Software Usage on Cray Systems across Three Centers (NICS, ORNL and CSCS)

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Contents

- **Introduction and Motivations**

- **Overview on ALTD Tool**

- **Data Mining over 3 centers (Kraken, Jaguar, Rosa)**

  - **Linkline**

  - **Execution**

- **Conclusions and Future Work**

Software Usage on Cray Systems across Three Centers (NICS, ORNL and CSCS) **NICS**

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Software Usage on Cray Systems across Three Centers (NICS, ORNL and CSCS)

NICS

Software/library/applications

Kraken, Jaguar and Rosa support:

- **Several categories of software/library**
  - Linear algebra
  - I/O
  - Performance tools
  - Debugger
  - Chemistry
  - Molecular dynamic
  - Materials
  - Communications
  - Visualization

- **Multiple versions**
  - hdf5 (1.6.10 - 1.8.3 - 1.8.4 - 1.8.5 - 1.8.6)
  - netcdf (3.6.2 - 4.0 - 4.0.1 - 4.1 - 4.1.1.0 4.1.2 4.1.3/
  - libsci (10.4.5/ 10.5.0/ 10.5.01/ 10.5.02/ 11.0.00/ 11.0.01 11.0.02/ 11.0.04 11.0.06/)

- **Multiple builds with different compiler:**
  - example with FFTW:
    cnl3.1_cray7.4.3/   cnl3.1_intel12.0.4.191/   sles11.1_cray7.4.3/   sles11.1_intel12.0.4.191/
    cnl3.1_gnu4.6.1/   cnl3.1_pgi11.6.0/   sles11.1_gnu4.6.1/   sles11.1_pgi11.6.0/

Issue !

