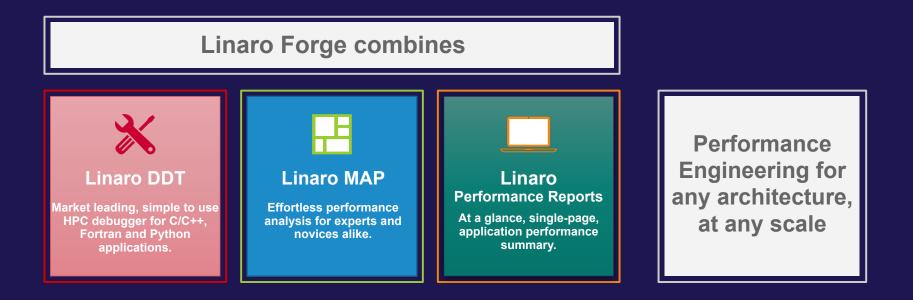
October 29-31, 2024



ALCF Hands-on HPC Workshop

HPC Development Solutions from Linaro

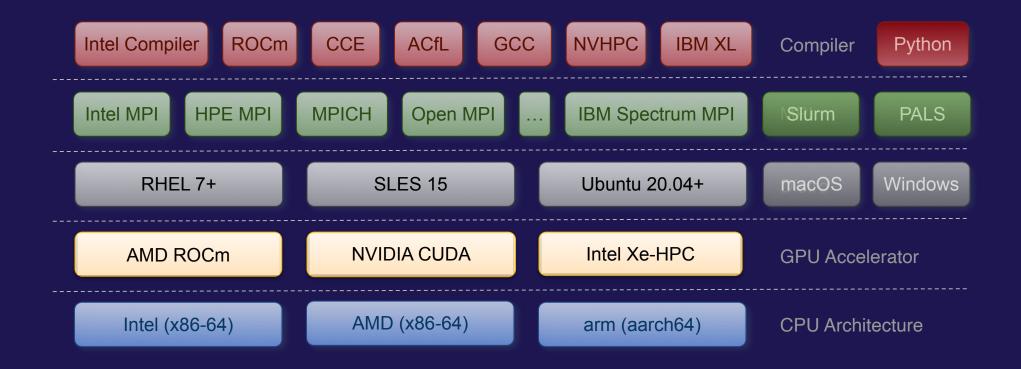
Best in class commercially supported tools for Linux and high-performance computing (HPC)





DDT Supported Platforms

Works across hardware architectures and HPC technologies





DDT UI

Intuitive and scalable user interface

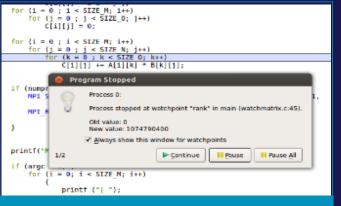
- 1 Process controls
- 2 Process groups
- 3 Source Code view
- 4 Variables
- 5 Evaluate window
- 6 Parallel Stack
- 7 Project files
- 8 Find a file or function

