory TBytes**
Kraken	NICS	Cray XT5	1030.00	129.00
Ranger	TACC	Sun Constellation	579.40	123.00
Abe	NCSA	Dell Intel 64 Linux Cluster	89.47	9.38
Lonestar	TACC	Dell PowerEdge Linux Cluster	62.16	11.60
Steele	Purdue	Dell Intel 64 Linux Cluster	60.00	12.40
Queen Bee	LONI	Dell Intel 64 Linux Cluster	50.70	5.31
Lincoln	NCSA	Dell/Intel PowerEdge 1950	47.50	3.00
Big Red	IU	IBM e1350	30.60	6.00
Frost	NCAR	IBM BlueGene/L	22.90	2.00
BigBen	PSC	Cray XT3	21.50	4.04
Mercury	NCSA	IBM Itanium2 Cluster	10.23	4.47
Cobalt	NCSA	SGI Altix	6.55	3.00
Pople	PSC	SGI Altix 4700	5.00	1.54
NSTG	ORNL	IBM IA-32 Cluster	0.34	0.07
		Total:	**2016.35**	**314.81**

Simulating “The Big One”

- Performed the largest earthquake simulation ever on the San Andreas Fault on Kraken
- Simulated in a 32 billion grid point subset of the SCEC Community Velocity Model (CVM) V4
- Used 96,000 processor cores



Slide info courtesy of Phil Maechling, Southern California Earthquake Center

NICS

Cosmology Simulations of the Lyman Alpha Forest

- Performed the largest hydrodynamic cosmology simulation ever done on Kraken
- Used ENZO (Hybrid MPI/ OpenMP code) for current model of $4{,}096^3$ = 64 billion dark matter particles
- *"The most productive platform in NSF portfolio for ENZO simulations, bar none."*

