

# Programming Environment for the Cray XT system

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#### Outline

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- Overview
- Modules
- Compilers
- Programming Environment User Guide

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# **Cray Programming Environment Focus**



- It is the role of the Programming Environment to close the gap between observed performance and peak performance
  - Help users achieve *highest possible performance* from the hardware
- The Cray Programming Environment addresses issues of scale and complexity of high end HPC systems.
  - The Cray Programming Environment helps users to be more productive
  - It is the place at which the complexity of a system is hidden from the user
- User productivity is enhanced with
  - Increased automation
  - · Ease of use
  - Extended *functionality* and improved *Reliability*
  - Close interaction with users for feedback targeting functionality enhancements

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#### **Cray Programming Environment**

- Programming Languages
  - Fortran
  - C
  - C++
  - ChapelPython #
- Compilers
  - Cray
  - PGI<sup>\*</sup>
  - GNU
- Programming models
  - Distributed Memory
    - > MPI
  - > SHMEM
  - Shared Memory
    - > OpenMP
  - PGAS & Global View
    - > UPC
    - > CAF
    - > Chapel
- I/O Libraries
  - NetCDF
  - HDF5

Tools

- Environment setup
  - Modules Debuggers
  - > TotalView
  - > DDT
- Debugging Support Tools
  - > Fast Track Debugger
  - > Abnormal Termination Process

#: Under development

- > STAT #
- > Comparative Debugger#
- Performance analysis
  - CrayPat
  - Cray Apprentice2
- Optimized Math Libraries
  - LibSci
    - > libgoto
    - > Iterative Refinement Toolkit
    - > LAPACK
    - Scalapck
    - > FFTW
  - > CRAFFT
  - Cray PETSc
    > CASK

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#### **Environment Setup**



- The Cray XT system uses modules in the user environment to support multiple software versions and to create integrated software packages
  - As new versions of the supported software and associated man pages become available, they are added automatically to the Programming Environment, while earlier versions are retained to support legacy applications
  - You can use the default version of an application, or you can choose another version by using Modules system commands
- By default, the PrgEnv-pgi and Base-opts modules are loaded into your user environment
  - You should **never unload the Base-opts module** because it contains the setup for CLE.

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# The module tool on the Cray XT



- How can we get appropriate Compiler, Tools, and Libraries?
  - The modules tool is used to handle different versions of packages
    - > e.g.: module load compiler\_v1
    - > e.g.: module switch compiler\_v1 compiler\_v2
    - > e.g.: module load xt-craypat
- Taking care of changing of PATH, MANPATH, LM\_LICENSE\_FILE,.... environment
  - Modules also provide a simple mechanism for updating certain environment variables, such as PATH, MANPATH, and LD\_LIBRARY\_PATH
  - In general, you should make use of the modules system rather than embedding specific directory paths into your startup files, makefiles, and scripts.
- It is also easy to setup your own modules for your own software

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#### Useful module commands



- Load software
  - · module load xt-craypat
- Change software version
  - module swap pgi/7.0.4 pgi/6.1.6
- Load Cray Compiling Environment
  - module swap PrgEnv-pgi PrgEnv-cray

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#### module list



#### users/ldr> module list

Currently Loaded Modulefiles:

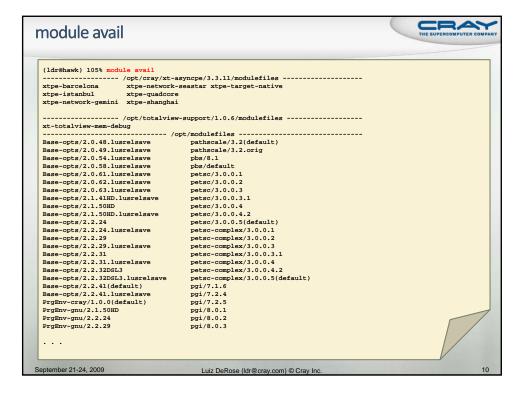
- 1) modules/3.1.6
  2) xtpe-target-cnl
  3) xt-service/2.2.41
  4) xt-os/2.2.41
  5) xt-boot/2.2.41
  6) xt-lustre-ss/2.2.41
  7) Base-opts/2.2.41
  10) xt-totalview/8.6.0
  11) xt-libsci/10.3.9
  12) xt-mpt/3.4.2
  13) xt-pe/2.2.41
  14) xt-asyncpe/3.3
  15) PrgEnv-pgi/2.2.41
  16) xt-craypat/5.0.0
- 8) pgi/9.0.3
- 9) totalview-support/1.0.6

