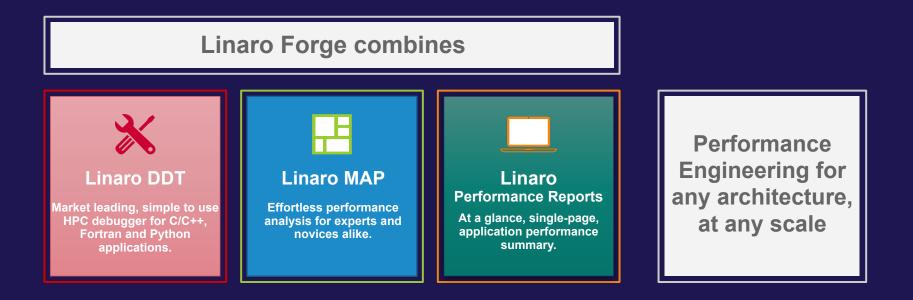
# October 29-31, 2024



# ALCF Hands-on HPC Workshop

# **HPC Development Solutions from Linaro**

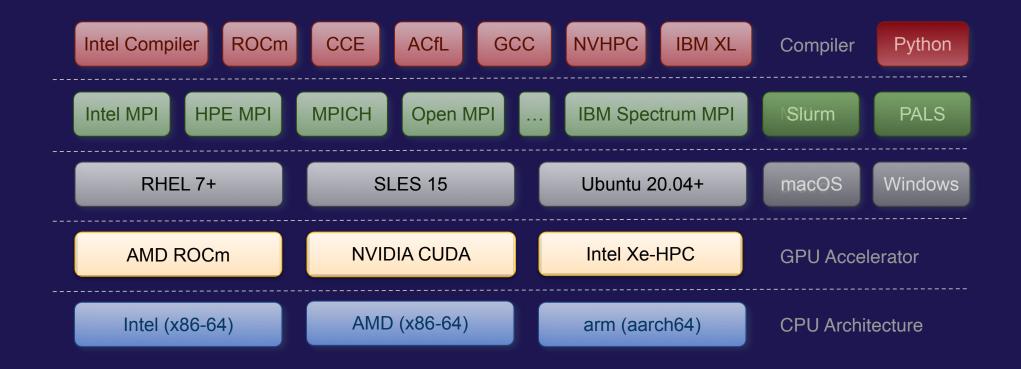
Best in class commercially supported tools for Linux and high-performance computing (HPC)





# **DDT Supported Platforms**

### Works across hardware architectures and HPC technologies





# DDT UI

# Intuitive and scalable user interface

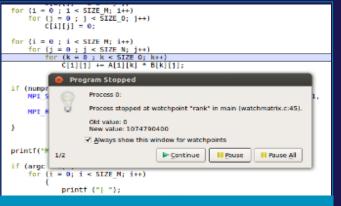
- 1 Process controls
- 2 Process groups
- 3 Source Code view
- 4 Variables
- 5 Evaluate window
- 6 Parallel Stack
- 7 Project files
- 8 Find a file or function

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
<ul> <li>Application Code</li> </ul>		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			
typeTwo		145	-								▶ t2		0	0x603050
		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	<b>•</b>	- 1	
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		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)														
$\mathbf{U}$														
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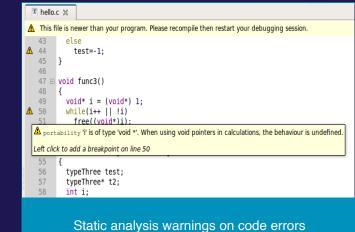
# Linaro DDT Debugger Highlights

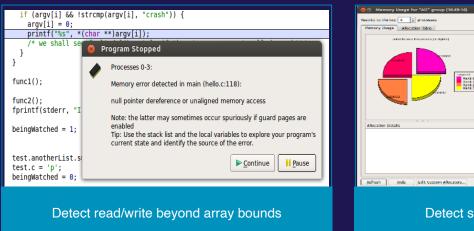
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Tracepoint Output					
Tracepoint	Processes	Values logged			
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vhone.f90:81	960, ranks 12,14-17,22-23,12	ks 1 kmax pez			
vhone.f90:85	942, ranks 12,14-17,22-23,12	mype 2172-3527 jcol: 44 2-83 mod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





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# **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						
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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

