# **alinea** Leaders in parallel software development tools

# **Debugging HPC Applications**

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www.allinea.com

# Agenda

- Bugs and Debugging
- Debugging parallel applications
- Debugging OpenACC and other hybrid codes
- Debugging for Petascale (and beyond)

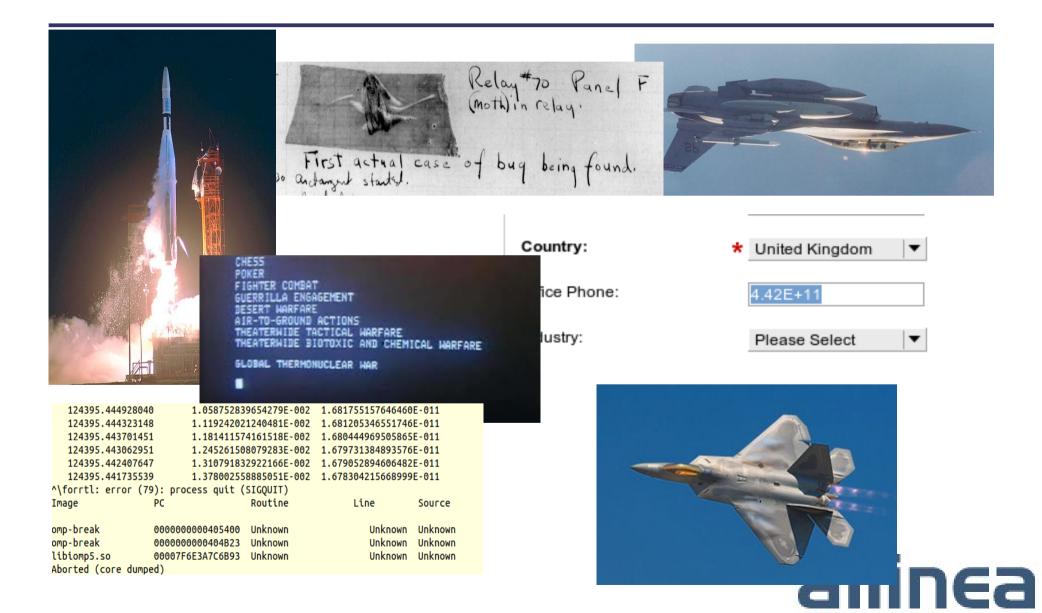


## About Allinea

- HPC development tools company
  - Flagship product Allinea DDT
    - Now the leading debugger in parallel computing
    - The scalable debugger
      - Record holder for debugging software on largest machines
      - Production use at extreme scale and desktop
    - Wide customer base
      - Blue-chip engineering, government and academic research
      - Strong collaborative relationships with customers and partners



## **Bugs in Practice**



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# Some types of bug

- Some Terminology
  - Bohr bug
    - Steady, dependable bug
  - Heisenbug
    - Vanishes when you try to debug (observe)
  - Mandelbug
    - Complexity and obscurity of the cause is so great that it appears chaotic
  - Schroedinbug
    - First occurs after someone reads the source file and deduces that it never worked, after which the program ceases to work



# Debugging

- Transforming a broken program to a working one
- How?
  - Track the problem
  - Reproduce
  - Automate (and simplify) the test case
  - Find origins where could the "infection" be from?
  - Focus examine the origins
  - Isolate narrow down the origins
  - Correct fix and verify the testcase is successful
- TRAFFIC
- Suggested Reading:
  - Zeller A., "Why Programs Fail", 2<sup>nd</sup> Edition, 2009



# How to focus and isolate

- A scientific process?
  - Hypothesis, trial and observation, ...
- Requires the ability to understand what a program is doing
  - Printf
  - Command line debuggers
  - Graphical debuggers
- Other options
  - Static analysis
  - Race detection
  - Valgrind
  - Manual source code review