Eile Edit View Control Iools Window Help														
Current Group:	* Focus on cur	rrent: 🖲 Gr	roup 🔿	Process O Three	ad I Step Threads	s Togethe								
All	512 processes (0-511) Currently selected:				Paused: 512 Playing: 0 Finished: 0 1 (on comp000, pid 1003)									
Group 1	256 processes	(0,2,4,6,8,1	0,12,14,1	16,18,20, (256 t	otal)) Pause	ed: 256	Playing: 0	Finis	ished: 0					
Group 2	171 processes	(0,3.6.9,12,	.15.18.21	.24,27,30, (171	total)} Pause	ed: 171	Playing: 0	Finis	ished: 0					
Create Group														
Project Files	3	c hello.c	×	hello.c 🗶							Locals	Current Line(s)	Curr	rent Stack
Search (Ctrl+K)	٩,	130		sprintf(messad	ge, "Greetings f	rom pro	cess %d!".	my	rank):		Locals			@ 18
 Application Code 		131			ng message from						Name		Value	
> = /		132		dest = 0;							argc		- 1	-
* 🖲 Sources		133			(message)+1 to i						Fargv			0x7fffffffd
hello.c		134				age) +	1, MPI_CHAP	R, de	lest, tag, MPI_COMM_WORL	.D)		Watched	— O	'
approvide app				eingWatched;			bigAm dest	ay	— o					
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func2() : int	t i	140							MPI COMM WORLD, &status	s) : :	messa	ae	_	
E func3(): vo	func3(): void 141 printf("%s\n", message				<u></u>	500100, 0				my_ra		/1	ε	
main(int argument)	gc,char ** arg	142		beingWatch							p		- 5	
typeOne		143		}	,						source	9	— 3	2767
typeThree		144	}	2							▶ status			
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		146	for	(i = 1; i < ar	rgc; i++)						tables			
		147			≨ !strcmp(argv[i], "nem	(crash*))				tag		5	io 👘
- 7		148		func3();							Itest	(4)		
•		149									х	•	- 1	
		150		(i = 1; i < ar							У		- 1	2
		151		1T (argv[1] 60	& !strcmp(argv[i	1, "gua	rdafter"))			Ŧ				
4	- F -									P.				
Input/Output Breakpoints Watchpoints Stacks (All) Tracepoints Tracepoint Output Logbook Evaluate @18														
Stacks (All)						aiue 	003		_					
Processes Function *							/ 1	005						
511 main (hello.c:141)														
1 main (hello.c:148)														
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-	•													

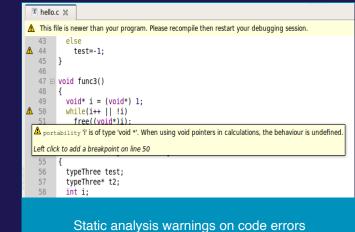
Linaro DDT Debugger Highlights

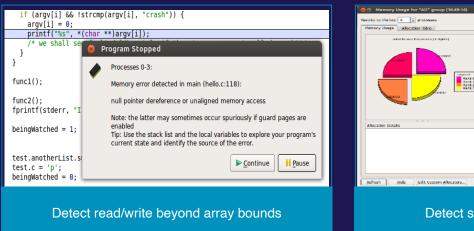
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Tracepoint Output					
Tracepoint	Processes	Values logged			
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vhone.f90:81	960, ranks 12,14-17,22-23,12	ks 1 kmax pez			
vhone.f90:85	942, ranks 12,14-17,22-23,12	mype 2172-3527 jcol: 44 2-83 mod 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: 44 2-83 mod pey			
vhone.f90:81	898, ranks 12,14-17,22-23,12	ks 1 kmax pez			

The scalable print alternative



Stop on variable change





A tenery large for full group (to the large function of the lar



GPU Debugging

<u>File Edit View Control Tools Window H</u> elp								
Focus on current: Process Threa	d 🗋 Step Threads Together							
Threads 1 2 K4								
GPU Threads (MatrixMulHIP(float*	Block 3 🗘 2 🗘 0 🗘 Thread 5 🗘 18 🗢 0 🌲 Go	Grid size: 4x4x1 Block size: 32x32x1						
Project Files	.срр 🗶	Lo Curre Curr GP						
Search (Ctrl+K) 🛛 🔧 19	<pre>int i = blockIdx.y * blockDim.y + threa</pre>	GPU Devices						
- Application Code	<pre>int j = blockIdx.x * blockDim.x + threa</pre>	Attribute Name Value						
k = / 21		✓ Ranks 0						
▼ Sources 22 ▼ 23	for(int k = 0; k < wA; k++)	vega20 2 Devices						
matrixMul.cp 23 24	{ temp += A[i * wA + k] * B[k* wB +	IDs 0-1 Threads 2400						
Constantly 25	}	Cores 240						
🖲 main(int al 🕥 26	C[i * wB + j] = temp;							
MatrixMul 27								
MatrixMul 28	<pre>syncthreads();</pre>							
MatrixMul 29 } External Code 30								
50	-label unid Materia WaluTDChanad (flast v							
31 • 32 {	<mark>global</mark> void MatrixMulHIPShared(float *(
32 1	// Block row and column							
34	int blockRow = blockIdx y	•						
	· · · · · · · · · · · · · · · · · · ·							
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Kernel Progress View	o x .	Name Value						
Kernel	Progress	i 82						
MatrixMul wA 128								
		wB 128 temp 1.27999914						
		temp 1.27555514						
not scheduled scheduled selected <u>How do I interpret GPU kernel progress?</u>								