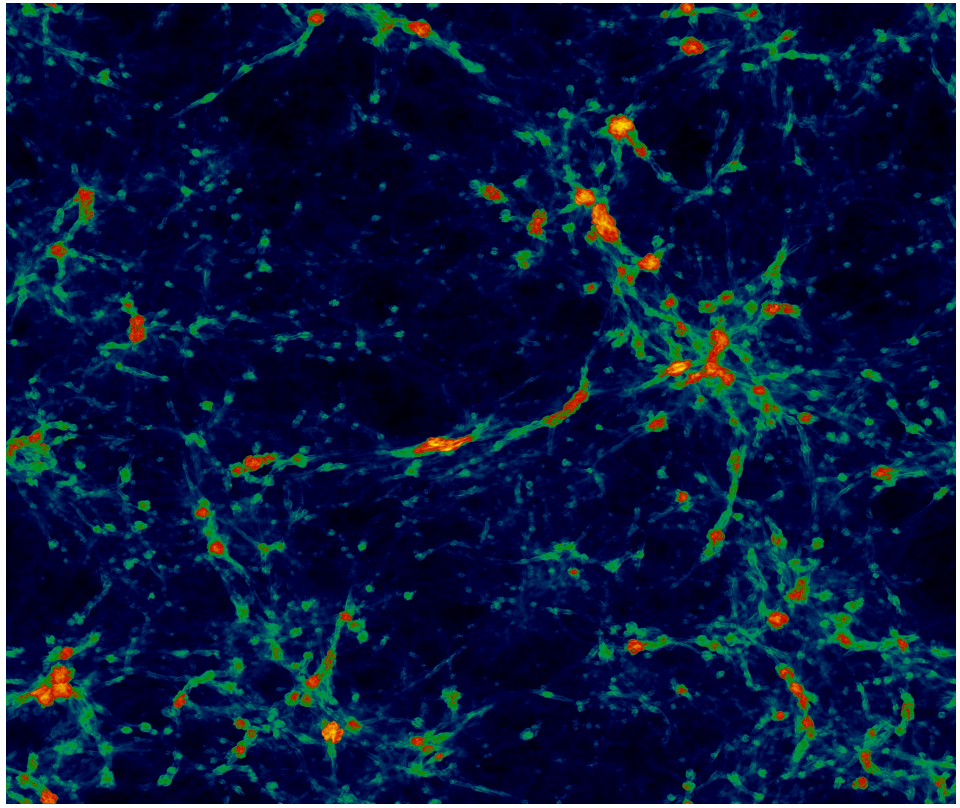
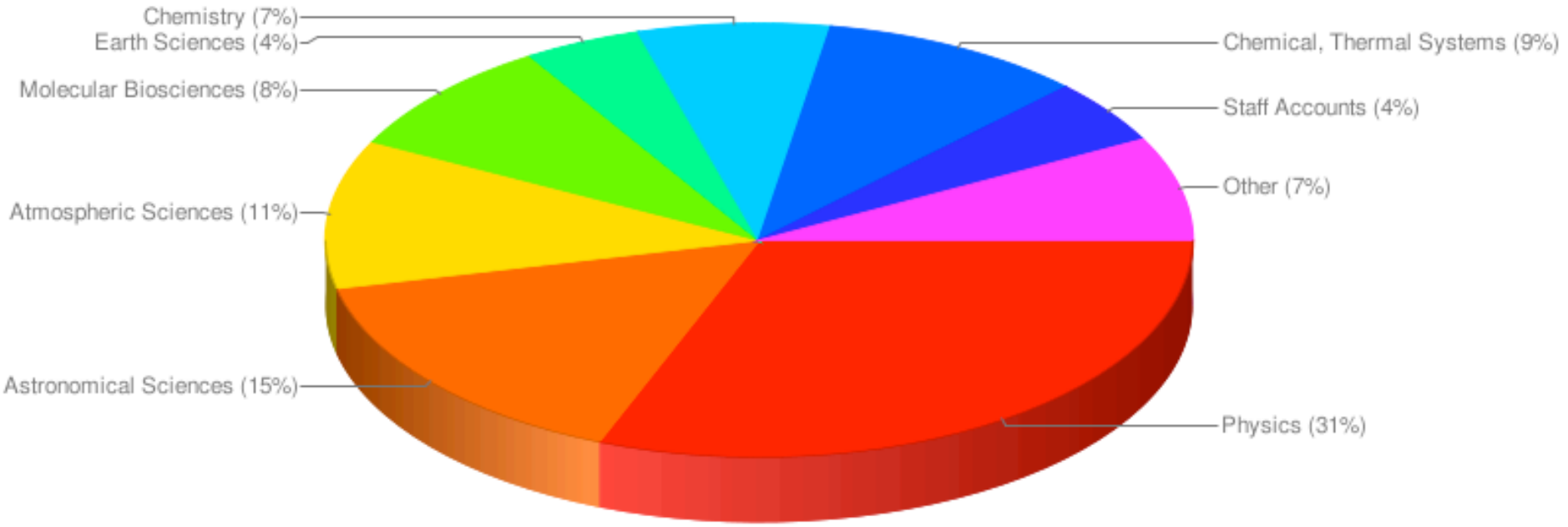


Image of the Lyman Alpha Forest showing the Baryon Acoustic Oscillation (BAO), which arises from sound waves becoming "frozen" when the matter and radiation decouple in the Big Bang.

Slide info courtesy of Robert Harkness, University of California, San Diego

Actual usage by discipline (’09)



Total Projects: 357

TG:291 + UT:66

Total Users: 1451

Active Users: ~400

Allocated 576M S.U. hours in ‘09

80% for TG – 20% for UT

Kraken System Configuration

- Cray XT5 running CNL 2.2.41
- 88 cabinets in 4 rows
- 8256 compute nodes (99,072 cores) & 96 service nodes
- 129TB of compute memory
- Two file systems available
  - NFS mounted home areas, 2TB
  - Lustre Scratch space, with 2.4PB of usable space
- 3D torus SeaStar2 interconnect.

Compute node configuration

- Two 2.6 Ghz Six-Core AMD (Istanbul) Processors
- Dual socket – 12 cores per node
- 16GB RAM per node
- Diskless nodes
- The ONLY accessible file system is Lustre scratch
- Runs a streamlined version of Linux-like OS called CLE
- Users cannot login to the compute nodes
- You need `qsub` & `aprun` to launch jobs in these nodes
- TORQUE/MOAB & ALPS control these resources