# What are debuggers?

- Tools to inspect the insides of an application whilst it is running
  - Ability to inspect process state
    - Inspect process registers, and memory
    - Inspect variables and stacktraces (nesting of function calls)
    - Step line by line, function by function through an execution
    - Stop at a line or function (breakpoint)
    - Stop if a memory location changes
  - Ideal to watch how a program is executed
    - Less intrusive on the code than printf
    - See exact line of crash unlike printf
    - Test more hypotheses at a time



#### **Debugging Parallel Applications**



# **Debugging Parallel Applications**

- Scalar bugs can be challenging: parallel even more so!
- The same need: observation, control
  - Complex environment with complex problems
    - More processes, more data
    - More Heisenbugs MPI communication library introduces potential non-determinism
  - Fewer options
    - Printf or command line debuggers are not quick enough



## First example

- Typical problem scenario: application ends abruptly
  - Example potential causes
    - Segmentation fault
    - Early termination due to invalid parameters
- Where do we start?



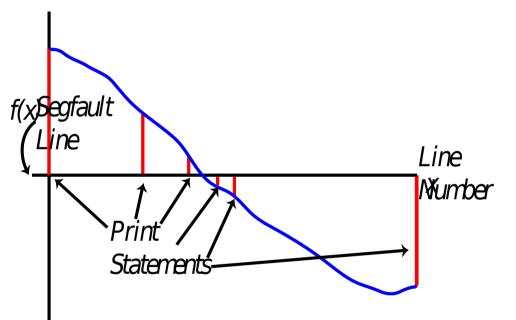
# Print statement debugging

#### • The first debugger: print statements

- Each process prints a message or value at defined locations
- Diagnose the problem from evidence
   and intuition
- A long slow process
  - Analogous to bisection root finding

Thanks to Rebecca Hartman-Baker of ORNL for the analogy and animation

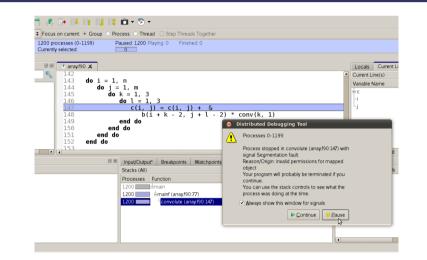
- Broken at modest scale
  - Too much output too many log files

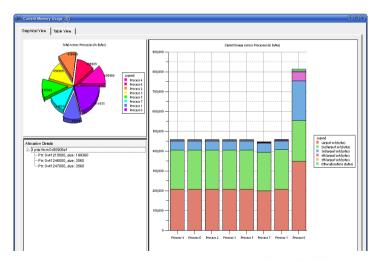




# Allinea DDT in a nutshell

- Graphical source level
   debugger for
  - Parallel, multi-threaded, scalar or hybrid code
  - C, C++, F90, Co-Array Fortran, UPC
- Strong feature set
  - Memory debugging
  - Data analysis
- Managing concurrency
  - Emphasizing differences
  - Collective control



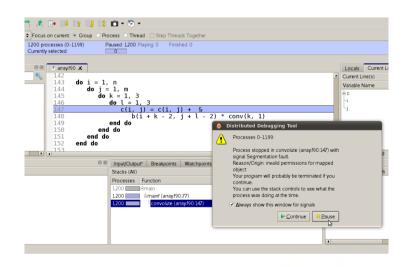


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# Fixing the everyday crash

- The typical application crash or early exit:
  - Run your program in the debugger ddt {application} {parameters}
  - Application crashes or starts to exit
- Where did it happen?
  - Allinea DDT merges stacks from processes and threads into a tree
  - Leaps to source automatically
- Why did it happen?
  - Some faults evident instantly from location(s)
  - But for others we need to look further at variables