- Support AMD, Intel and Nvidia GPUs
- Debug simultaneously on GPU and CPU
- Look and feel exactly the same
- Main Features work in GPU
- Key (additional) GPU features:
 - Kernel Progress View
 - GPU thread in parallel stack view
 - GPU Thread Selector
 - GPU Device Pane
- For NVIDIA's nvcc compiler, kernels must be compiled with the -g -G flags



Python Debugging

Debug Features

- Sparklines for Python variables
- Tracepoints
- MDA viewer
- Mixed language support

Improved Evaluations:

- Matrix objects
- Array objects
- Pandas DataFrame
- Series objects

• Python Specific:

- Stop on uncaught Python exception
- Show F-string variables
- Mpi4py, NumPy, SciPy

ddt --connect mpiexec -n 8 python3 %allinea_python_debug% ./mmult.py

Current Group: All	Image: Solution of the second state		
Create Group			
🗶 🗗 🛛 Project Files	P mmult	Locals Current Line(s)	Current Stacl
Search (೫K)	124 if mr == 0:	× 🗗 🛛 Local	s
	125 if fortran_style_array_order: 126 mat.a = numpy.ndarray(shape=(sz, sz), dtype='d', order='F	Name	Value
C lseek64.c	126 mat_a = numpy.ndarray(shape=(sz, sz), dtype='d', order='F 127 mat b = numpy.ndarray(shape=(sz, sz), dtype='d', order='F		mpi4py
> 💀 Ismr.py	128 mat c = numpy.ndarray(shape=(sz, sz), dtype='d', order='F		"res_Py
	129 else:	fortran style array	False
> 📴 Isqr.py	130 mat_a = numpy.ndarray(shape=(sz*sz), dtype='d', order='C')	Interco
Istat64.c	131 mat_b = numpy.ndarray(shape=(sz*sz), dtype='d', order='C' 132 mat_c = numpy.ndarray(shape=(sz*sz), dtype='d', order='C'		"C"
> 💀 Izma.py	132 mat_c = humpy.hdarray(shape=(sz^sz), dtype='d', order='c'		
> 💀 machinery.py	<pre>133 print("{}: Initializing_matrices".format(mr))</pre>	> mat_a	numpy
> 💀 main.py	135 minit(sz, fortran_style_array_order, mat_a)	─ v mat_b	ndarray
> 💀 matfuncs.py	136 minit(sz, fortran_style_array_order, mat_b)	[0]	0.0
> 💀 matfuncs.py	137 minit(sz, fortran_style_array_order, mat_c) 138	[1000]	
memchr.S	138 print("{}: Sending matrices".format(mr))	[100]	0.0
memchr.S	140 for i in range (1, nproc):	[101]	0.0
memcmp.S	141 # Get a slice from the mat_a and mat_c matrix	[102]	0.0
	142 if fortran_style_array_order:	[103]	0.0
memcmp.S	143mat_a_slice = mat_c[:, i*mslice_r:(i+1)*mslice_r]144mat c slice = mat c[:, i*mslice r:(i+1)*mslice r]	[103]	0.0
> 💀 memmap.py	144 mat_c_slice = mat_c[:, 1^mslice_r:(1+1)^mslice_r]		
		<u></u>	
	oints Watchpoints Stacks (All) Tracepoints Tracepoint Output Logbook 🗴 🖻	Evaluate	
K 0	Stacks (All) Name Value		
Processes Function	n mslice mslice	512	



DDT in offline mode

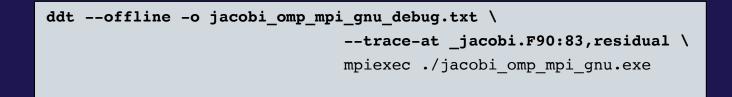
Run the application under DDT and halt or report when a failure occurs

You can run the debugger in non-interactive mode

- For long-running jobs / debugging at very high scale
- For automated testing, continuous integration...