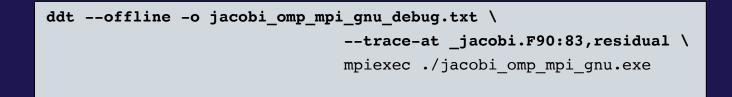
# Run the application under DDT and halt or report when a failure occurs

#### 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:

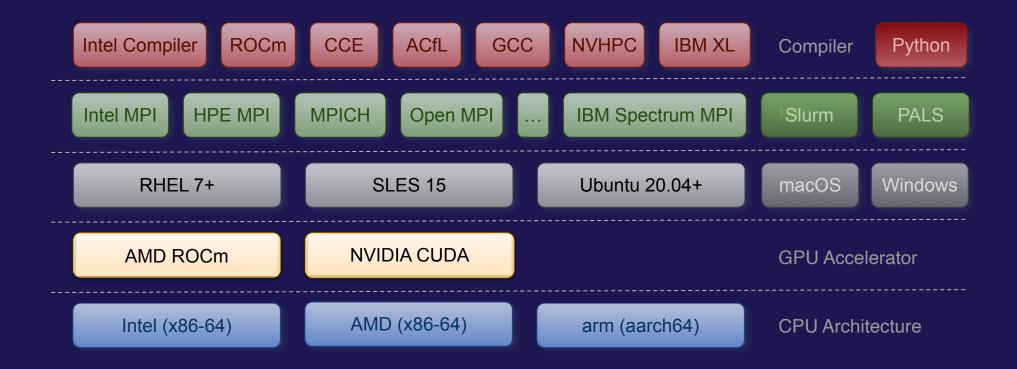
- \$ ddt --offline --output=report.html mpirun ./jacobi\_omp\_mpi\_gnu.exe
  - --offline enable non-interactive debugging
  - --output specifies the name and output of the non-interactive debugging session (HTML or Txt)
  - Add --mem-debug to enable memory debugging and memory leak detection





# **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



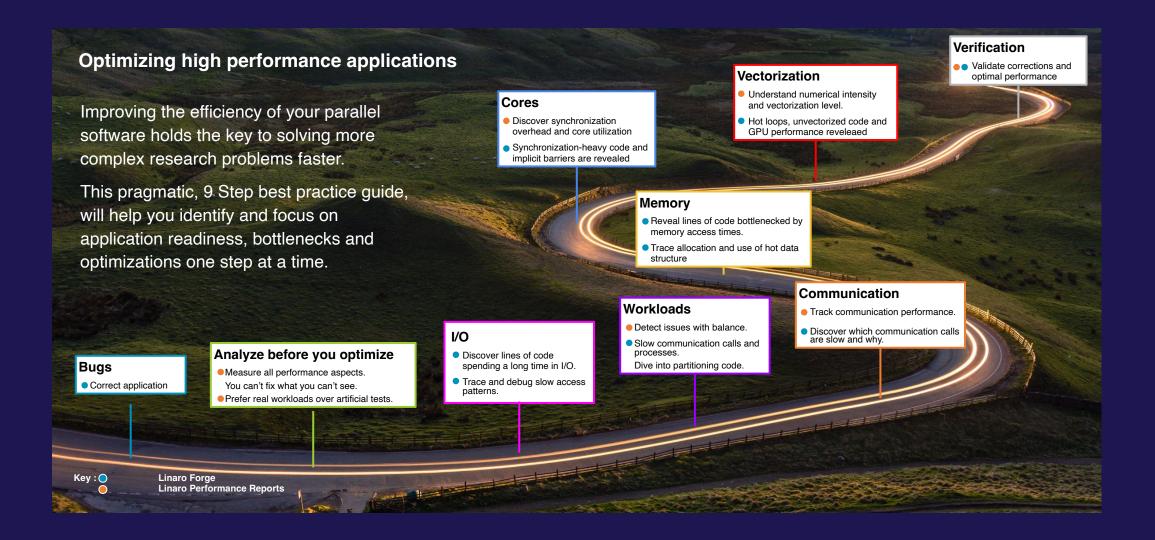
Relevant advice to avoid pitfalls

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	<b>Resources:</b>	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