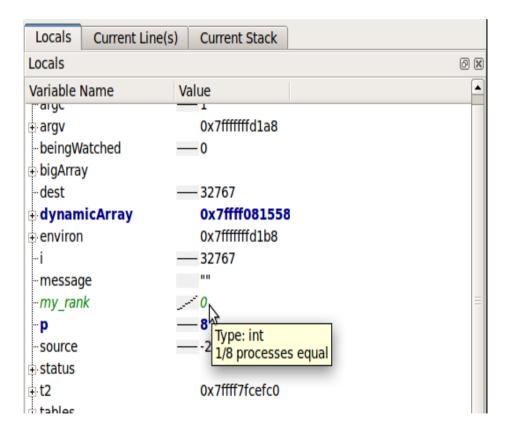
Stacks (AII)	
Processes	Function
150120	🚊_start
150120	Ėlibc_start_main
150120	Ėmain
150120	Ėpop (POP.f90:81)
150120	⊡initialize_pop (initial.f90:119)
150120	⊟init_communicate (communicate.f90:87)
150119	<ul> <li>create_ocn_communicator (communicate.f90:300)</li> </ul>
1	create_ocn_communicator (communicate.f90:303)





# Simplifying data divergence

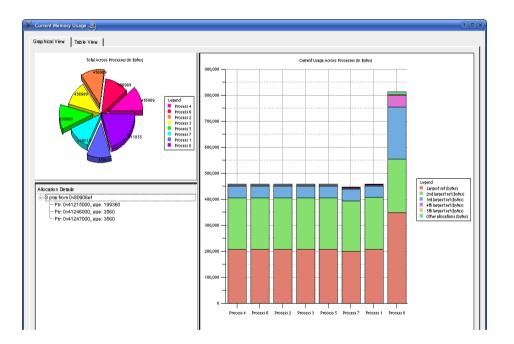
- Need to understand the data
  - Too many variables to trawl manually
  - Allinea DDT compares data automatically
- Smart highlighting
  - Subtle hints for differences and changes
  - With sparklines!
- More detailed analysis
  - Full cross process comparison
  - Historical values via tracepoints





# Memory debugging

- Random errors are the worst kind
  - You can't fix a bug that doesn't repeat memory debugging can force the bug
  - Better to crash every time, than only during product demos
- Allinea DDT helps eliminate random memory bugs
  - Enable memory debugging by ticking an option
  - Monitors usage: detects memory leaks
  - Automatically protects ends of arrays
  - Trigger instant stop on touching invalid memory
  - Also with CUDA support





#### Interlude: Fixing a simple MPI bug



## Second example

- More subtle issue
  - Not an immediately obvious crash
    - Crash occurs in self-evidently correct code
    - Something went wrong somewhere else!
- How can a debugger help here?
  - Observation: we can watch things go bad



# **Controlling execution**

- Observe application behaviour by controlling execution
  - Step, play or run to line based on groups
  - Change interleaving order by stepping/playing selectively
  - Set breakpoints
  - Set data watchpoints
- Examine data and progress at each point
- Group creation is easy
  - Integrated throughout Allinea DDT
     eg. stack and data views

All	0 1	2
ddt.bin	1 2	
licenceserver	0	
	• • • • • • • • • • • • • • • • • • • •	• •• •• •
Current Group: All	Focus on current:   Group	O Process O Thread
All	200004 processes (0-200003) Currently selected:	Paused: 200004 Running: 0
Create Group		Ş

Stacks (AII)	
Processes	Function
150120	start
150120	Ėlibc_start_main
150120	idimain
150120	≟pop (POP.f90:81)
150120	Ėinitialize_pop (initial.f90:119)
150120	Ėinit_communicate (communicate.f90:87)
150119	-create_ocn_communicator (communicate.f90:300)
1 🗖	create_ocn_communicator (communicate.f90:303)



# **Exploring large arrays**

<u>A</u> rray E	Ξx	ore	ssion: (	bigArray	/[\$i]								•
<u>D</u> istrib	Distributed Array Dimensions: 1 😫 How do I view distributed arrays?												
Range	Range of \$x (Distributed) Range of \$i Auto- <u>u</u> pdate												
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3	-	+				-						-	
4			1										
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												•	
	Visualize in <u>3</u> D Export to Spreadsheet/HDF5												