- 7) Base-opts/2.2.41 16) xt-craypat/5.0.0
  - 17) apprentice2/5.0.0

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```
module show
  users/ldr> module show cce
  /opt/modulefiles/cce/7.1.3:
  setenv
                     CRAYLMD_LICENSE_FILE /opt/cray/cce/cce.lic
                     CRAY_BINUTILS_ROOT /opt/cray/cce/7.1.3/cray-binutils
  setenv
                     CRAY BINUTILS VERSION /opt/cray/cce/7.1.3
                     CRAY_BINUTTLS_BIN /opt/cray/cce/7.1.3/cray-binutils/x86_64-unknown-linux-gnu/bin LINKER_X86_64 /opt/cray/cce/7.1.3/cray-binutils/x86_64-unknown-linux-gnu/bin/ld
  setenv
  setenv
                     ASSEMBLER_X86_64 /opt/cray/cce/7.1.3/cray-binutils/x86_64-unknown-linux-gnu/bin/as
  setenv
                     CRAYLIBS_X86_64 /opt/cray/cce/7.1.3/craylibs/x86-64 FTN_X86_64 /opt/cray/cce/7.1.3/cftn/x86-64
  setenv
                     CC_X86_64 /opt/cray/cce/7.1.3/CC/x86-64 CRAY_FTN_VERSION 7.1.3
  setenv
  setenv
                     CRAY CC VERSION 7.1.3
                     PE_LEVEL 7.1
                     FORTRAN_SYSTEM_MODULE_NAMES ftn lib definitions
  prepend-path
  prepend-path
  /opt/cray/cce/7.1.3/man:/opt/cray/cce/7.1.3/craylibs/man:/opt/cray/cce/7.1.3/CC/man:/opt/cray/cce/7.
  prepend-path
                    NLSPATH /opt/cray/cce/7.1.3/CC/x86-
  64/nls/En/%N.cat:/opt/cray/cce/7.1.3/craylbs/x86-64/nls/En/%N.cat:/opt/cray/cce/7.1.3/cftn/x86-
  64/nls/En/%N.cat
  prepend-path
                     INCLUDE_PATH_X86_64 /opt/cray/cce/7.1.3/craylibs/x86-64/include
  prepend-path
                    PATH /opt/cray/cce/7.1.3/cray-binutils/x86_64-unknown-linux-
  gnu/bin:/opt/cray/cce/7.1.3/craylibs/x86-
  64/bin:/opt/cray/cce/7.1.3/cftn/bin:/opt/cray/cce/7.1.3/CC/bin
  append-path
                    MANPATH /usr/share/man
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```



# **Release Notes** (ldr@hawk) 112% module help xt-craypat ----- Module Specific Help for 'xt-craypat/5.0.0' -----Release Date: August 20, 2009 Purpose: Differences: Changes from CrayPat 4.4.1 release to 5.0.0 release CrayPat 4.4.1 release revision: 2380 CrayPat 5.0.0 release revision: 2686 -DCRAYPAT is added to compilation options when the xt-craypat module is loaded. (Add -UCRAYPAT to a compiler invocation will undefine the macro.) modulefile pat\_hwpc pat\_build pat\_build pat\_build removed - no longer supported removed - no longer supported more complete evaluation of DWARF DIEs no longer control tracing symbols in file by write permissions add 'trace-file' directive to control tracing symbols in file Bugz closed since 4.4.1 release (following fixed in revs <=2686 == 5.0 release) September 21-24, 2009 Luiz DeRose (ldr@cray.com) © Cray Inc.