To do so, use following arguments:

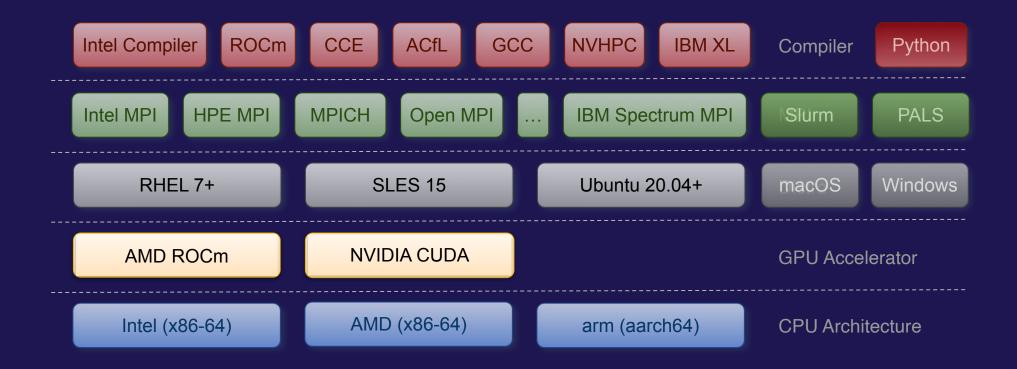
- \$ ddt --offline --output=report.html mpirun ./jacobi_omp_mpi_gnu.exe
 - --offline enable non-interactive debugging
 - --output specifies the name and output of the non-interactive debugging session (HTML or Txt)
 - Add --mem-debug to enable memory debugging and memory leak detection





MAP and Performance Reports Supported Platforms

Works across hardware architectures and HPC technologies





Linaro Performance tools

Characterize and understand the performance of HPC application runs



Commercially supported by Linaro



- Analyses metric around CPU, memory, IO, hardware counters, etc.
- Possibility for users to add their own metrics



Build a culture of application performance & efficiency awareness

- Analyses data and reports the information that matters to users
- Provides simple guidance to help improve workloads' efficiency