- **How do HPC centers monitor/measure software usage and forecast needs?**

- **How do**
  - **we know when to change defaults? (to newer versions)**

  - **we know when we can get rid of old versions ?**

  - **we know which software is not used ? (reduce cost)**

  - **we find who is using**
    - **deprecated software?**
    - **non-optimal [math] libraries?**
    - **software with bugs?**
    - **software funded by NSF/DOE …?**

```
-------------------------------------------------- /opt/cray/modulefiles --------------------------------------------------
atp/1.1.3                                              perftools/5.2.0
atp/1.4.1(default)                                     perftools/5.2.3(default)
atp/1.4.2                                              petsc/3.1.05
atp/1.4.3                                              petsc/3.1.09
ccm/2.0.0-1.0301.27363.11.17(default)                  petsc/3.2.00(default)
fftw/2.1.5.3                                           petsc-complex/3.1.05
fftw/3.2.2.1                                           petsc-complex/3.1.09
fftw/3.3.0.0(default)                                  petsc-complex/3.2.00(default)
ga/4.3.5(default)                                      pmi/2.1.4-1.0000.8596.15.1.ss(default)
gdb/7.2(default)                                       stat/1.1.3
hdf5/1.8.5.0                                           stat/1.2.1.1(default)
hdf5/1.8.6                                             tpsl/1.0.0
hdf5/1.8.7(default)                                    tpsl/1.1.01
hdf5-parallel/1.8.5.0                                  tpsl/1.2.00(default)
hdf5-parallel/1.8.6                                    trilinos/10.6.2.0
hdf5-parallel/1.8.7(default)                           trilinos/10.6.4.0
iobuf/2.0.2(default)                                   trilinos/10.8.3.0(default)
libfast/1.0.9(default)                                 xt-lgdb/1.4(default)
lustre-cray_ss_s/1.8.4_2.6.27.48_0.12.1_1.0301.5943.18.1-1.0301.27524.1.24(default)   xt-libsci/10.6.02
netcdf/4.1.1.0                                         xt-libsci/11.0.04(default)
netcdf/4.1.2                                           xt-libsci/11.0.05
netcdf/4.1.3(default)                                  xt-libsci/11.0.06
netcdf-hdf5parallel/4.1.1.0                            xt-mpich2/5.2.3
netcdf-hdf5parallel/4.1.2                              xt-mpich2/5.3.5(default)
netcdf-hdf5parallel/4.1.3(default)                     xt-mpt/5.2.3
papi/4.1                                               xt-mpt/5.3.5(default)
papi/4.1.2                                             xt-shmem/5.2.3
papi/4.1.4(default)                                    xt-shmem/5.3.5(default)
perftools/5.1.3

----------------------------------------------------- /opt/modulefiles -----------------------------------------------------
Base-opts/1.0.2-1.0301.25878.4.1.ss(default)   gcc/4.6.1                      petsc-complex/3.1.09
PrgEnv-cray/3.1.72(default)                    gcc/4.6.2(default)             petsc-complex/3.2.00(default)
PrgEnv-gnu/3.1.72(default)                     intel/11.1.038                pgi/11.4.0
PrgEnv-intel/3.1.72(default)                   intel/12.1.2.273(default)     pgi/11.9.0(default)
PrgEnv-pgi/3.1.72(default)                     intel/12.1.3.293              pgi/12.1.0
acml/4.4.0(default)                            java/jdk1.6.0_24(default)      pgi/12.2.0
acml/5.0.0                                     java/jdk1.7.0_02              torque/2.5.7(default)
acml/5.1.0                                     java/jdk1.7.0_03              xt-asyncpe/4.9
admin-modules/1.0.2-1.0301.25878.4.1.ss(default)  libfast/1.0.8             xt-asyncpe/5.05
apprentice2/5.1.3(default)                     maxama/6.1.0(default)          xt-asyncpe/5.06(default)
cce/7.3.4                                      moab/6.1.4(default)            xt-asyncpe/5.07
cce/7.4.4(default)                             modules/3.2.6.6(default)       xt-asyncpe/5.08
cce/7.4.5                                      mrnet/3.0.0(default)           xt-craypat/1.0(default)
chapel/1.3.0                                   petsc/3.1.05                   xt-craypat/5.1.3(default)
chapel/1.4.0(default)                          petsc/3.1.09                   xt-papi/4.1.0.0.2
gcc/4.4.4                                      petsc/3.2.00(default)          xt-papi/4.1.2
gcc/4.6.3                                      petsc-complex/3.1.06           xt-papi/4.1.4(default)

--------------------------------------------------- /sw/xt-cle3.1/modulefiles ---------------------------------------------------
DefApps                cue-hdf4          ghostscript/8.64(default)      lammps/6April11_icms      q-espresso/4.3.1
adios/1.2.2a           cue-hdf5          git/1.7.4.2(default)           lapack/3.1.1(default)     qbox/1.50
altd/1.0               cue-hypre         glib/2.27.0(default)           lapack/3.1.1-dualcore     qbox/1.54.4(default)
amber/11(default)      cue-lammps        glib/2.31.10                   lapack/3.1.1-FPIC         qt/4.6.2
ambertools/1.4(default) cue-lapack       globalarrays/5.0.2             libarch/2.3.19            ruby/1.9.1
apache-ant/1.6.5       cue-login-env     globalarrays/5.1(default)      m4/1.4.11                 saga/1.6.0
arpack/2008.03.11      cue-math          marmot/2.3.0(default)          matrix/2.3.3(default)     scalasca/1.3.3(default)
atk/1.32.0(default)    cue-metis         globus/4.0.8                   matplotlib/1.0.1          scipy/0.6.0
atlas/3.8.3            cue-mpt           globus/5.0.4(default)          mercurial/1.6.4           silo/4.8(default)
atlas/3.8.3-FPIC-dualcore cue-namd       gmake/3.82                     metis/4.0.1               sprng/2.0b
autoconf/2.66          cue-netcdf        gnuplot/4.4.3(default)         mpe2/1.3.0                subversion/1.6.9(default)
autoconf/2.68(default) cue-nwchem        gotoblas2/2.1.13               mpip/3.1.2                sundials/2.3.0
automake/1.11.1        cue-parmetis      gptl/3.5(default)              numpe/4.9.2               superlu/4.0
aztec/2.1              cue-petsc         grace/5.1.21                   msmb/2.6                  superlu_dist/2.4
bbcp/10.07.26.00.0     cue-phdf5         grads/2.0.47.1                 namd/2.8(default)         szip/2.1
bbcp/10.08.29.00.0     cue-python        graphviz/2.26.3                nano/2.2.5                tau/2.20
boost/1.44.0           cue-scalapack     gromacs/4.0.7                  ncl/5.0.0_source          tau/2.20.3(default)
budget/2.0             cue-tau           gromacs/4.0.7_fprelaxed        ncl/5.2.1                 tau/2.21.2
busybox/1.1.0          cue-top           gromacs/4.5.3                  nco/4.0.7                 tgusage/3.0-r2
cairo/1.10.0           cue-totalview     gromacs/4.5.3_mpt4.1.1         ncview/1.93g              tgusage/3.0-r3(default)
casino/2.5             cue-uberftp       gsl/1.14                       nedit/5.5                 tiff/3.9.4(default)
cdo/1.4.5(default)     cue-vmd           gv/3.7.1                       netcdf/3.6.3              tkdiff/4.1.4
charm++/6.1.3          desmond/2.2.7.3_dbl hdf4/4.2.5                   netcdf/4.1.3(default)     totalview/8.10.0-4-beta(default)
cmake/2.8.2            desmond/2.2.7.3_sngl hdf4/4.2.6                  netcdf-parallel/3.6.3     udunits/1.12.9
cmake/2.8.7(default)   doxygen/1.7.1     hdf5/1.6.10                    netcdf-parallel/4.1.3     udunits/2.1.13
cp2k/2_2-branch        espresso/2.1.2-gnu(default) hdf5/1.8.5           nose/0.11.3               umfpack/5.4.0
cpmd/3.13.2            espresso/2.1.2-pgi hdf5/1.8.6                    numpy/1.6.1               upc/2.10.2(default)
cue                    ferret/6.72(default) hdf5-parallel/1.6.10        nwchem/6.0                valgrind/3.5.0
cue-amber              fftw/2.1.5        hdf5-parallel/1.8.6            nwchem/6.1                vasp/4.6
cue-atlas              fftw/2.1.5-dualcore hpctoolkit/5.1.0             octave/3.4.2              vasp/5.2
cue-blas               fftw/3.1.2        hsp-dn-nr/20120320             cmaes/7.10.1              vim/7.3
cue-boost              fftw/3.1.2-dualcore hsp-dn-nr/20120320           ncl/5.0.0                 vina/1.1.2
cue-build              fftw/3.1.2-dualcore-fpic hsp-dn-pfam/24.0        pacman/3.26-r1            visit/current
cue-charm++            fftw/3.3          hsp-ncbi/0.4.0                 pango/1.28.3(default)     vmd/1.9
cue-cpmd               fftw/3.3-dualcore hypre/2.0.0                    paraview/3.10.0           yt/2.1
cue-compiler           fftw/3.3_alpha    hypre/2.7.0b                   parmetis/3.1              yt/2.2(default)
cue-cpmd               fpmpi/1.1         hypre/2.8.0b                   pgplot/5.2                yt/2.3
cue-fftw               fpmpi_papi/1.1    imagemagick/6.6.9-1(default)   pixman/0.21.8             yt/2.3-local
cue-globus             fsplit/1.0        ipm/0.983                      pepline/1.0               yt/dev
cue-globus             gamess/2010Aug10  lammps/11Apr11                 python/2.7.1(default)
cue-gromacs            gdlib/2.0.35      lammps/14Aug11                 python/2.7.1-cnl
cue-gsl                gempak/5.11.4     lammps/24Jan10                 python/3.1.1
```