Service node configuration

- One 2.6 Ghz Dual-Core AMD Processors
- One socket – 2 cores per node
- 8GB RAM per node
- Diskless nodes
- Both NFS home areas & Lustre scratch accessible
- Runs a complete Linux-like OS called SLES10
- There are 16 login nodes
- 11 OTP only + 4 GSISSH only + 1 Experimental
- 4 GridFTP only with 10GigE internet connection
- 16 Aprun nodes & 48 I/O nodes

How to get access

You can apply for an account on Kraken in two ways:

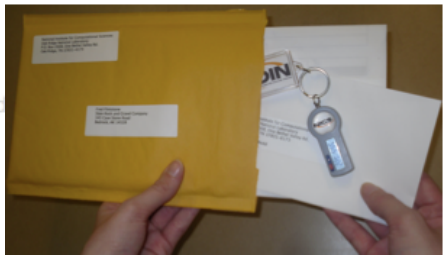
-Via a Teragrid allocation
(Four times a year proposals are reviewed)

http://www.teragrid.org/userinfo/access/dac.php

- Via a Director's Discretionary allocation
(Only for courses and workshops)

http://www.nics.tennessee.edu/user-support/request-an-account

You will receive from us a welcome package, that includes both your token and login instructions.



What do you get with your account

- A Unix account (userid and Project account)
- A One Time Password generator (token) to login via ssh
- Access through Globus Grid tools (gssissh, GridFTP)
- A NFS home area (default 2GB quota)
- Lustre scratch space (<2.4PT)
- HPSS mass storage archival via `hsi/htar` (OTP only)
- >100 applications ready to run on Kraken
- Up to 99,072 cores
- User Assistance
- Bash as default Unix shell

2. HowTo

How to login

Via SSH, BBCP using OTP

```
% ssh userid@kraken.nics.tennessee.edu
Enter PASSCODE:
```

PASSCODE = PIN + TokenCode

4 digit 6 digit

Changes every 30s

Via GSISSH

```
login3$ myproxy-logon
Enter MyProxy pass phrase:
A credential has been received for user userid in /tmp/x509up_u974.
login3$ gsissh kraken-gsi.nics.tennessee.edu
userid@kraken-pwd4(XT5):~>
```

Via GridFTP, UBERFTP

```
gsiftp://gridftp.nics.utk.edu:2811
```

HowTo use modules

- All software/packages are managed via modules
- This allows environment variables, libraries, include paths to be cleanly entered and/or removed from your software environment.
- Conflicts are detected and loads that would cause conflicts are not allowed
- There are a number of basic modules loaded by default

```
  1) modules/3.1.6.5
  2) torque/2.4.1b1
  3) moab/5.2.5.s12399
  4) /opt/cray/xt-asyncpe/default/modulefiles/xtpe-
istanbul
  5) tgusage/3.0-r2
  6) DefApps
  7) cray/MySQL/5.0.64-1.0000.2342.16.1
  8) xtpe-target-cnl
  9) xt-service/2.2.41A
 10) xt-os/2.2.41A
 11) xt-boot/2.2.41A
 12) xt-lustre-ss/2.2.41A_1.6.5
 13) cray/job/1.5.5-0.1_2.0202.18632.46.1
 14) cray/csa/3.0.0-1_2.0202.18623.63.1
 15) cray/account/1.0.0-2.0202.18612.42.3
 16) cray/projdb/1.0.0-1.0202.18638.45.1
 17) Base-opts/2.2.41A
 18) pgi/9.0.3
 19) totalview-support/1.0.5
 20) xt-totalview/8.4.1b
 21) xt-libsci/10.3.9
 22) xt-mpt/3.5.0
 23) xt-pe/2.2.41A
 24) xt-asyncpe/3.3
 25) PrgEnv-pgi/2.2.41A
 26) /sw/altd/modulefiles/altd
```

HowTo use modules

The complete list of all available modules can be viewed with the command `module avail`. The 3rd party list of software can also be viewed from our website at:

http://www.nics.tennessee.edu/user-support/software/Kraken

Loading commands

`module [load|unload] <my_module>`
Loads/unloads module

`module swap <module1> <module2>`
Replaces <module1> with <module2>

```
> module swap PrgEnv-pgi PrgEnv-gnu
```

Informational commands

`module help [my_module]`
Lists available commands and usage

`module show <my_module>`
Displays the actions upon loading the module <my_module>

`module list`
Displays all currently loaded modules

`module avail <name>`
Lists all modules (beginning with name)