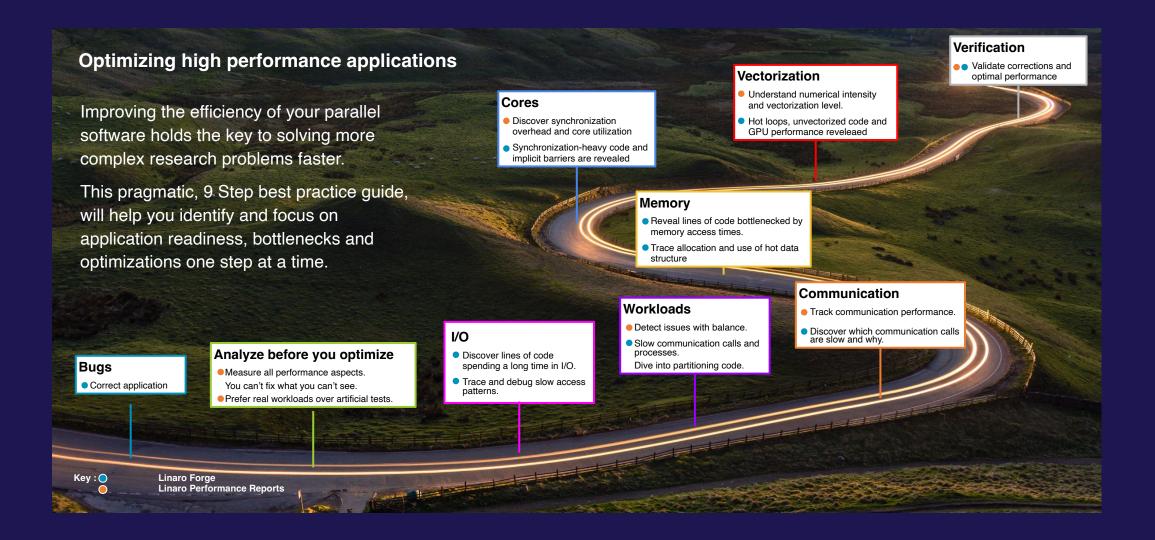
Relevant advice to avoid pitfalls

Adds value to typical users' workflows

- Define application behaviour and performance expectations
- Integrate outputs to various systems for validation (eg. continuous integration)
- Can be automated completely (no user intervention)



9 Step guide for optimising code





Linaro Performance Reports

A high-level view of application performance with "plain English" insights

	Command:	mpiexec.hydra -host node-1,node-2 -map-by socket -n 16 -ppn 8 ./Bin/low_freq///Src//hydro -i
Performance		/Bin/low_freq////Input/input_250x125_corner.nml
REPORTS	Resources:	2 nodes (8 physical, 8 logical cores per node)
	Memory:	15 GiB per node
	Tasks:	16 processes, OMP_NUM_THREADS was 1
	Machine:	node-1
	Start time:	Thu Jul 9 2015 10:32:13
	Total time:	165 seconds (about 3 minutes)
	Full path:	Bin//Src

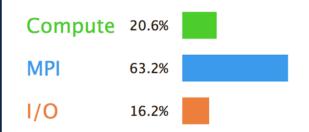
I/O

A breakdown of the 16.2% I/O time:

Time in reads	0.0%	
Time in writes	100.0%	
Effective process read rate	0.00 bytes/s	
Effective process write rate	1.38 MB/s	

Most of the time is spent in write operations with a very low effective transfer rate. This may be caused by contention for the filesystem or inefficient access patterns. Use an I/O profiler to investigate which write calls are affected.

Summary: hydro is MPI-bound in this configuration



Time spent running application code. High values are usually good. This is **very low**; focus on improving MPI or I/O performance first

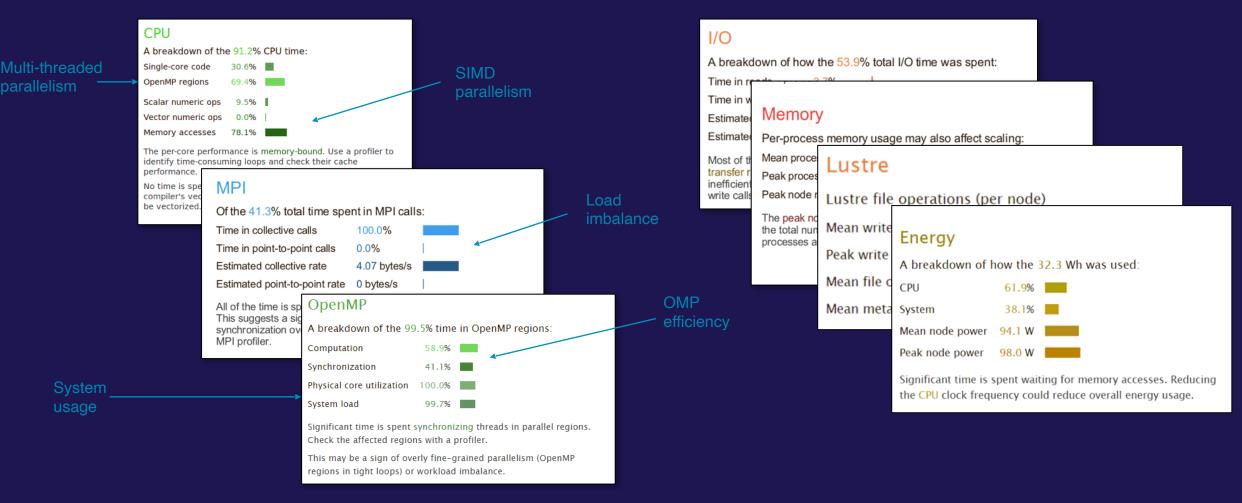
Time spent in MPI calls. High values are usually bad. This is **high**; check the MPI breakdown for advice on reducing it

