

## The Automatic Library Tracking Database

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NATIONAL INSTITUTE FOR COMPUTATIONAL SCIENCES

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## Outline

- NICS/OLCF
- Motivation for tracking library use
- Design/Implementation
- Results
- Conclusions



#### National Institute for Computational Sciences University of Tennessee

- NICS is the latest NSF HPC center
- Kraken #3 on Top 500
  - 1.030 Petaflop peak; 831.7 Teraflops Linpack

#### First academic PF





#### **Kraken XT5**



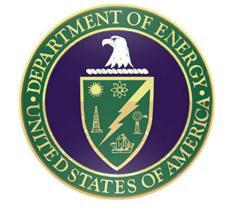
	Kraken
Compute processor type	AMD 2.6 GHz Istanbul
Compute cores	99,072
Compute sockets	16,512 hex-core
Compute nodes	8,256
Memory per node	16 GB (1.33 GB/core)
Total memory	129 TB

### Oak Ridge Leadership Computing Facility



- JaguarPF #1 on Top 500
  - 2.331 Petaflops peak, 1.759 Petaflops Linpack
- Center (40,000 ft<sup>2</sup>)









Cray User Group, May 24-27, 2010

### **JaguarPF XT5**

.

	JaguarPF	
Compute processor type	AMD 2.6 GHz Istanbul	
Compute cores	224,256	
Compute sockets	37,376 hex-core	
Compute nodes	18,688	
Memory per node	16 GB (1.33 GB/core)	
Total memory	362 TB	



## **Motivation**

#### Issues

- Centers support >100 software packages
- Supporting multiple compilers (>=3)
- Multiple versions of each library

#### Want to

- have the software users need; "stay ahead" of user requests
- change default versions as needed
- clean up; keep list of software presented to users reasonable

#### • How do

- we know when to change defaults (to newer versions)
- we know when we can get rid of old versions
- we find out who is using
  - deprecated software?
  - software with bugs?
  - software funded by NSF/DOE?



### **Software maintained on Kraken**

CTSSV4 DefApps MiscApps abinit/6.0.2 altd/1.0 amber/10 amber/9 ambertools/1.3 apache-ant/1.6.5 aprun-wrapper/0.1 apwrap/0.1(default) apwrap/0.2 arpack/2008.03.11 atk/1.24.0 atlas/3.8.3 atlas/3.8.3-fPIC-dualcore aztec/2.1 blas/ref(default) blas/ref-dualcore bugget/2.0 cairo/1.8.6 casino/2.5 cdo/1.3.2 cdo/1.4.1 charm++/6.1.3 cmake/2.6.4(default) cmake/2.8.0 condor/7.0.4-r1 cpmd/3.13.2 desmond/2.2.7.3\_dbl desmond/2.2.7.3\_sngl espresso/2.1.0gnu(default) espresso/2.1.0pgi espresso/2,1,2,j-gnu espresso/2,1,2j-pgi ferret/6.1 fftpack/5-r4i4 fftpack/5-r8i4 fftpack/5-r8i8 fftw/2.1.5 fftw/2.1.5-dualcore

fftw/3.1.2 fftw/3.1.2-dualcore fftw/3.3 alpha fpmpi/1.1 fpmpi\_papi/1.1 fsplit/1.0 gamess/2008Mar04 gamess/2009Jan12 odlib/2.0.35 gempak/5.11.4 ghostscript/8.64(default) gimp/2.6.4 git/1.6.4.3 glib/2.18.3 globalarrays/4.1.1 globus/4.0.8 omake/3.81 gnuplot/4.2.6(default) gpt1/3.5(default) grace/5.1.21 grads/2.0.a7.1 gromacs/4.0.5 gromacs/4.0.7(default) gromacs/4.0.7\_fprelaxed osl/1.13 gsl/1.13-dualcore gtk/2.14.6 gv/3.6.8 hdf4/4.2r4 hdf5/1.6.10 hdf5/1.8.3 hdf5/1.8.4 hdf5-parallel/1.6.10 hdf5-parallel/1.8.3 hdf5-parallel/1.8.4 hypre/2.0.0 imagemagick/6.5.3 imagemagick/6.6.1(default) iobuf/beta java-jdk/1.5.0.06 java-jdk/1.6.0.06