HowTo compile

- Available C, C++ and Fortran compilers: PGI, GNU, Pathscale
- Use the Cray compiler wrappers `cc`, `CC` and `ftn`, to compile programs for the compute nodes.
- The compiler wrappers know where most of the correct Cray provided libraries and include files are, if the corresponding module is loaded.
- You do not need to know where the MPI libraries are.
- The wrappers automatically add the correct tuning parameters for the Istanbul Processor.
- Use module help <name> to learn what you need to manually add for 3rd party modules

HowTo compile

This example shows that a user needs to add ${SUPER_LU} to the compile line

```
lucio@krakenpf2(XT5):~> module help superlu
----------- Module Specific Help for 'superlu/4.0' ----------------
Sets up environment to use parallel SUPERLU 4.0.
Usage:   ftn test.f90 ${SUPERLU_LIB}
    or   cc test.c ${SUPERLU_LIB}
```

Example of what the wrappers do for you

```
/sw/altd/bin/ld /usr/lib64/crt1.o /usr/lib64/crti.o /opt/pgi/9.0.3/linux86-64/9.0-3/lib/trace_init.o /
usr/lib64/gcc/x86_64-suse-linux/4.1.2/crtbeginT.o -m elf_x86_64 -dynamic-linker /lib64/ld-linux-
x86-64.so.2 /opt/pgi/9.0.3/linux86-64/9.0-3/lib/pgi.ld -L/opt/mpt/3.5.0/xt/mpich2-pgi/lib -L/opt/xt-
libsci/10.3.9/pgi/lib -L/opt/mpt/3.5.0/xt/sma/lib -L/opt/mpt/3.5.0/xt/util/lib -L/opt/mpt/3.5.0/xt/pmi/
lib -L/opt/xt-pe/2.2.41A/lib -L/opt/xt-pe/2.2.41A/lib/snos64 -L/usr/lib/alps -L/opt/pgi/9.0.3/
linux86-64/9.0-3/lib -L/usr/lib64 -L/usr/lib64/gcc/x86_64-suse-linux/4.1.2 -Bstatic -rpath=/opt/xt-pe/
2.2.41A/lib -rpath=/opt/mpt/3.5.0/xt/mpich2-pgi/lib -rpath=/opt/xt-libsci/10.3.9/pgi/lib -rpath=/opt/
mpt/3.5.0/xt/sma/lib -rpath=/opt/mpt/3.5.0/xt/util/lib -rpath=/opt/mpt/3.5.0/xt/pmi/lib -lsci_istanbul
-lsma -lmpich -lrt --start-group -lpmi -lalpslli -lalpsutil -lportals -lpthread -lm --end-group -
rpath /opt/pgi/9.0.3/linux86-64/9.0-3/lib -lpgf90 -lpgf90_rpm1 -lpgf902 -lpgf90rtl -lpgftnrtl -lnspgc -
lpgc -lrt -lpthread -lm -lgcc -lgcc_eh -lc -lgcc -lgcc_eh -lc /usr/lib64/gcc/x86_64-suse-linux/4.1.2/
crtend.o /usr/lib64/crtn.o
```

How to compile

MPI Hello World example

```
/* C Example */
#include <stdio.h>
#include <mpi.h>


int main (argc, argv)
     int argc;
     char *argv[];
{
  int rank, size;

  MPI_Init (&argc, &argv);       /* starts MPI */
  MPI_Comm_rank (MPI_COMM_WORLD, &rank);    /* get current process id */
  MPI_Comm_size (MPI_COMM_WORLD, &size);    /* get number of processes */

  printf( "Hello2 world2 from process %d of %d\n", rank, size );

  MPI_Finalize();

  return 0;
}
```

```
> cc -o hello hello.c
```

How to compile

MPI Hello World example with another compiler

```
> module swap PrgEnv-pgi PrgEnv-gnu
> cc –o hello hello.c
```

MPI Hello World example with an older compiler version

```
> module swap pgi/9.0.3 pgi/7.2.5
> module swap xtpe-istanbul xtpe-barcelona
> cc –o hello hello.c
```