Time spent in filesystem I/O. High values are usually bad. This is **average**; check the I/O breakdown section for optimization advice



Linaro Performance Reports Metrics

Lowers expertise requirements by explaining everything in detail right in the report





MAP Capabilities

MAP is a sampling based scalable profiler

- Built on same framework as DDT
- Parallel support for MPI, OpenMP, CUDA
- Designed for C/C++/Fortran

Designed for 'hot-spot' analysis

- Stack traces
- Augmented with performance metrics

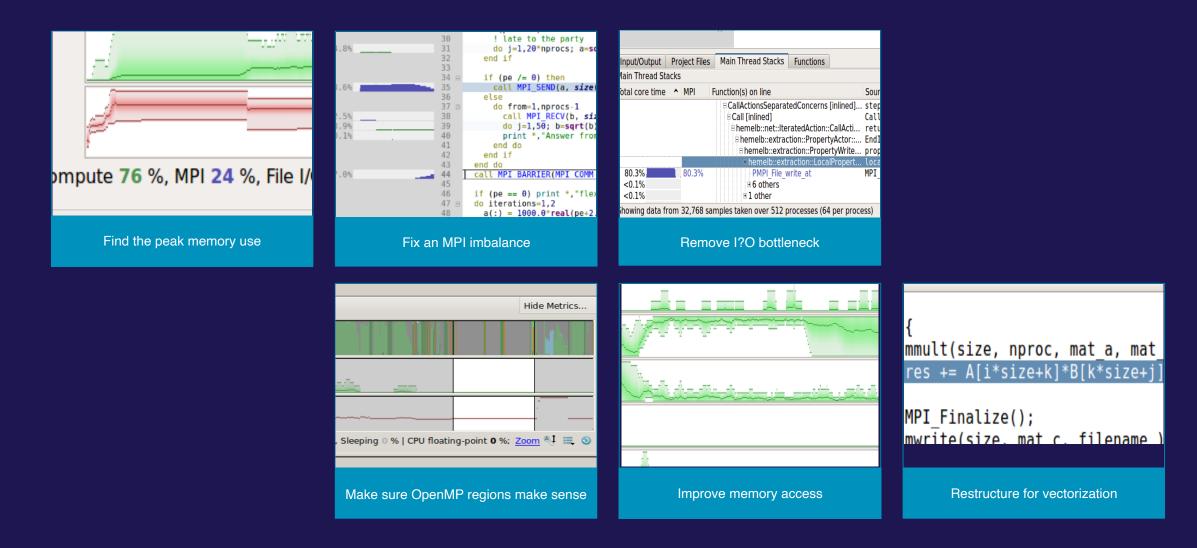
Adaptive sampling rate

- Throws data away 1,000 samples per process
- Low overhead, scalable and small file size