Issue

- **As of today:**
  - **Rule of the thumbs from the staff:**
    - **not strictly accurate and reliable**
  - **Modulefile, logs, Surveys:**
    - **Incomplete data**

"Questions were raised around whether other techniques such as user survey, and gathering of library requirements a priori rather than as forensics would be more cost effective and achieve similar goals."

→ Solution ALTD: Automatic Library Tracking Database

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NICS

Objectives and Goals

- **A primary objective of ALTD :**
  - **track only libraries linked into the applications (not the function calls)**
  - **track parallel executables launched (how often are the libraries used?)**

- **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**

- **Intercept the whole library path to retrieve valuable information on :**
  - **Package name**
  - **Version number**
  - **Build configuration**

ALTD design

- Intercepting the GNU linker (ld) to get the linkage information

- Intercepting the job launcher (aprun)

→ **Wrapping the linker and the job launcher through scripts is a simple and efficient way to obtain the information automatically and transparently.**

- ld - Intercept link line
  - Update tags table
  - Call real linker (with tracemap option)
  - Use output from tracemap to find libraries linked into executable
  - Update linkline table

- aprun- Intercept job launcher
  - Pull information from ALTD section header in executable
  - Update jobs table
  - Call real job launcher

→ **Storing information about compilation and execution into a database that can be mined to provide reports.**

ALTD database results

- **ALTD generates records into 3 tables:**
  - **Tags: entry for every link executed**
  - **Linkline: entry for each unique link line**
  - **Jobs: entry for each executable launched**

a) linkline table

b) tag_id table

c) job_id table

Software Usage on Cray Systems across Three Centers (NICS, ORNL and CSCS)

NICS

Linktable

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/gcc/x86_64-suse-linux/4.1.2/libgcc_eh.a /usr/lib64/libc.a /usr/lib64/gcc/x86_64-suse-linux/4.1.2/crtend.o /usr/lib64/crtn.o
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

Software Usage on Cray Systems across Three Centers (NICS, ORNL and CSCS) **NICS**

Job table

run_inc	tag_id	executable	username	run_date	Job_launch_id	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
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/CH4/vasp_vtst.x	user5	2010-04-28	548638	kraken

NICS

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NICS

OMG ! What are they doing !?