- Browse arrays
  - 1, 2, 3, ... dimensions
  - Table view
- Filtering
  - Look for an outlier
- Export
  - Save to a spreadsheet
- View and search arrays from multiple processes
  - Search terabytes for rogue data – in parallel

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# Static analysis

```
29
   30
          threads = calloc(sizeof(pthread t), nthreads);
   31
          ids = calloc(sizeof(int), nthreads);
   32
   33
          init mutex();
   34
   35
          pthread mutex lock(mutley);
   36
          for (i = 0; i < nthreads; ++i) {</pre>
   37
               ids[i] = i:
   38
               pthread create (threads + i, NULL, &thread,
   39
   40
          pthread mutex unlock(mutley);
   41
          for (i = 0; i < nthreads; ++i)</pre>
   42
               pthread join (threads[i], NULL);
   43
   44
          return 0:
 error Memory leak: threads
                      oid *a)
 error Memory leak: ids
          volatile int busy = 0;
   49
          volatile int locker = 0; /* to be amended by
50
   51
          int i, j;
▲ 52
          double k = 1:
   53
          int tid = *(int*) q;
   54
۰
  55
          usleep(rand() % 31);
   56
```

- Analyzes source code
  - Detects some common errors (eg.)
    - Memory leaks
    - Buffer overflow
    - Unused variables
  - Not exhaustive but a useful hint for debugging



## Tracepoints

	Breakpoints Watchp	points Tracepoints Tracepoint Output Stacks (All)							
Fracepoint Output	racepoint Output								
Tracepoint	Processes	Values logged							
vhone.f90:85	976, ranks 12,14-17,22-23,12	mype 2172-3527 jcol: 42-83 mod pey							
vhone.f90:81	960, ranks 12,14-17,22-23,12	ks — 1 kmax pez							
vhone.f90:85	942, ranks 12,14-17,22-23,12	mype 2172-3527 jcol: 2-83 mod pey							
vhone.f90:81	929, ranks 12,14-17,22-23,12	ks — 1 kmax pez							
vhone.f90:85	919, ranks 12,14-17,22-23,12	mype 2172-3527 jcol: 2-83 mod pey							
vhone.f90:81	898, ranks 12,14-17,22-23,12	ks — 1 kmax pez							
vhone.f90:85	884, ranks 12,14-17,22-23,12	mype 2172-3527 jcol: 4 2-83 mod pey							
vhone.f90:81	880, ranks 12 14-17 22-23 12	ks — 1 kmax pez							

- A scalable print alternative
  - Merged print with a sparkline graph showing distribution
  - Change at runtime no recompilation required



# Offline debugging

- Machine access can be a problem
  - New offline mode
    - Set breakpoints, tracepoints from command line
    - Memory debugging
    - Record variables, stacks crashes and breakpoints
  - Submit and forget
    - Post-mortem analysis
    - HTML/plain text
  - Debug while you sleep

9	Δ	01:42.176	1-15	Reason/Origin: ki Your program wil	Process stopped in sched_yield (syscall-template.5:82) with signal SIGSEGV (Segmentation fau Reason/Origin: kill, sigsend or raise Your program will probably be terminated if you continue. You can use the stack controls to see what the process was doing at the time. V Stacks				
				Processes	Threads	Function			
				1-15	15	applu (lu.f:118)			
				1-15	15	ssor (ssor.f:131)			
				1-15	15	blts (blts.f:55)			
				1-3,5-7,9-11,13,15	11	exchange_1 (exchange_1.f:37)			
				1-3,5-7,9-11,13,15	11	pmpi_recv			
				1-3,5-7,9-11,13,15	11	PMPI_Recv			
				1-3,5-7,9-11,13,15		mca_pml_obl_recv			
				1-3,5-7,9-11,13,15		opal_progress			
				1-3,5-7,9-11,13,15	11	sched_yield (syscall-template.S:82)			
				4, 8, 12, 14	4	exchange_1 (exchange_1.f:55)			
				4, 8, 12, 14	4	pmpi_recv			
				4, 8, 12, 14	4	PMPI_Recv			
1				4,8,12,14	4	mca_pml_obl_recv			
				4,8,12,14	4	opal_progress			
				4,8,12,14	4	sched_yield (syscall-template.S:82)			
				► Stack for proce	ess 1				
כ	8	01:46.488	n/a	Every process in	your pro	gram has terminated.			
-		-							
N	lessa	dos Tra	acepoints	Output		5			