#### **Setting Your Target Architecture**



- Before you begin to compile programs, you must verify that the target architecture is set correctly
- The compilers and linker use the target architecture in creating executables to run on compute nodes
- The target architecture is set automatically when you log in
  - The xtpe-target-cnl module should be loaded and the XTPE\_COMPILE\_TARGET environment variable set to linux

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# Using the Compiler Driver Commands



- You use compiler driver commands to launch all Cray XT compilers
- The syntax for the compiler driver is:
  - cc | CC | ftn [Cray\_options | PGI\_options | GNU\_options] files [-lhugetlbfs]
- For example, to use the PGI Fortran compiler to compile prog1.f90
  - First use the **module list** command to verify that these modules have been loaded:
    - > PrgEnv-pgi
    - > xtpe-target-cnl
  - Then use this command:
    - > % ftn prog1.f90

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# Compiler man Pages



- The cc(1), CC(1), and ftn(1) man pages contain information about the compiler driver commands
- The pgcc(1), pgCC(1), and pgf95(1) man pages contain descriptions of the PGI compiler command options
- The craycc(1), crayCC(1), and crayftn(1) man pages contain descriptions of the Cray compiler command options
- The gcc(1), g++(1), and gfortran(1) man pages contain descriptions of the GNU compiler command options
- To verify that you are using the correct version of a compiler, use:
  - · -V option on a cc, CC, or ftn command with PGI and CCE
  - · --version option on a cc, CC, or ftn command with GNU

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# **Cross Compiling Environment**



- Compiling on a Linux service node
- Generating an executable for a CLE compute node
- Do not use pgf90, pgcc, gcc, g++, ..., unless you want a Linux executable for the service node
- Information message:
  - > ftn: INFO: linux target is being used

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#### **Using PGI Compilers**



- To use the PGI compilers, run the module list command to verify that the PrgEnv-pgi module is loaded
  - If it is not, use a module swap command, such as:
    - > % module swap PrgEnv-gnu PrgEnv-pgi
    - PrgEnv-pgi loads the product modules that define the system paths and environment variables needed to use the PGI compilers

Compiler File	Command	Source
C compiler	сс	filename.c
C++ compiler	сс	filename.CC filename.cc filename.cpp filename.cxx
Fortran 90/95 compiler	ftn	filename.f (fixed source, no preprocessing) filename.f90 (free source, no preprocessing) filename.f95 (free source, no preprocessing) filename.F (fixed source, preprocessing) filename.F90 (free source, preprocessing) filename.F95 (free source, preprocessing)

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### PGI Basic Compiler Usage



- A compiler driver interprets options and invokes preprocessors, compilers, assembler, linker, etc.
- Options precedence: if options conflict, last option on command line takes precedence
- Use -Minfo to see a listing of optimizations and transformations performed by the compiler
- Use -help to list all options or see details on how to use a given option, e.g. pgf90 -Mvect -help
- Use man pages for more details on options

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# PGI compiler flags for a first start



#### **Preprocessor Options:**

-Mpreprocess runs the preprocessor on Fortran files

(default on .F, .F90, or .fpp files)

**Optimization Options:** 

-fast (or -fastsse) chooses generally optimal flags

for the target platform

-Mipa=fast,inline Inter Procedural Analysis

-Minline=levels:number number of levels of inlining (default 1)