- **Early 2010, on Kraken, a new recent tree has been put in place, /sw/xt/ instead of /sw/xt5/**

- **End 2010, still some users are using old builds:**

```
/sw/xt5/lapack/3.1.1/cnl2.1_pgi7.2.3/lib/liblapack.a      18
/sw/xt5/szip/2.1/sles10.1_pgi7.2.3/lib/libsz.a    16
/sw/xt5/gsl/1.11/cnl2.1_pgi7.2.3/lib/libgsl.a     15
/sw/xt5/hdf5/1.8.2/cnl2.1_pgi7.2.5/lib/libhdf5.a       5
/sw/xt5/blas/ref/cnl2.1_pgi7.2.3/lib/libblas.a    4
/sw/xt5/fftw/3.1.2/sles10.1_gnu4.2.4/lib/libfftw3f.a      3
/sw/xt5/fpmpi/1.1/cnl2.1_pgi7.2.5/lib/libfpmpi_papi.a     2
/sw/xt5/hdf4/4.2r4/cnl2.1_pgi7.2.5/lib/libdf.a    1
/sw/xt5/hdf5/1.6.7/cnl2.1_pgi7.2.3/lib/libhdf5.a       1
/sw/xt5/netcdf/3.6.2/sles10.1_pgi7.2.3/lib/libnetcdf.a   1
/sw/xt5/hdf4/4.2r4/cnl2.1_pgi7.2.5/lib/libmfhdf.a      1
```

- **Some users not using the modulefiles**

- **Usage of reference BLAS and LAPACK on Kraken**

ALTD : full paths

- **ALTD can detect also the location of the library used and subpackages**

/opt/cray/hdf5-parallel/1.8.4.1/hdf5-parallel-pgi/lib/libhdf5.a   1538
/opt/cray/hdf5-parallel/1.8.4.1/hdf5-parallel-pgi/lib/libhdf5_fortran.a   1407   **HDF5 installed by vendor**
/opt/cray/hdf5-parallel/1.8.5.0/hdf5-parallel-pgi/lib/libhdf5.a   1365
/opt/cray/hdf5-parallel/1.8.5.0/hdf5-parallel-pgi/lib/libhdf5_fortran.a   1356

/sw/xt/hdf5/1.6.10/cnl2.2_pgi10.4.0_par/lib/libhdf5.a   266
/sw/xt/hdf5/1.8.5/cnl2.2_pgi10.4.0/lib/libhdf5.a   230   **HDF5 installed by staff**
/sw/xt/hdf5/1.8.5/cnl2.2_gnu4.4.3/lib/libhdf5.a   192

/nics/b/home/usr1/hdf5-1.8.7/src/.libs/libhdf5.a   37
/nics/b/home/usr2/deploy/lib/libhdf5.a   32   **HDF5 installed by users**
/nics/b/home/usr3/hdf5-1.6.5/hdf5/lib/libhdf5.a   31
/nics/d/home/usr4hdf5patch1/lib/libhdf5_fortran.a   17

/opt/petsc/3.1.00/real/gnu/linux/lib/44/libparmetis_quadcore.a   337
/opt/petsc/3.1.00/real/gnu/linux/lib/44/libcraypetsc_quadcore.a   337
/opt/petsc/3.1.00/real/gnu/linux/lib/44/libpord_quadcore.a   337
/opt/petsc/3.1.00/real/gnu/linux/lib/44/libsuperlu_dist_2.3_quadcore.a   337
/opt/petsc/3.1.00/real/gnu/linux/lib/44/libmumps_common_quadcore.a   337
/opt/petsc/3.1.00/real/gnu/linux/lib/44/libsuperlu_4.0_quadcore.a   337   **PETSc subpackages usage**
/opt/petsc/3.1.00/real/gnu/linux/lib/44/libdmumps_quadcore.a   337
/opt/petsc/3.1.00/real/gnu/linux/lib/44/libmetis_quadcore.a   337
/opt/petsc/3.1.00/real/gnu/linux/lib/44/libhypre_quadcore.a   328

Why quadcore for Istanbul ?

NICS

Data mining

- **ALTD has recorded the following data at each site for Year 2011:**
  - **Kraken:**
    - 456,437 successful compilations by 860 users
    - 1,434,972 application executions by 919 users.
  - **Jaguar:**
    - 1,024,793 successful compilations performed by 684 users
    - 1,325,538 application executions by 671 users.
  - **Rosa:**
    - 103,451 successful compilations by 254 users,
    - 501,102 application executions by 309 users.