#	Time	Tracepoint	Processes	Values
1	00:13.451	subdomain.f:96	0	jend: — 0 ny: — 9
2	00:13.453	ssor.f:177	0-15	delunm(5): 0.25
3	00:13.455	ssor.f:177	0-15	delunm(5): — 0.25



# Interlude: Fixing a more unusual bug Hands on: A first exercise with Allinea DDT

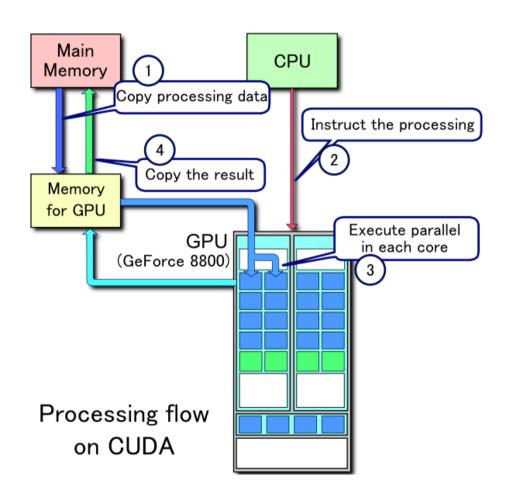


#### Debugging OpenACC and other hybrid codes



# HPC's current challenge

- GPUs a rival to traditional processors
  - AMD and NVIDIA
  - OpenCL, CUDA
- New languages, compilers, standards
- Great bang-for-bucks ratios
- A big challenge for HPC developers
  - Data transfer
  - Several memory levels
  - Grid/block layout and thread scheduling
  - Synchronization
- Bugs are inevitable



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# How do we fix GPU bugs?

- Print statements
  - Too intrusive
- Command line debugger?
  - A good start:
    - Variables, source code
    - Large thread counts overwhelming
  - Too complex
- A graphical debugger...

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	(140 90	-		0,0,0)	(143,		(63,0,6	4.77		0000b4da			
1	(147 90 (156			0, 0, 0) 0, 0, 0)	(151,		(63,0,6	10		00000b4da	dau		a
	90 (167 90			0,0,0)	(168,		(63,0,0	to		0000b4da	mo		
10	(176 90	9,0,	0) (0	0,0,0)	(172,	0,0)	(63,0,0	) 192	0x00000	0000b4da	a848 pr	efix.cu	
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# **GPU Debugging**

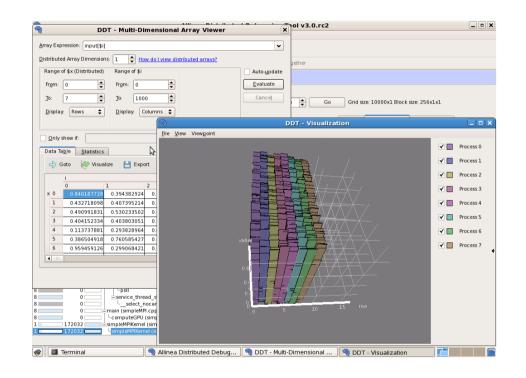
- Almost like debugging a CPU we can still:
  - Run through to a crash
  - Step through and observe
- CPU-like debugging features
  - Double click to set breakpoints
  - Hover the mouse for more information
  - Step a warp, block or kernel
  - Follow threads through the kernel
- Simultaneously debugs CPU code
- CUDA Memcheck feature detects read/write errors