/sw/xt/modulefiles -.java-.jre/1.5.0.06 lammps/Jan10 lammps/Mar09(default) lammps/Oct09 lapack/3.1.1(default) lapack/3.1.1-dualcore lapack/3.1.1-fPIC libart/2.3.19 marmot/2.3.0 mercurial/1.3 metis/4.0.1 mpe2/1.0.6 mpip/3.1.2 mumps/4.7.3\_par mumps/4.9.2 par namd/2.6namd/2.7b1 namd/2.7b1-09Jul21 namd/2.7b2 nano/2.0.9 nc1/5.0.0 nc1/5.0.0\_source nco/3.9.9 nco/4.0.0 ncview/1.939 nedit/5.5 netcdf/3.6.2 netcdf/3.6.3 netcdf/4.1 netcdf-parallel/4.1 numpy/1.3.0 nwchem/5.1 p-netcdf/1.0.3 p-netcdf/1.1.1 pacman/3.26-r1 pango/1.20.5 parmetis/3.1 petsc/2.3.3-debug petsc-complex/2.3.3-debug pgplot/5.2 pixman/0.13.2

pspline/1.0 python/2.5.2 python/2.6.4(default) puthon/3.1.1 q-espresso/4.1.2 qbox/1.47 abox/1.50 qt/4.3.4 qt/4.5.2 ruby/1.9.1 scalasca/1.1 scalasca/1.2(default) sprng/2.0b srb-client/3.4.1-r3(default) subversion/1.4.6(default) subversion/1.5.0 subversion/1.6.9 sundials/2.3.0 superlu/3.1 superlu/4.0 superlu\_dist/2.3 swig/1.3.36 szip/2.1 tau/2.19(default) tg-policy/0.2-r1 tginfo/1.1.0-r1 tgusage/3.0-r2(default) tiff/3.8.2 tkdiff/4.1.4 totalview/8.6.0-1 totalview/8.7.0-1(default) trilinos/10.0.2 trilinos/9.0.3 udunits/1.12.9 udunits/2.1.13 umfpack/5.1.1 umfpack/5.4.0 upc/2.8.0 valgrind/3.4.1 valgrind/3.5.0 vim/7.2(default)



### **Objective**

- Track libraries that are linked into executables
- Track executables run (and by inference) how often are the libraries used?
  - Of course, not necessarily true



## **Assumptions/Requirements**

- Must support statically linked executables – Shared library support desirable as well
- Have as little impact on user as possible
  - Lightweight solution
    - No runtime increase
    - Only link time and job launch have marginal increase in time
  - Do not change user experience
    - Linker and job launcher work as expected
- Tracking libraries
  - Not function calls
- Only libraries actually linked into executable



## Design

- Wrap binutils "Id" and job launcher "aprun"
  - This allows us to track libraries at link time
  - This allows us to track executables that we can tie back to the actually link and thus the libraries

#### • Id - Intercept link line

- Update tags table
- Create altd.o to link into executable
- Call real linker (with tracemap option)
- Use output from tracemap to find libraries linked into executable
- Update linkline table
- (Could stop here)
- aprun- Intercept job launcher
  - Pull information from altd section header in executable
  - Update jobs table
  - Call real job launcher



### altd.o

Assembly code inserted into binaries

```
.section .altd
.asciz "ALTD_Link_Info"
.byte 0x00, 0x00, 0x00, 0x00, 0x00, 0x00, 0x00
.asciz "Version:0.7:"
.asciz "Machine:athena:"
.asciz "Tag_id:38:"
.asciz "Year:2009:"
.byte 0x00, 0x00, 0x00, 0x00, 0x00, 0x00, 0x00
.asciz "ALTD_Link_Info_End"
```



## **MySQL** database

#### • 3 tables: tags, linkline, and jobs

- Tags entry for every link executed
  - Id wrapper does 2 steps
    - First pass, entry added to include user name, date stamp
    - On the final pass of the Id wrapper, previous entry is updated with the linkline table "id"
  - This gives first count of library usage => # times used in link
- Linkline entry for each unique link line
  - Inserted if new on 2<sup>nd</sup> pass of Id wrapper
- Jobs entry for each executable launched
  - The "tag id" and "build machine" is pulled from the binary and stored
  - This table gives us another way to count library "usage"
    - Usage => how many times code was run



## tags table

tag_id	linkline_id	username	exit_code	link_date
91126	14437	user1	0	2010-04-28
91127	0	user2	-1	2010-04-28
91128	14435	user3	0	2010-04-28
91129	6835	user2	0	2010-04-28
91130	14438	user4	0	2010-04-28
91131	14439	user1	0	2010-04-28
91132	14439	user1	0	2010-04-28