- **The percentage of active users who have never compiled a code is about 18% and 6%, on Rosa and Kraken, respectively.**

- **The presence of these "black-box" users, (running applications installed either by the centers' staff or by their colleagues) needs to be taken into account when center staff are considering the installation and maintenance of third-party applications for their users.**

Compiler usage with MPI

USAGE OF COMPILERS (NUMBER OF INSTANCES)

Compiler	Kraken	Jaguar	Rosa
GNU	26689	70854	**9407**
PGI	**51154**	**132345**	6116
Intel	6321	55182	1729
CCE	69	343	1415
Pathscale	14	1486	389

USAGE OF COMPILERS (NUMBER OF USERS)

Compiler	Kraken	Jaguar	Rosa
GNU	189	190	85
PGI	**609**	**524**	**87**
Intel	146	64	41
CCE	3	3	39
Pathscale	3	38	20

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ALTD - Cray

- **Detected in 2011 that ALTD was not tracking when Cray Compiler was used:**
  - CCE uses its own linker not the GNU linker located in /usr/bin
  - /opt/cray/cce/7.3.3/cray-binutils/x86_64-unknown-linux-gnu/bin/ld
  - Is there a reason ?

- **Fix:**
  - setenv LINKER_X86_64   /sw/altd/bin/ld
  - Modify the PrgEnv-Cray: unload/load   ALTD
  - Ticket to CRAY : response "for user who want to use an alternative linker path, the environment variable ALT_LINKER is created." This environment variable is added to xt-asyncpe 5.05

- **Recent usage of Cray in 2012:**
  - Kraken : 198 out of 42649 instances with 8 unique users out of 504 total users.
  - Jaguar(TITAN): 11336 (140637) instances by 7users (373)

Software usage during linking process

- **Top 10 most used libraries fall into three major categories (on all machines):**
  - numerical libraries (LibSci, FFTW, ACML, PETSc),

  - I/O software (HDF5, NetCDF),

  - Performance analysis tools (Craypat, PAPI, TAU).

Numerical Libraries

Library usage ranked by number of instances and number of users on Kraken

Library	instances	users	Library/ version	instances	users
Libsci	42271	291	libsci/10.5.02	29787	220
atlas	35954	8	fftw/3.2.2.1	15987	128
fftw	24494	235	xt-libsci/10.4.5	12167	169
acml	3537	59	fftw/2.1.5	3710	64
petsc	2460	20	acml/4.4.0/	3088	39
sprng	1745	13	sprng/2.0b/	1739	12
arpack	1721	11	petsc/3.1.05	1571	13
tspl	1517	14	arpack/2008	1543	1
gsl	1451	48	tpsl/1.0.0/	1517	14
fftpack	1317	35	gsl/1.14	1063	39

Installed by staff

Jaguar

Library	instances	users	Library/ version	instances	users
libsci	74970	317	libsci/10.4.4/	47383	245
fftw	48728	163	fftw/3.2.2.1/	44779	109
acml	17198	58	libsci/10.5.0/	26303	208
trilinos	7518	25	acml/4.3.0/	9360	43
petsc	6008	58	acml/4.4.0/	7727	32
parmetis	1810	19	petsc/3.0.0.10/	1882	29
umfpack	1773	24	fftw/3.2.2/	1832	15
arpack	1166	12	parmetis/3.1 .1	1793	15
fftpack	1069	21	trilinos/10.4.0/	1786	10
pspline	1066	16	petsc/3.1.04/	1152	25

Rosa

Library	instances	users	Library/ version	instances	users
libsci	6240	109	fftw/3.2.2.1	4497	53
fftw	6042	84	libsci/11.0.01/	2806	33
acml	2020	48	libsci/10.5.02	1919	55
trilinos	1090	9	acml/4.4.0/	1123	44
tpsl	974	7	libsci/11.0.04/	974	33
parmetis	913	8	trilinos/10.6.0	731	1
umfpack	865	9	fftw/3.3.0.0	721	27
petsc	469	11	tpsl/1.0.0/	532	3
mkl	145	7	libsci/11.0.03/	512	24
Gsl	116	4	fftw/2.1.5	346	16

Software Usage on Cray Systems across Three Centers (NICS, ORNL and CSCS)

NICS

Application linked with different versions of LibSci

Usage of LibSci versions			
Month	11.0.3	11.0.4	11.0.5	11.0.6
Dec 11	**2326**	18	0	0
Jan 12	**4875**	2387	0	0
Febr12	**6388**	4459	0	0
March 12	**2280**	1693	4	0
Number of users using LibSci versions			
Dec 11	**33**	4	0	0
Jan 12	17	**29**	0	0
Febr12	12	**30**	0	0
March 12	12	**26**	2	0

Rosa

Kraken

	Usage of LibSci versions					
Month	10.4.5	10.5.0	10.5.02	11.0.01	11.0.4	11.0.6
Dec 11	2977	0	**18886**	1930	0	0
Jan 12	4625	4	**20370**	621	77	0
Febr12	2794	17	**14262**	692	1	0
March 12	520	0	8582	979	**8890**	7
	Number of users using LibSci versions					
Dec 11	17	0	**71**	5	0	0
Jan 12	14	1	**76**	4	2	0
Febr12	17	1	**95**	7	1	0
March 12	11	0	47	7	**75**	2