-Minline= [name:]function A non-numeric option is assumed to be

a function name

-Minfo Compiler optimization information

**Overall Options:** 

-Mlist creates a listing file

-help displays command-line options

e.g., pgf95 -fast -help

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## -help users/ldr> pgf90 -fast -help Reading rcfile /opt/pgi/9.0.3/linux86-64/9.0-3/bin/.pgf90rc Common optimizations; includes -O2 -Munroll=c:1 -Mnoframe -Mlre -Mautoinline == -Mvect=sse -Mscalarsse -Mcache\_align -Mflushz M[no] vect[=[no] altcode|[no] assoc|cachesize: <<>|[no] fuse|[no] gather|[no] idiom|levels: <n>|[no] partial|[no] sizelimit[:n]|prefetch| function | fu|[no]short|[no]sse|[no]uniform] Control automatic vector pipelining [no]altcode Generate appropriate alternative code for vectorized loops [no]assoc Allow [disallow] reassociation levels:<n> Maximum nest level of loops to optimize [no]partial Enable [disable] partial loop vectorization via inner loop distribution [no]sizelimit[:n] Limit size of vectorized loops prefetch Generate prefetch instructions [no]short Enable [disable] short vector operations [no]sse Generate [don't generate] SSE instructions [no]uniform Perform consistent optimizations in both vectorized and residual loops; this may affect the performance of the residual loop -M[no]scalarsse Generate scalar sse code with xmm registers; implies -Mflushz -Mcache\_align Align long objects on cache-line boundaries -M[no]flushz Set SSE to flush-to-zero mode

# PGI Flags for Debugging Aids

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-g generates symbolic debug information used by a debugger

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- -gopt generates debug information in the presence of optimization
- -Mbounds adds array bounds checking
- -v gives verbose output, useful for debugging system or build problems
- -Mlist will generate a listing
- -Minfo provides feedback on optimizations made by the compiler
- -S or –Mkeepasm to see the exact assembly generated

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# Basic optimization switches



- Traditional optimization controlled through -O[<n>]
  - n is 0 to 4.
- -fast switch combines common set into one simple switch, is equal to -O2 -Munroll=c:1 -Mnoframe -Mlre
  - Same as -fastsse
  - For -Munroll, c specifies completely unroll loops with this loop count or less
  - -Munroll=n:<m> says unroll other loops m times
  - -Mlre is loop-carried redundancy elimination
- -Mcache\_align aligns top level arrays and objects on cacheline boundaries
- -Mflushz flushes SSE denormal numbers to zero

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# Node level tuning



- Vectorization packed SSE instructions maximize performance
- Interprocedural Analysis (IPA) use it!
- Function Inlining especially important for C and C++
- Parallelization for Cray multi-core processors
- Miscellaneous Optimizations hit or miss, but worth a try

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# What can Interprocedural Analysis and Optimization with –Mipa do for You?



- Interprocedural constant propagation
- Pointer disambiguation
- Alignment detection, Alignment propagation
- Global variable mod/ref detection
- F90 shape propagation
- Function inlining
- IPA optimization of libraries, including inlining

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# **Using Interprocedural Analysis**



- Must be used at both compile time and link time
- Non-disruptive to development process edit/build/run
- Speed-ups of 5% 10% are common
- –Mipa=safe:<name> safe to optimize functions which call or are called from unknown function/library name
- –Mipa=libopt perform IPA optimizations on libraries
- –Mipa=libinline perform IPA inlining from libraries

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-Minline[=[lib:]<inlib> | [name:]<func> | except:<func> | size:<n> | levels:<n>]

[lib:]<inlib> Inline extracted functions from inlib

[name:]<func> Inline function func

except:<func> Do not inline function func

size:<n> Inline only functions smaller than n statements (approximate)

levels:<n> Inline n levels of functions

 For C++ Codes, PGI Recommends IPA-based inlining or –Minline=levels:10!

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#### Effect of IPA on the WUPWISE Benchmark



PGF95 Compiler Options	Execution Time in Seconds			
-fastsse	156.49			
-fastsse -Mipa=fast	121.65			
-fastsse -Mipa=fast,inline	91.72			

- -Mipa=fast => constant propagation =>
  - compiler sees complex matrices are all 4x3 => completely unrolls loops
- -Mipa=fast,inline => small matrix multiplies are all inlined

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#### Other C++ recommendations



- Encapsulation, Data Hiding small functions, inline!
- Exception Handling use –no\_exceptions until 7.0
- Overloaded operators, overloaded functions okay
- Pointer Chasing -Msafeptr, restrict qualifer, 32 bits?
- Templates, Generic Programming now okay
- Inheritance, polymorphism, virtual functions runtime lookup or check, no inlining, potential performance penalties