## linkline table

linkline _id	linkline
14437	/bin/cg.B.4 /usr/lib//lib64/crt1.o /usr/lib//lib64/crti.o /opt/gcc/4.4.2/snos/lib/gcc/x86_64-suse-linux/4.4.2/crtbeginT.o /sw/xt/tau/2.19/cnl2.2_gnu4.4.1/tau-2.19/craycnl/lib/libTauMpi-gnu-mpi-pdt.a /sw/xt/tau/2.19/cnl2.2_gnu4.4.1/tau-2.19/craycnl/lib/libtau-gnu-mpi-pdt.a /usr/lib//lib64/libpthread.a /opt/cray/mpt/4.0.1/xt/seastar/mpich2-gnu/lib/libmpich.a /opt/cray/pmi/1.0-1.0000.7628.10.2.ss/lib64/libpmi.a /usr/lib/alps/libalpslli.a /usr/lib/alps/libalpsutil.a /opt/xt-pe/2.2.41A/lib/snos64/libportals.a [ gcc 4.4.2 libraries] /usr/lib//lib64/libc.a /usr/lib//lib64/crtn.o
14438	highmass3d.Linux.CC.ex /usr/lib64/crt1.o /usr/lib64/crti.o /opt/pgi/9.0.4/linux86-64/9.0-4/lib/trace_init.o /usr/lib64/gcc/x86_64-suse-linux/4.1.2/crtbeginT.o /sw/xt/hypre/2.0.0/cnl2.2_pgi9.0.1/lib/libHYPRE.a /opt/cray/pmi/1.0-1.0000.7628.10.2.ss/lib64/libpmi.a /usr/lib/alps/libalpslli.a /usr/lib/alps/libalpsutil.a /opt/xt-pe/2.2.41A/lib/snos64/libportals.a /usr/lib64/libpthread.a /usr/lib64/libm.a /usr/local/lib/libmpich.a [ pgi 9.0.4 libraries] /usr/lib64/librt.a /usr/lib64/libpthread.a /usr/lib64/libm.a /usr/lib64/librt.a /usr/lib64/libpthread.a /usr/lib64/libm.a /usr/lib64/librt.a /usr/lib64/libpthread.a /usr/lib64/libm.a
14439	probeTest /usr/lib//lib64/crt1.o /usr/lib//lib64/crti.o /opt/gcc/4.4.2/snos/lib/gcc/x86_64-suse-linux/4.4.2/crtbeginT.o /opt/cray/mpt/4.0.1/xt/seastar/mpich2-gnu/lib/libmpich.a /opt/cray/pmi/1.0-1.0000.7628.10.2.ss/lib64/libpmi.a /usr/lib/alps/libalpslli.a /usr/lib/alps/libalpsutil.a /opt/xt-pe/2.2.41A/lib/snos64/libportals.a /usr/lib//lib64/libpthread.a [ gcc 4.4.2 libraries] /usr/lib//lib64/libc.a /usr/lib//lib64/crtn.o



## jobs table

run_inc	tag_id	executable	usern ame	run_date	job_launc h_id	build_ma chine
144091	91126	/nics/b/home/user1/ NPB3.3/bin/cg.B.4	user1	2010-04-28	548346	kraken
144099	91131	/nics/b/home/user1/ probeTest	user1	2010-04-28	548357	kraken
144102	91132	/nics/b/home/user1/ probeTest	user1	2010-04-28	548357	kraken
144179	91128	/lustre/scratch/user3/CH4/ vasp_vtst.x	user3	2010-04-28	548444	kraken
144192	91128	/lustre/scratch/user3/CH4/ vasp_vtst.x	user3	2010-04-28	548488	kraken
144356	91128	/lustre/scratch/user5/src/ CH4/vasp_vtst.x	user5	2010-04-29	548638	kraken