One of the most powerful aspects of ALTD is its ability to identify users running codes that were built with legacy versions of libraries (particularly ones that are known to provide suboptimal performance, or are known to contain bugs)

Software Usage on Cray Systems across Three Centers (NICS, ORNL and CSCS)

NICS

I/O and Performance tools

I/O usage on Kraken

Library/ version	instances	users
iobuf/beta	5763	16
hdf5/1.8.4.1	2023	48
hdf5/1.8.5.0	1931	50
hdf5-par/1.8.5.0	1811	23
netcdf/3.6.2/	1600	25
szip/2.1	1533	51
hdf5-par/1.8.4.1	1467	17
netcdf/3.6.3/	868	5
netcdf/4.0.1.3/	593	16
hdf5/1.6.10	505	18

Performance tools usage on Jaguar

Library/ version	instances	users
papi/3.7.2	3787	121
craypat/5.1.0/	1331	29
vampirtrace/5.11	782	16
vampirtrace/5.12	780	4
craypat/5.1.3	767	19
papi/3.6.2.2	388	7
papi/4.1.0.0.2	285	17
craypat/5.0.2/	275	20
vampirtrace/5.13	160	2
hpctoolkit/5.1.0	143	8

Performance tools usage on Kraken

Library/ version	instances	users
perftools/5.2.0	3352	21
craypat/5.1.3/	2950	30
craypat/5.1.0/	1674	11
papi/4.1.2/	339	34
tau/2.20	315	38
fpmpi/1.1	295	11
papi/4.1.0.0.2	229	17
papi/3.6.2.2	200	8
papi/3.7.2	133	19
mpip/3.1.2	113	3

Performance tools usage on Rosa

Library	instances	users
craypat	3465	32
papi	577	35
scalasca	163	7
tau	27	2

Software Usage on Cray Systems across Three Centers (NICS, ORNL and CSCS)

NICS

Usage during executions

Kraken

Application	instances	users	Application / version	instances	users
namd	368349	109	namd/2.7/	294547	19
aprs	192749	20	namd/2.7b2	16237	10
amber	71261	18	namd/2.7b1-09	7834	4
hmc	51541	10	gromacs/4.5.3	3162	12
vasp	17884	33	namd/2.7b1/	2576	3
wrf	20141	19	amber/10	1830	7
espresso	14597	20	amber/11	1081	4
lammps	7035	40	namd/2.8	1052	10
gromacs	6345	28	cpmd/3.13.2	1047	6
cpmd	1773	6	q-espresso/4.2.1	950	1

MD applications

Jaguar

Application	instances	users	Application / version	instances	users
ior_bench	496352	2	vasp/4.6	16333	8
lammps	105345	31	lammps/9sep10	2899	6
esmf	86480	9	namd/2.7b1	1400	4
amber	64725	4	namd/2.6	692	1
vasp	45533	26	lammps/1jui11	477	4
nwpar	33484	1	spdcp/1.0.0	121	17
ccsm	25557	61	adios/1.3	46	4
espresso	19605	20	esmf/5.2.0	25	3
gromacs	8443	9	namd/2.7b4	14	1
namd	5143	14	gromacs/4.0.5/	12	1

Rosa

Application	instances	users	Application / version	instances	users
namd	74952	22	namd/2.8	29351	12
int2lm1	65274	8	namd/2.7b4	22160	6
parfe	52167	13	espresso/4.2.1	17296	7
cp2k	52010	37	cp2k/21.11.2011	11006	10
siba	37443	4	cp2k/17.08.2010	7838	5
gromacs	32573	13	vasp/5.2	2965	5
echam	28480	11	vasp/4.6	2053	3
espresso	21133	15	espresso/4.3.2	987	7
dlpoly	8535	4	Cpmd/3.13	680	4
vasp	5071	10	espresso/4.1	599	2