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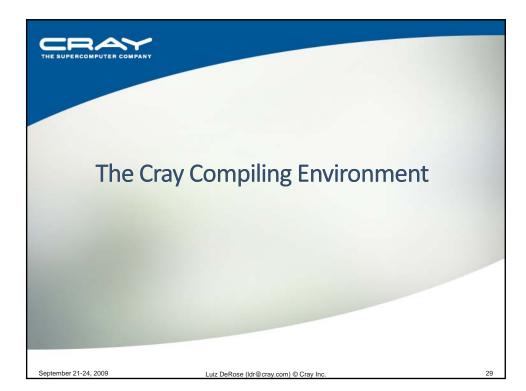
#### **SMP Parallelization**



- Mconcur for auto-parallelization on multi-core
  - Compiler strives for parallel outer loops, vector SSE inner loops
  - –Mconcur=innermost forces a vector/parallel innermost loop
  - -Mconcur=cncall enables parallelization of loops with calls
- –mp to enable OpenMP parallel programming model
  - OpenMP programs compiled w/out –mp=nonuma
- –Mconcur and –mp can be used together!

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# The Cray Compiling Environment



- Ability and motivation to provide high-quality support for custom Cray network hardware
- Cray technology focused on scientific applications
  - Takes advantage of Cray's extensive knowledge of automatic vectorization
  - Takes advantage of Cray's extensive knowledge of automatic shared memory parallelization
  - Supplements, rather than replaces, the available compiler choices
- Standard conforming languages and programming models
  - Fortran 2003 Compliant Working on Fortran 2008
  - OpenMP
    - > Fully integrated with other compiler optimizations, including automatic shared memory parallelization
  - UPC & CoArray Fortran
    - > Fully optimized and integrated into the compiler
    - > No preprocessor involved
    - Target the network appropriately:
      - GASNet with Portals
      - o DMAPP with Gemini

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#### **CCE Main Features**



- Fortran 2003 standard compliant
  - Selected F2008 features
- C99 and C++ support
- PGAS functional support
  - UPC 1.2
  - Fortran 2008 CAF
- OpenMP 3.0 support (with limitations)
- Vectorization
- Cache optimizations
  - Automatic Blocking
  - · Automatic Management of what stays in cache
- Automatic multithreading
- Prefetching, Interchange, Fusion
- Cray performance tools and debugger support

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### **OpenMP**



- CCE 7.1 supports the OpenMP 3.0 specification, with minor limitations:
  - C++ random access iterator loops marked for work sharing may not get work shared
  - · Task switching is not implemented
  - Limitations to be removed in future releases
- OpenMP and automatic multithreading are fully integrated with the compiler
  - Share the same runtime and resource pool
  - Aggressive loop restructuring and scalar optimization is done in the presence of OpenMP
  - · Consistent interface for managing OpenMP and automatic multithreading
- Nested parallelism and OpenMP tasks can be used to take advantage of increasing numbers of cores within a node

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# Performance Tests – May 11, 2009



Speedup	Language	Compiler 1		Compiler 2		Compiler 3	
	FTN	193	48.1%	182	45.4%	186	46.4%
CCE better	С	15	14.6%	9	8.7%	17	16.5%
(> 105%)	C++	1	11.1%	1	11.1%	0	0.0%
	Total	209	40.7%	192	37.4%	203	39.6%
CCE on par or better (> 95%)	FTN	281	70.1%	282	70.3%	265	66.1%
	С	60	58.3%	55	53.4%	49	47.6%
	C++	3	33.3%	5	55.6%	1	11.1%
	Total	344	67.1%	342	66.7%	315	61.4%
CCE worst (< 95%)	FTN	120	29.9%	119	29.7%	136	33.9%
	С	43	41.7%	48	46.6%	54	52.4%
	C++	6	66.7%	4	44.4%	8	88.9%
	Total	169	32.9%	171	33.3%	198	38.6%

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#### CCE: How to use it



- Make sure it is available
  - module avail PrgEnv-cray
- To access the Cray compiler
  - module load PrgEnv-cray
  - or module switch PrgEnv-xxx PrgEnv-cray
- To target the shanghai chip
  - module load xtpe-shanghai
- Once you have loaded the module "cc" and "ftn" are the Cray compilers
  - Recommend just using default options
  - Use -rm (fortran) and -hlist=m (C) to find out what happened