	+		
14437	/bin/cg.B.4 /usr/lib//lib64/crt1.o /usr/lib//lib64/crt1.o		
	<pre>//opt/gcc/4.4.2/snos/lib/gcc/x86_64-suse-linux/4.4.2/crtbeginT.o</pre>		
	<pre>//sw/xt/tau/2.19/cnl2.2_gnu4.4.1/tau-2.19/craycnl/lib/libTauMpi-gnu-mpi-pdt.a</pre>		
	<pre>//sw/xt/tau/2.19/cn12.2_gnu4.4.1/tau-2.19/craycn1/lib/libtau-gnu-mpi-pdt.a /usr/lib//lib64/libpthread.a</pre>		
	<pre>//opt/cray/mpt/4.0.1/xt/seastar/mpich2-gnu/lib/libmpich.a /opt/cray/pmi/1.0-1.0000.7628.10.2.ss/lib64/libpmi.a  </pre>		
	<pre>//usr/lib/alps/libalpslli.a /usr/lib/alps/libalpsutil.a /opt/xt-pe/2.2.41A/lib/snos64/libportals.a</pre>		
	<pre>//opt/gcc/4.4.2/snos/lib/gcc/x86_64-suse-linux/4.4.2/libgfortranbegin.a</pre>		
	//opt/gcc/4.4.2/snos/lib/gcc/x86_64-suse-linux/4.4.2/libgcc.a [		
	<pre>//opt/gcc/4.4.2/snos/lib/gcc/x86_64-suse-linux/4.4.2/libgcc_eh.a /usr/lib//lib64/libc.a</pre>		
	<pre>//opt/gcc/4.4.2/snos/lib/gcc/x86_64-suse-linux/4.4.2/crtend.o /usr/lib//lib64/crtn.o</pre>		
	I I I	a)	
14438	highmass3d.Linux.CC.ex /usr/lib64/crt1.o /usr/lib64/crt1.o /opt/pgi/9.0.4/linux86-64/9.0-4/lib/trace_init.o	,	
	<pre>//usr/lib64/gcc/x86_64-suse-linux/4.1.2/crtbeginT.o /sw/xt/hypre/2.0.0/cnl2.2_pgi9.0.1/lib/libHYPRE.a</pre>		
	<pre>//opt/cray/pmi/1.0-1.0000.7628.10.2.ss/lib64/libpmi.a /usr/lib/alps/libalpslli.a /usr/lib/alps/libalpsutil.a</pre>		
$\mathbf{A}$	<pre>//opt/xt-pe/2.2.41A/lib/snos64/libportals.a /usr/lib64/libpthread.a /usr/lib64/libm.a</pre>		
	<pre>//usr/local/lib/libmpich.a /opt/pgi/9.0.4/linux86-64/9.0-4/lib/libstd.a /opt/pgi/9.0.4/linux86-64/9.0-4/lib/libC.a/</pre>		
	<pre>//opt/pgi/9.0.4/linux86-64/9.0-4/lib/libpgf90.a /opt/pgi/9.0.4/linux86-64/9.0-4/lib/libpgc.a /</pre>		
	<pre>//usr/lib64/librt.a /usr/lib64/libpthread.a /usr/lib64/libm.a /usr/lib64/gcc/x86_64-suse-linux/4.1.2/libgcc_eh.a  </pre>		
	<pre>//usr/lib64/libc.a /usr/lib64/gcc/x86_64-suse-linux/4.1.2/crtend.o /usr/lib64/crtn.o</pre>		
14439	probeTest /usr/lib//lib64/crt1.o /usr/lib//lib64/crti.o		
	/opt/gcc/4.4.2/snos/lib/gcc/x86 64-suse-linux/4.4.2/crtbeginT.o		
	/opt/cray/mpt/4.0.1/xt/seastar/mpich2-qnu/lib/libmpich.a /opt/cray/pmi/1.0-1.0000.7628.10.2.ss/lib64/libpmi.a		
	/usr/lib/alps/libalpslli.a /usr/lib/alps/libalpsutil.a /opt/xt-pe/2.2.41A/lib/snos64/libportals.a		
	/usr/lib//lib64/libpthread.a /opt/gcc/4.4.2/snos/lib/gcc/x86 64-suse-linux/4.4.2/libgcc eh.a		
	//usr/lib//lib64/libc.a /opt/gcc/4.4.2/snos/lib/gcc/x86 64-suse-linux/4.4.2/crtend.o /usr/lib//lib64/crtn.o		

- 1

a) Linkline table

run_inc	tag_id	executable	username	-		build_machine
144091	91126	/nics/b/home/user1/NPB3.3/bin/cg.B.4	user1	2010-04-28	548346	kraken
144099	91131	/nics/b/home/user1/probeTest	user1	2010-04-28	548357	kraken
144102	91132	/nics/b/home/user1/probeTest	user1	2010-04-28	548357	kraken
		<pre>/lustre/scratch/user3/CH4/vasp vtst.x</pre>	user3	2010-04-28	548444	kraken