How to compile

Using 3rd party hdf5/1.6.7 library example

```
> module load hdf5/1.6.7
> module help hdf5/1.6.7

----------- Module Specific Help for 'hdf5/1.6.7' -----------------

Sets up environment to use serial HDF5 1.6.7 with any compiler.
Usage:  ftn test.f90 ${HDF5_FLIB}  OR  h5fc test.f90
    or   cc test.c ${HDF5_CLIB}    OR  h5cc test.c
The hdf5 module must be reloaded if you change the PrgEnv
   or you must issue a 'module update hdf5' command.
This version is deprecated and will soon be no longer available.

> cc -o myhdf5test  h5_copy18.c ${HDF5_CLIB}
```

How to run a job

Remember that the compute nodes can only access the Lustre scratch file system. Therefore all input/output files for your program must be within Lustre.
Non interactive jobs are launched with a batch job script with the help of the 'qsub' command.

Job script example

```
#PBS -A UT-NTNLEDU
#PBS -l size=12
#PBS -l walltime=00:05:00

cd $PBS_O_WORKDIR
aprun -n 4 ./hello
```

1. *Specify project account*
2. *Specify number of cores to allocate for this job. It must always be a multiple of 12*
3. *$PBS_O_WORKDIR is set to the directory from where you issued the qsub command*

HowTo run a job

Before submitting your job, make sure your current directory is somewhere in Lustre. Here is an example when it is not:

Error from submitting a job from home directory

```
lucio@krakenpf11(XT5):~> qsub /lustre/scratch/lucio/helloMPI/ hello_mpi.pbs
384515.nid00016
lucio@krakenpf11(XT5):~> ls hello_mpi.pbs*
-rw------- 1 lucio nicsstaff 104 2009-12-07 09:14 hello_mpi.pbs.e384515
-rw------- 1 lucio nicsstaff   0 2009-12-07 09:14 hello_mpi.pbs.o384515
lucio@krakenpf11(XT5):~> cat hello_mpi.pbs.e384515
[NID 16327] 2009-12-07 09:14:41 Exec ./hello failed: chdir /nics/a/home/
lucio No such file or directory
```

HowTo run a job

The scheduler will assign your job to the right queue based upon the number of cores and walltime allocated. Do not specify a queue (except for jobs that archive files).

HPSS batch script example

```
#!/bin/bash
#PBS -A TG-EXAMPLE
#PBS -l size=0
#PBS -l walltime=10:00:00
#PBS -q hpss
#PBS -W depend=afterok:123456.nid00016

cd $PBS_O_WORKDIR
hsi put file
htar cvf this_run.tar dir/
```

Batch jobs that use the `hpss` queue must request zero cores

HowTo run a job

Hello world example

```
lucio@krakenpf3(XT5):~> cd /lustre/scratch/lucio/helloMPI
lucio@krakenpf3(XT5):/lustre/scratch/lucio/helloMPI> qsub hello_mpi.pbs
384361.nid00016
lucio@krakenpf3(XT5):/lustre/scratch/lucio/helloMPI> qstat 384361
Job id                    Name             User            Time Use S Queue
------------------------- ---------------- --------------- -------- - -----
384361.nid00016           hello_mpi.pbs    lucio           00:00:00 C small
lucio@krakenpf3(XT5):/lustre/scratch/lucio/helloMPI> ls
hello  hello_mpi.c  hello_mpi.pbs  hello_mpi.pbs.e384361  hello_mpi.pbs.o384361
lucio@krakenpf3(XT5):/lustre/scratch/lucio/helloMPI> cat hello_mpi.pbs.o384361
Hello world from process 1 of 4
Hello world from process 2 of 4
Hello world from process 0 of 4
Hello world from process 3 of 4
Application 1529031 resources utime 0, stime
```

HowTo run a job

Using a 3rd party application like NAMD

```
#!/bin/bash
#PBS -A TG-DMR090083
#PBS -j oe
#PBS -m abe
#PBS -N
#PBS -l walltime=3:00:00,size=144

module load namd/2.71-09Jul21

cd $PBS_O_WORKDIR

export MPICH_PTL_SEND_CREDITS=-1
export MPICH_MAX_SHORT_MSG_SIZE=8000
export MPICH_PTL_UNEX_EVENTS=80000
export MPICH_UNEX_BUFFER_SIZE=100M

aprun -n 144 namd2 start.namd 2>&1 > start .log
```

HowTo use Lustre

Interesting facts:

- Kraken has 1.73PB of data with ~300M files
- Jaguar has 1.43PB of data with ~201M files

Configuration:

- 2.4PB of total space
- 48 OSS servers
- 7 OST per OSS (336 OSTs total)
- Peak sustained bandwidth: ~30GB/s
- Defaults: Stripe count 4, Stripe size 1MB
- Location: `/lustre/scratch/userid`

HowTo use Lustre

Best practices:

- Change your default stripe count to one! Specially if doing one file per process.
- Use stripe count of more than one only when needed.
- Use single/multiple shared files, and stripe counts multiple of 48 to get the best bandwidth
- Avoid using in Lustre: `ls -lt`
- If you need to monitor the progress, you want to use instead something like: `ls -t1 $destination | head`
- Learn to use the `lfs` command
- Visit our I/O page for more information

http://www.nics.tennessee.edu/io-tips

HowTo debug and profile

The following tools are available on Kraken for debugging, profiling and analysis parallel programs

Debugging	Profiling and Analysis
Totalview, lgdb	CrayPAT, pgprof, TAU, FPMPI, PAPI

Always check the compatibility of the compiler options you want to use. For example, the following PGI compiler options are not supported:

```
-Mprof=mpi, -Mmpi, and -Mscalapack
```

HowTo transfer & archive

There are five ways to transfer files to/from Kraken:

globus-url-copy (GridFTP)	The fastest way to transfer files to/from other (TG) systems. Can only be used with Kraken's GridFTP nodes. Requires GSI authentication. Use `gsiftp://gridftp.nics.utk.edu:2811`
Uberftp	Convenient FTP/SFTP like client, that uses the GridFTP protocol. Same requirements as 'globus-url-copy'.
BBCP	Yields much better performance than standard scp. Recommended if GridFTP is not available. *The right transfer parameters are critical for getting the best transfer rates!*
SCP (HPN)	A modified version of `scp` that uses dynamic flow control buffers which yields better transfer rates than the vanilla version that comes with OpenSSH. Available at all OTP/GSI nodes.
HSI/HTAR	Used to archive files and extract to/from the mass storage HPSS system. Only available at the OTP login nodes. *Highly desirable to bundle files together when archiving files!*

3. NICS survival kit

NICS survival kit

This is a list of Unix commands available on Kraken that all users should be aware of:

`module <command>`	All software packages like compilers, libraries and applications, are handled via modules
`qsub <jobscript>`	All jobs are submitted with the `qsub` command
`aprun -{n|N|S|d|cc}`	Programs get executed on the compute nodes with this command
`showq [-r]`	Shows the state of the queue

NICS survival kit

`qstat <jid>`	Shows the status of a job with job id `<jid>`
`glsjob <jid>`	It can be used to query information about a previous job or all previous jobs with `-u <uid>`
`showstart <jid>`	Shows approximate start time for job with job id `<jid>`
`showusage`	Displays the current balance of all the project accounts on Kraken a user has access to
`showbf`	Shows what resources are available for "immediate" use.

Other commands include: `checkjob, apstat, glsuser, glsproject`

NICS survival kit

A better/faster way to work with files in Lustre, can be done with the help of the `lfs` instead of the standard Unix commands: `ls`, `find`, `df`.

```
lfs <command> [options]
```

`setstripe/getstripe`	Used to manipulate the striping of files and directories in Lustre
`find`	A much faster way to find files in Lustre. Example: `lfs find /lustre/scratch/lucio --name *.c`
`df`	Shows how much space is left in Lustre
`quota`	Shows how much space I am using in Lustre. Example: `lfs quota -u lucio/lustre/scratch | sed -n 3p`

4. Important policies

Important Policies

- Large core count (i.e. capability) jobs have more priority
- Dedicated mode of the whole system is possible on Wednesdays
- Jobs using an account with negative balance will run only as backfill jobs
- Refunds can be provided for jobs that failed because of a system failure
- When Lustre gets 70% full we contact users to ask them to delete files. When 80% full, we will start deleting oldest files as an emergency procedure

5. Docs & Reference

More information

Cray Inc. offers most of their documentation online at

http://docs.cray.com/

Two excellent documents for new users are:

- Cray XT System Overview (S-2423-22)
- **Cray XT Programming Environment User's Guide** (S-2396-22)