MAP Highlights





Argonne Leadership Computing Facility

GPU profiling

Profiled: <u>tea_leaf</u> on 12 proc	esses,2 nodes, <u>72 cores</u>	(6 per process) for	46.1s Sampled from:	We 🌍 🗸 🚺 🚦	Main Thread	Only Hide Metrics
Main thread activity		ang balang kanalang k	an alanta and to be	a santanyi wanananyi walan	n da dinanadah	aba panan bibidi, p
Memory usage	563					
531 MB	1. A.					
GPU utilization	0 100					
11.8 %						
GPU memory usage	0					
3.5 %						
3.3 %	0					
10:58:49-10:59:35 (46.086	6s): Main thread comput	e 0.4 %,MPI 77.0	%,Waiting for Accelerato	or 22.6 %,File I/O 0.0 %		Zoom 🔍 📃 💿
📕 diffuse	pack_kernel_cud	l				
4.68	18	cuda	_chunk.packUr	npackAllBuffer	rs(fields,	offsets, *de
	19	}				
		time (25.53s) wa	ing instructions on this li s waiting for accelerator Learcudachun	ne <::packUnpack#	AllBuffe <u>rs</u>	
	22			DS], int offse		ELDS],
			—	nst int face,	—	
	24					
	Input/Output	Project Files 🖡 M	ain Thread Stacks 🛛 Fu	nctions GPU Kernels	Libraries	
×ø			GPU Kernels			
Breakdown	 Selected 	Blocked GPU	Kernels	Source	e Pos	ition
			tea_leaf [program]		line-level inf	
4.4%	- Alexandress	4	device_tea_leaf_ppcg			
4.2%		4	🖌 device_tea_leaf_ppcg	_solve_calc_sd		

Profile

- Supports both AMD and Nvidia GPUs
- Able to bring up metadata of the profile
- Mixed CPU [green] / GPU [purple] application
- CPU time waiting for GPU Kernels [purple]
- GPU Kernels graph indicating Kernel activity

GUI information

- GUI is consistent across platforms
- Zoom into main thread activity
- Ranked by highest contributors to app time



Python Profiling

19.0 adds support for Python

- Call stacks
- Time in interpreter

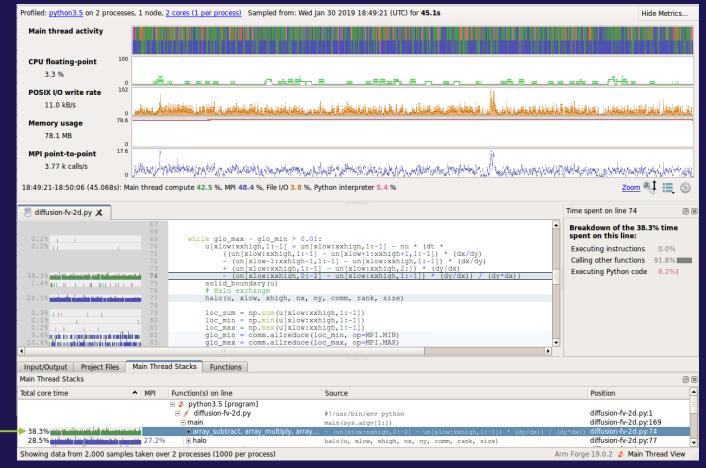
Works with MPI4PY

• Usual MAP metrics

Source code view

• Mixed language support

Note: Green as operation is on numpy array, so backed by C routine, not — Python (which would be pink)



map --profile mpiexec -n 2 python ./diffusion-fv-2d.py



Compiler Remarks

Annotates source code with compiler remarks

- Remarks are extracted from the compiler optimisation report
- Compiler remarks are displayed as annotations next to your source code

Colour coded

- Their colour indicates the type of remark present in the following priority order:
- Red: failed or missed optimisations
- Green: successful or passed optimisations
- White: information or analysis notes

Compiler Remarks menu.

- Specify build directories for non-trivial build systems
- Filter out remarks

207 * #pragma omp parallel shared (newval, values) wave_openmp.c:207 __kmpc_fork_call will not be inlined into update wave_openmp.c:167 because its definition is unavailable [inline] wave_openmp.c:207 __kmpc_fork_call will not be inlined into update wave_openmp.c:167 because its definition is unavailable [inline] wave_openmp.c:207 __kmpc_fork_call will not be inlined into update wave_openmp.c:167 because its definition is unavailable [inline] wave_openmp.c:207 _ kmpc_fork_call will not be inlined into update copies cost generated in function [regalloc] wave_openmp.c:207 'update.omp_outlined_debug__' inlined into 'update.omp_outlined wave_openmp.c:207': always inline attribute at callsite update.omp_outlined:0:1; [inline] wave_openmp.c:207 96 stack bytes in function [prologepilog] wave_openmp.c:207 80 instructions in function [asm-printer]