All	0 1 2 3 4 5 6 7
Create Group	
CUDA Threads (Process 0,	simpleMPIKernel) Block 0 + 0 + 0 + Thread 0 + 0 + 0 +
Project Files 🛛 🕅	🐨 simpleMPI.cpp 💥 🐨 simpleMPI.cu 🎗
Search (Ctrl+K)	34 my_abort(err); }
🛓 🗈 signal.c	36
• m simpleMPI.cpp	37 // Device code 38 // Very simple GPU Kernel that computes square roots of input numbe:
🗉 🎹 simpleMPI.cu	39global void simpleMPIKernel(float * input, float * output)
+ C slist.c	40 { 41 int tid = blockIdx.x * blockDim.x + threadIdx.x;
+ C snapc base clos	<pre>41 int tid = blockIdx.x * blockDim.x + threadIdx.x; 42 output[tid] = sqrt(input[tid]);</pre>
	43 ]
I snapc_base_ope	44 45
	46 // Initialize an array with random data (between 0 and 1)
	47 <b>void</b> initData( <b>float</b> * data, int dataSize)
🕂 🗊 stacktrace.c 📃	
I	$48 \{ 49 \text{ for (int i = 0, i < dataSize, i+t)} \}$
stacktrace.c	48 { 48 { 49 for(int i = 0. i < dataSize. i++) 10 mmmmm
I	48 {
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Input/Outp Breakpo Stacks (All)	48 {
Input/Outp Breakpo Stacks (All) Processes Threads	48 { 49 for (int i = 0 · i < dataSize · i++) (     for (int i = 0 · i < dataSize · i++) ints Watchpoi Tracepoints Tracepoint Out Stacks (All) Kernel Progress V
Input/Outp Breakpo Stacks (All) Processes Threads 8 8 8	48 {       49       for (int i = 0. i < dataSize. i++)
Input/Outp Breakpo Stacks (All) Processes Threads 8 8 8	48 {       49 for (int i = 0 · i < dataSize · i++)
Input/Outp Breakpo Stacks (All) Processes Threads 8 8 8 8 8 8 8	48 {       for (int i = 0.i < dataSize.i+t)
Input/Outp Breakpo Stacks (All) Processes Threads 8 8 8 8 8 8 8	48 {       for (int i = 0.i < dataSize.i++)



# Examining GPU data

- Debugger reads host and device memory
  - Shows all memory classes: shared, constant, local, global, register..
  - Able to examine variables
  - ... or plot larger arrays directly from device memory





## New overviews of GPUs

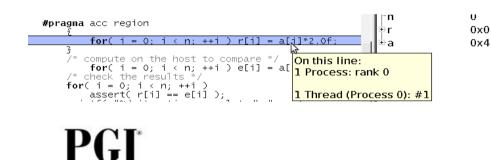
	Locals	Current Line(s)	Current Sta	ck	GPU Devices			
	GPU Devi	ces				0 X		
	Attribute Name Value							
L	🚊 🛛 Ranks	s 0,21,35,98						
L	⊟ gf	100		2 D (	evices			
L		···· IDs		0-1				
L		— Compute Capabili	ty	sm_	20			
		···· Number of SMs		14				
		···· Warps per SM		48				
		···· Lanes per Warp		32				
L		Registers per Lane		64				
L	Ranks	s 1-20,22-34,36-55,	57-97,99-119	No [	Device			

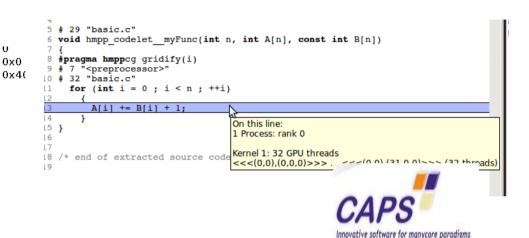
Kernel Prog	ress Vie	W	0 X			
Kernel		Progress				
simpleM						
		Kernels: 7 CUDA thread: <<<(1080,0,0),(0,0,0)>>> Dimensions: <<<(10000,1,1),(256,1,1)>>>				

- Device overview shows system properties
  - Helps optimize grid sizes
  - Handy for bug fixing and detecting hardware failure!
- Kernel progress view
  - Shows progress through kernels
  - Click to select a thread