Software Usage on Cray Systems across Three Centers (NICS, ORNL and CSCS)
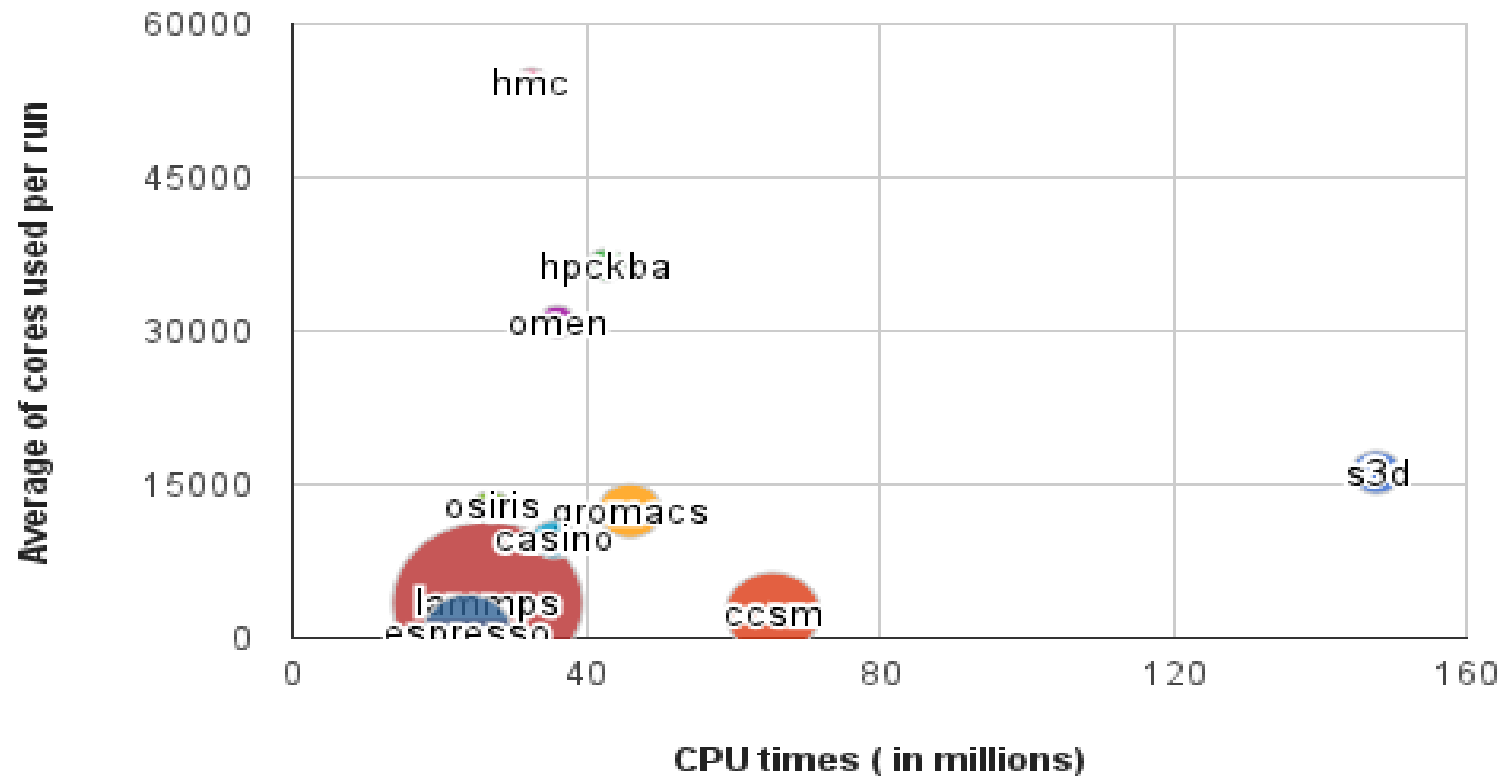
NICS