14437 | user1 0 | user2

14435 | user3

6835 | user2

14438 | user4

L4439

91126

91127 |

91128 |

91129 |

91130

91131

T

L

c) job\_id table

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<mark>0 | 2010-04-28 |</mark> -1 | 2010-04-28 |

0 | 2010-04-28 |

0 | 2010-04-28 |

0 | 2010-04-28 0 | 2010-04-28 b) tag\_id table



Most used libraries provided by Cray

Rank	Kraken	JaguarPF
1	CrayPAT/5.0	CrayPAT/4.x
2	Libsci/10.4	PETSc/3.0
3	PETSc/3.0	PAPI/3.6
4	FFTW/3.2	ACML/4.2
5	HDF5/1.8	HDF5/1.8

3 months of Kraken data, JaguarPF data is for all of 2009



Most used libraries provided by centers

Rank	Kraken	JaguarPF
1	SPRNG/2.0b	SZIP/2.1
2	PETSc/2.3	HDF5/1.6
3	lobuf/beta	Trilinos/9
4	TAU/2.19	PSPLINE/1.0
5	SZIP/2.1	NetCDF/3.6

3 months of Kraken data, JaguarPF data is for all of 2009



Most used applications on Kraken (last 3 months)

Rank	Library	# instances
1	interpo**	60,032
2	namd*	8,389
3	amber*	5,784
4	chimera	4,000
5	mpiblast	2,917

ALTD

From Torque job scripts

Rank	Library	# instances
1	arps	11,844
2	amber	6,789
3	namd	6,450
4	chimera	4,473
•••		
8	mpiblast	2,919

Absolute number of executions, not CPU hours! And only "launched jobs".

\* Counting both center-provided and user-built applications

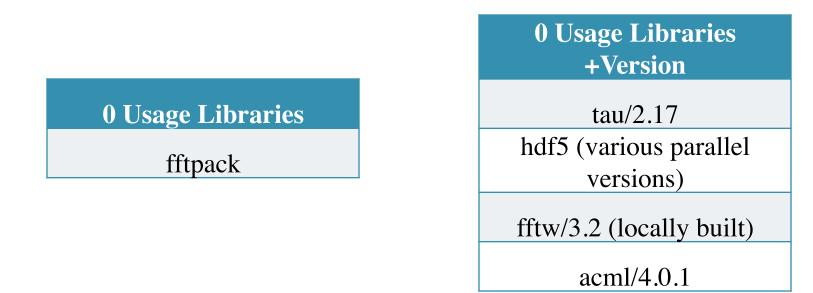
\*\* Compiled on athena and run on Kraken

• Typically job script mining counts more because includes staff and matches strings that can appear in multiple places; and ALTD will miss some early after being turned on

• ALTD counted more for namd because we catch it each time it is launched, the scripts searching for namd in job scripts can't tell if it is inside a loop.



Least used libraries on JaguarPF for 2009



Clearly, supporting fftpack can stop Old versions of tau and acml, for example, can be removed. Locally built hdf5 and fftw/3 libraries are not being used because there is a Cray analogue!



#### Miscellaneous

- If a library is unused (or used very little)
  - How do we really know if we can stop support
    - Maybe the users "went away" for awhile
    - Need long duration and "recent" usage views
- Found we can't just ignore all .o files

– lobuf – IO buffering library is a .o



## **Installation details**

- Written in Python, original version in C
- Actual mode of interception
  - Modulefiles (prepend PATH)
  - Move/rename Id and aprun
  - Tied into admin's "aprun wrapper" as an aprun-prologue
    - See Matt Ezell's talk on Tuesday at 3:30
- Built in ability to turn tracking on/off with env vars
  - Per person if desired
- Gets complicated with tools like Totalview
  - Either "fix" Totalview or unload ALTD
    - Modified Totalview on JaguarPF
  - Unload ALTD modulefile on Kraken



## Conclusions

#### In production and tracking usage

- We don't *really* know if the libraries were used
- We do know they were linked into the application

#### Almost unnoticed by users

One or two hiccups along the way, but were addressed quickly

#### Mining the data is hard

Even with mostly consistent software installations, many exceptions when looking for patterns

#### Can start making decisions about software support based on real usage

- 1. Stop providing FFTPACK and an old version of ACML, TAU
- 2. Users linking with Cray provided libraries
- Will be preparing a release of ALTD soon