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## **Cray Opteron Compiler: Directives**



- Cray compiler supports a full and growing set of directives and pragmas
  - > !dir\$ concurrent
  - > !dir\$ ivdep
  - > !dir\$ interchange
  - > !dir\$ unroll
  - > !dir\$ loop\_info [max\_trips] [cache\_na] ... Many more
  - > !dir\$ blockable
  - See
    - > man directives
    - > man loop\_info

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# Loopmark: Compiler Feedback



- Compiler can generate a "filename.lst" file
  - ftn -rm ... or cc -hlist=m
  - Contains annotated listing of your source code with letter indicating important optimizations

%%% Loopmark Legend %%%

Primary Loop Type Modifiers

\_\_\_\_\_

a - vector atomic memory operation

A - Pattern matched b - blocked

C - Collapsed

f - fused

 $\mbox{ D - Deleted } \mbox{ i -- interchanged }$ 

E - Cloned m - streamed but not partitioned
I - Inlined p - conditional, partial and/or computed
M - Multithreaded r - unrolled

P - Parallel/Tasked

s - shortloop

V - Vectorized

t - array syntax temp used

W - Unwound

w - unwound

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```
Example: Cray loopmark messages for Resid
    29. b----<
                    do i3=2.n3-1
    30. b b----<
                      do i2=2,n2-1
    31. b b Vr--<
                         do i1=1,n1
    32. b b Vr
                         u1(i1) = u(i1,i2-1,i3) + u(i1,i2+1,i3)
    33. b b Vr
                               + u(i1,i2,i3-1) + u(i1,i2,i3+1)
    34. b b Vr
                        u2(i1) = u(i1,i2-1,i3-1) + u(i1,i2+1,i3-1)
    35. b b Vr >
                               + u(i1,i2-1,i3+1) + u(i1,i2+1,i3+1)
    36. b b Vr-->
                         enddo
                       do i1=2,n1-1
    37. b b Vr--<
    38. b b Vr
                        r(i1,i2,i3) = v(i1,i2,i3)
                                 - a(0) * u(i1,i2,i3)
    39. b b Vr
    40. b b Vr
                                 -a(2)*(u2(i1)+u1(i1-1)+u1(i1+1))
                >
    41. b b Vr >
                                  -a(3)*(u2(i1-1)+u2(i1+1))
    42. b b Vr-->
                       enddo
    43. b b---->
                      enddo
    44. b---->
                  enddo
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```

#### Example: Cray loopmark messages for Resid (cont) ftn-6289 ftn: VECTOR File = resid.f, Line = 29 A loop starting at line 29 was not vectorized because a recurrence was found on "U1" between lines 32 and 38. ftn-6049 ftn: SCALAR File = resid.f, Line = 29 A loop starting at line 29 was blocked with block size 4. ftn-6289 ftn: VECTOR File = resid.f, Line = 30 A loop starting at line 30 was not vectorized because a recurrence was found on "U1" between lines 32 and 38. ftn-6049 ftn: SCALAR File = resid.f, Line = 30 A loop starting at line 30 was blocked with block size 4. ftn-6005 ftn: SCALAR File = resid.f, Line = 31 A loop starting at line 31 was unrolled 4 times. ftn-6204 ftn: VECTOR File = resid.f, Line = 31 A loop starting at line 31 was vectorized. ftn-6005 ftn: SCALAR File = resid.f, Line = 37 A loop starting at line 37 was unrolled 4 times. ftn-6204 ftn: VECTOR File = resid.f, Line = 37 A loop starting at line 37 was vectorized. September 21-24, 2009 Luiz DeRose (ldr@cray.com) © Cray Ind

#### **On-line Documentation**



- http://docs.cray.com/latest.html
  - Cray XT Programming Environment User's Guide
     S-2396-22 · Jul 2009
  - Using Cray Performance Analysis Tools
     ➤ S-2376-50 · Sep 2009

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# Programming Environment for the Cray XT system

# Questions / Comments Thank You!

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