# **Debugging for Directives**





 Supporting the environments that you use for hybrid development

ргоуган натт 2 integer, parameter :: n = 1000 3 real.dimension(n) :: input 4 real.dimension(n) :: result 5 integer :: i 6 **do** i = 1,n 7 input(i) = i\*4.0 8 enddo **!\$omp** acc region 10 **!Somp** acc loop do i.= 1.n result(i) = input(i) \* 4.0 enddd On this line: 13 1 Process: rank 0 14 **!Som** 15 \$0M Kernel 1: 32 GPU threads print<<<<(0,0),(0,0,0)>>> ... <<<(0,0),(31,0,0)>>> (32 threads) 16 17 end program

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# **OpenACC** debugging

CUDA Threads (main\$ck_L51	
Proj Fortran	C reduction.c 🗵
Project Files 🗗 🗙 Search (Ctrl+K)	41         plot.height = 25;           42         plot.xoffset = 0;           43         plot.yoffset = 0;
Froject Files     Fource Tree     Fource Tree     Fource Tree     Fource Tree     Fource Files	44       45     int j;       46     float dist;       47     float total;       48     coords_3d temp;
÷. C reduction.c	49 50 <b>#pragma omp</b> acc_region_loop <b>reduction</b> (+:tota 51 <b>for</b> (j=0; j <n; ++j)="" {<br="">52 temp = nodes[j]; 53 dist = distance(temp,plot.origin);</n;>
	▲ 55 coords_3d* ptr = &nodes[j]; 56 57 total = dist;
	<pre>58  } 59 60  printf("total = %f\n",total); 61 62 63 64 64 65 65 65 65 65 65 65 65 65 65 65 65 65</pre>
	62 return (0); 63 }
	۲
Input/Output* Breakpoin	nts Watchpoints Stacks Kernel Progress View Tracepoints Tracepoint O
Stacks	
1     96       1     10       1     22	nction nain\$ck_L51_1 (reduction.c:58) main\$ck_L51_1 (reduction.c:51) main\$ck_L51_1 (reduction.c:52) main\$ck_L51_1 (reduction.c:58) nain (reduction.c:58)

- OpenACC for C and F90
  - Straightforward CUDA compute power
  - Getting code onto the GPU quickly

     Optimization may still be required
- On device debugging with Allinea DDT
  - Variables arrays, pointers, full F90 and C support
  - Set breakpoints and step warps and blocks
- Requires Cray compiler for on device debugging
  - Other compilers to follow



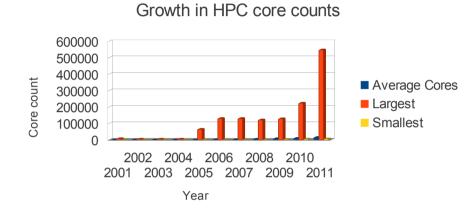
#### Interlude: CUDA Debugging



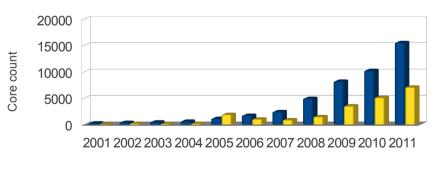
#### **Debugging for Petascale**



#### Extreme machine sizes



HPC core counts



Average Cores Smallest

- Progress requires ever more CPU hours
  - Machine sizes are exploding
  - Skewed by largest machines
  - ... but a common trend everywhere else
  - Software is changing to exploit the machines