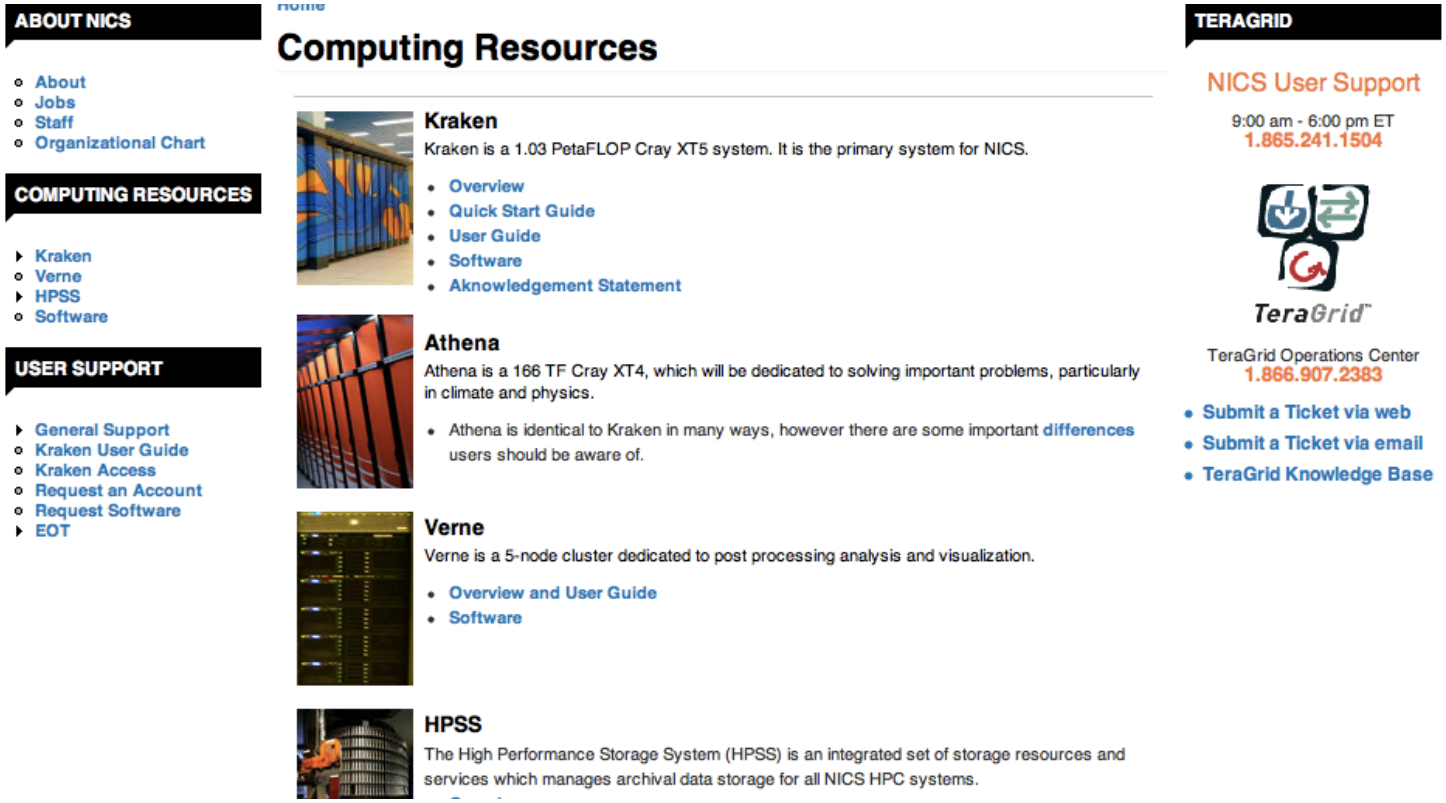
Specific information about Kraken, tools, software and FAQs can be found at:

http://www.nics.tennessee.edu/computing-resources/kraken/user-guide

Other NICS HPC resources

For more information on other NICS HPC resources, please visit

http://www.nics.tennessee.edu/computing-resources



6. Q&A

How to get help

Send your questions via email to

help@teragrid.org

Or contact us by phone

1.865.241.1504

or

to the TG helpdesk

1.866.907.2383 (off hours)