5.0%	if ((first + j - 1 == 1) (first + j - 1 == tpoints))	^
214	<pre>newval[j] = 0.0;</pre>	
215	else	
43.6% at http://databashindbooking 7 216	do_math(j);	
217	}	
218	}	
219		
220	/* swap arrays */	*
4		P I





Cheat sheet

Job Script

#!/bin/bash -l

#PBS -I select=1
#PBS -I filesystems=home:eagle
#PBS -I walltime=0:30:00
#PBS -q HandsOnHPC
#PBS -A alcf_training

module use /soft/modulefiles module load forge cray-cti

Debug in reverse connect mode ddt --connect mpiexec -n 4 ./simple

Debug in offline mode ddt --offline -o offline-debugging.html --break-at=simple.c:32 --break-at=simple.c:43 mpiexec -n 4 ./simple

Profile a Python application module load conda conda activate base

MPICH_GPU_SUPPORT_ENABLED=0 map --profile mpiexec -n 8 python myscript.py -s 3072

Interactive Session

qsub -I -I select=1 -I filesystems=home:eagle -I walltime=0:30:00 -q HandsOnHPC -A alcf_training

module use /soft/modulefiles module load forge cray-cti

Forge commands

ddtconnect	# Reverse connect
ddtoffline	# Run DDT without GUI
mapprofile	# Profile without GUI
perf-report	# Generate Performance Repor

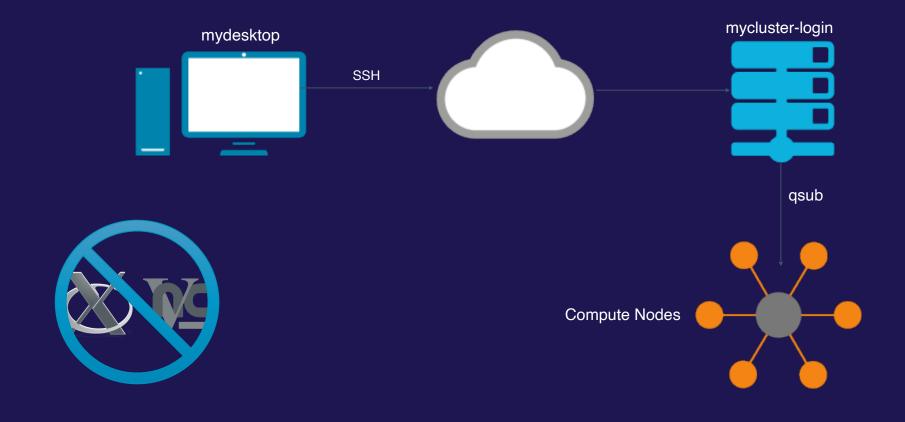


Forge userguide



The Forge GUI and where to run it

Forge provides a powerful GUIs that can be run in a variety of configurations





Remote connection to Polaris

$\bullet \bullet \bullet$	Linaro DDT - Linaro Forge 23.1	
Linaro Forge	• • •	Remote Launch Settings
10180	RUN Run and debug a program. ATTACH	Polaris <username>@polaris.alcf.anl.gov</username>
Linaro DDT	Attach to an already running program. OPEN CORE Remote Installation Directory: Open a core file from a previous run. Remote Installation Directory: MANUAL LAUNCH (ADVANCED) Remote Script:	How do I connect via a gateway (multi-hop)? /soft/debuggers/forge-24.0.3 Optional
Linaro MAP	Private Key: Private Key: Remote Launch: Configure KeepAlive Packets:	Optional Always look for source files locally Enable
	QUIT Interval:	30 seconds
Get trial licence Support linaroforge.com		Test Remote Launch
Remote Client ?	Help	OK Cancel





- <u>www.linaroforge.com</u>
- <u>support@forge.linaro.com</u>
- <u>https://docs.linaroforge.com/24.0.5/html/forge/index.html</u>