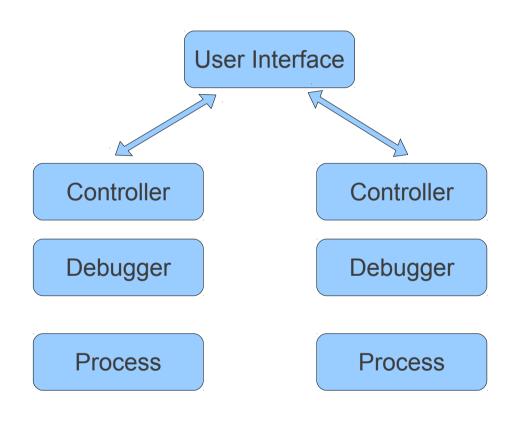
## Bug fixing as scale increases

- Can we reproduce at a smaller scale?
  - Attempt to make problem happen on fewer nodes
    - Often requires reduced data set the large one may not fit
      - Smaller data set may not trigger the problem
    - Does the bug even exist on smaller problems?
      - Didn't you already try the code at small scale?
    - Is it a system issue eg. an MPI problem?
  - Is probability stacking up against you?
    - Unlikely to spot on smaller runs without many many runs
    - But near guaranteed to see it on a many-thousand core run
- Debugging at extreme scale is a necessity



# A simple parallel debugger

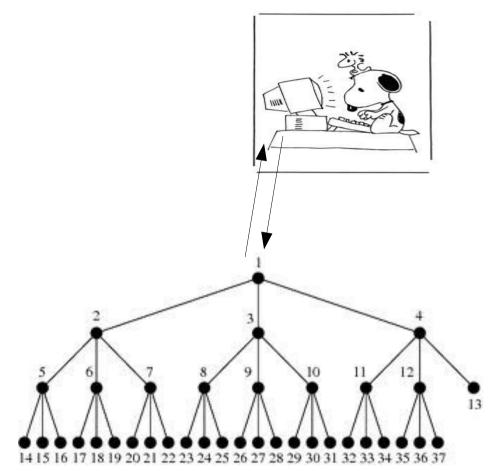
- A basic parallel debugger
  - Aggregate scalar debuggers and control asynchronously
  - Implement support for many platforms and MPI implementations
  - Develop user interface: simplify control and state display
- Initial architecture
  - Scalar debuggers connect to user interface
  - Eventual scalability bottlenecks
    - Operating system limitations: file handles, threads, processes
    - I/O limitations, memory and computation limitations
  - Machines still getting bigger...





#### How to make a Petascale debugger

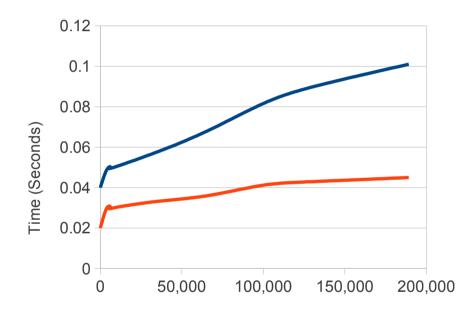
- A control tree is the solution
  - Ability to send bulk commands and merge responses
    - 100,000 processes in a depth 3 tree
  - Compact data type to represent sets of processes
    - eg. For message envelopes
    - An ordered tree of intervals?
    - \_ Or a bitmap?
  - Develop aggregations
    - Merge operations are key
    - Not everything can merge losslessly
    - Maintain the essence of the information
      - eg. min, max, distribution





#### For Petascale and beyond

#### DDT 3.0 Performance Figures





- All Step

----- All Breakpoint

- Scale doesn't have to be hard
  - 100,000 cores should be as easy as 100 cores
  - The user interface is vital to success
- Scale doesn't have to be slow
  - High performance debugging even at 200,000 cores
  - Step all and display stacks: 0.1 seconds
  - Logarithmic performance
- Stable and in production use
  - Routinely used by end users at over 100,000 cores



# Key features at scale

- Top 5 features at scale
  - Parallel stack view
    - Ideal for divergence or deadlock
  - Automated data comparison: sparklines
    - Rogue data is easily seen
  - Parallel array searching
    - Data is too large to examine manually
  - Process control with step, play, and breakpoints
    - Still essential
  - Offline debugging
    - Access to machine may be hard try offline debugging instead

	Locals	Current Line(s)	Current Stack	
•	Current Lin	e(s)		8×
	Variable N	lame	Value	
	jcol		36	
	туре		···· 2724	



#### Interlude: Petascale demonstration