Most CPU hours applications on Kraken
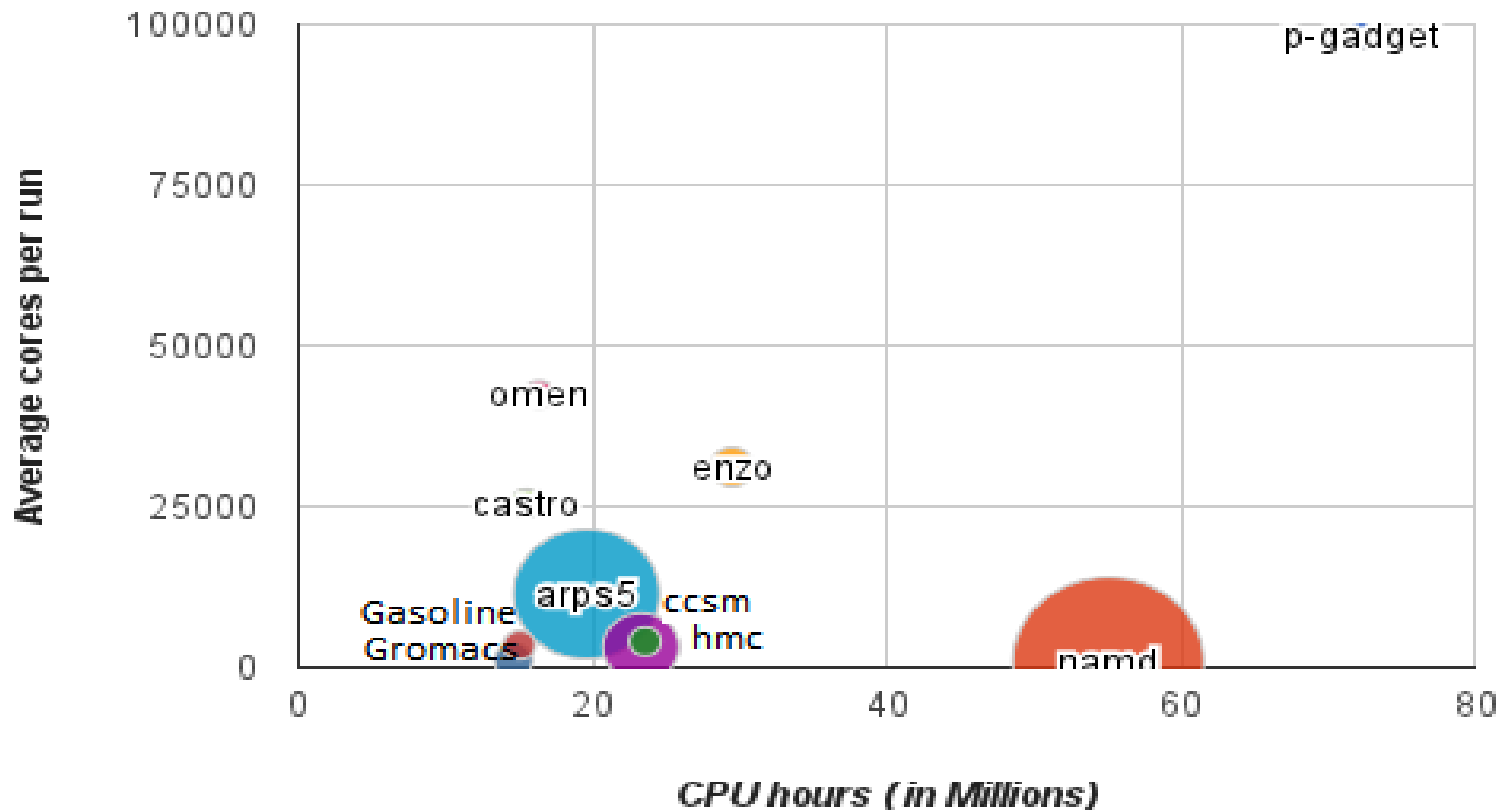
The top 10 most CPU consuming codes on Kraken in 2011, showing CPU hours consumed vs the average cores per run.

Software Usage on Cray Systems across Three Centers (NICS, ORNL and CSCS) NICS

Most CPU hours applications on Jaguar

Contents

● **Conclusions and Future Work**

NICS

Conclusions

- **ALTD tracks automatically and transparently library usage at compilation and at execution**
  - **Wrapping the linker and the job launcher**
  - **In production on several Cray XT/XE machines at NICS and OLCF (ORNL), CSCS**
  - **Alpha version is available if interested, please contact us !**

- **Track the most used libraries and it facilitates decisions for removing old/non-used libraries**

- **Data mining:**
  - **Usage at linking:**
    - **Linear algebra, (LibSci, FFTW, ACML, PETSc)**
    - **I/O (HDF5, NetCDF)**
    - **Performance tools (Craypat, PAPI, TAU)**
  - **Usage at execution**
    - **Molecular dynamic (NAMD, LAMMPS, GROMACS, ESPRESSO), climate modeling(US),bone structures simulation (EU) for the number of executions**
    - **Cosmology code for the CPU hours, (Kraken), Combustion (Jaguar)**

Conclusions

- **How ALTD has been useful to NICS?**
  - Detected bad behavior
  - Dropped Pathscale support
  - Upgrade to CLE3.1: prioritize tasks according to the high usage and choose the most used version along with the most recent one.

- **The results of our data mining have shown that a significant number of users are using their own libraries/executables even where there is a centrally installed application available:**
  - a user might require a non-standard version

  - prefer to use a version built by them

  - unaware that a centrally installed version exists. (need more TEO)

  - Don't use optimized version

    → **Greengineering the present for the Future !**

NICS

Future Work

- **We need support to continue the efforts.**

- **The data mining has confirmed that there is extensive use made of numerical libraries (particularly LibSci, ACML, and PETSc).**
  - envision adding functionality to track individual routines and correlate them back to "logical" libraries
    - → assist library develops and vendors (and centers) to tune the most used functions for current and upcoming architectures, including multicore and accelerators.

- **At present the data mining of ALTD is a manual process(python scripts) that generate a few simple SQL queries.**
  - envision to provide tools that automate the querying process: support staff would thus be alerted immediately to cases where, for example, a user is running a code that is linked against a deprecated or buggy library

Thank You !

Software Usage on Cray Systems across Three Centers (NICS, ORNL and CSCS)

NICS