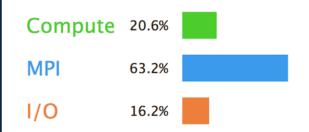
#### I/O

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

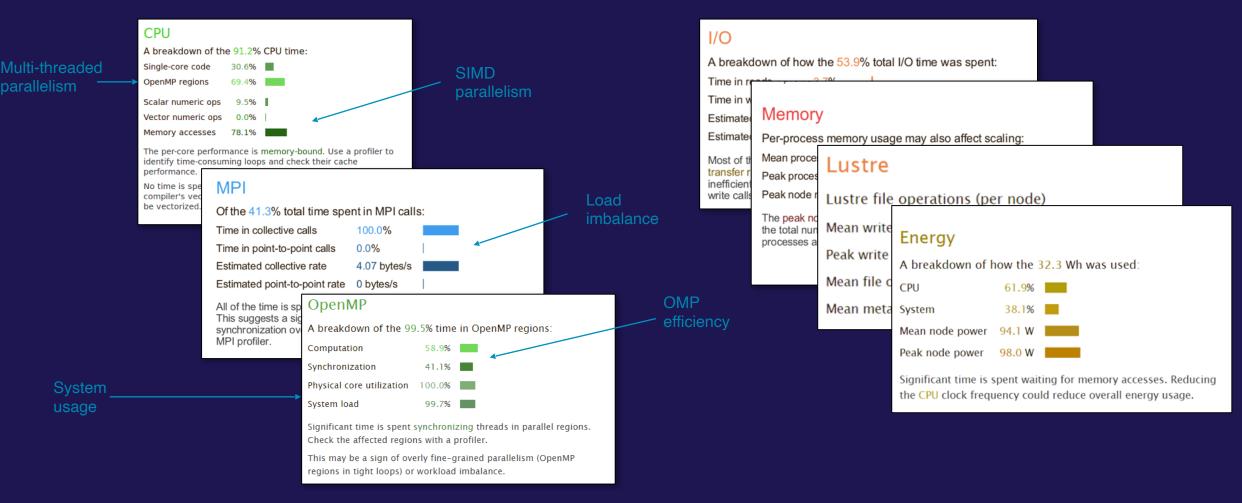
Time spent in MPI calls. High values are usually bad. This is **high**; check the MPI breakdown for advice on reducing it

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

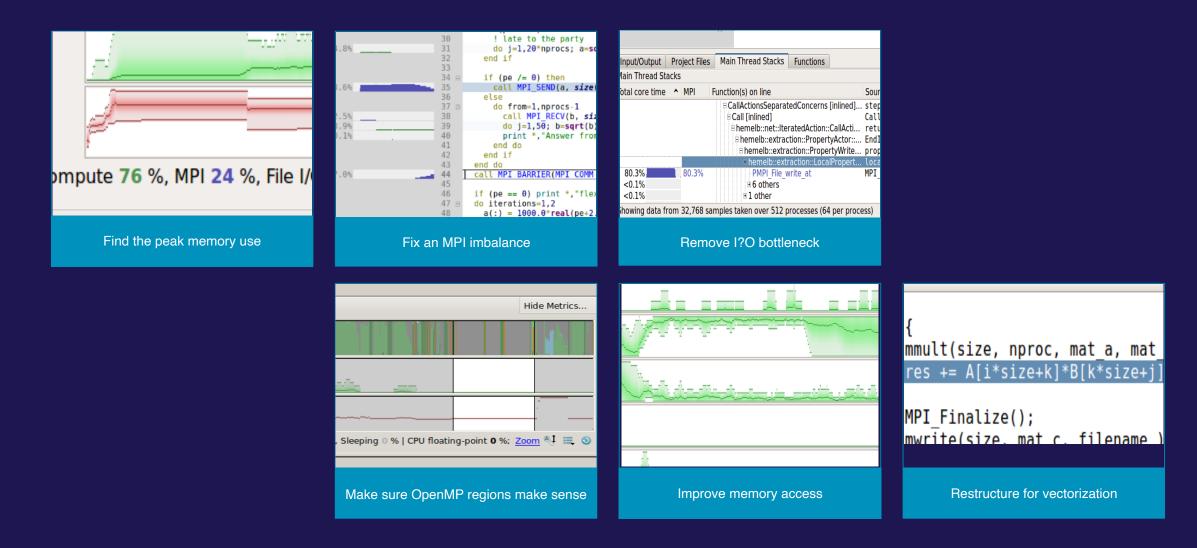
#### Adaptive sampling rate

- 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	<b>46.1s</b> 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	<ul> <li>Selected</li> </ul>	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

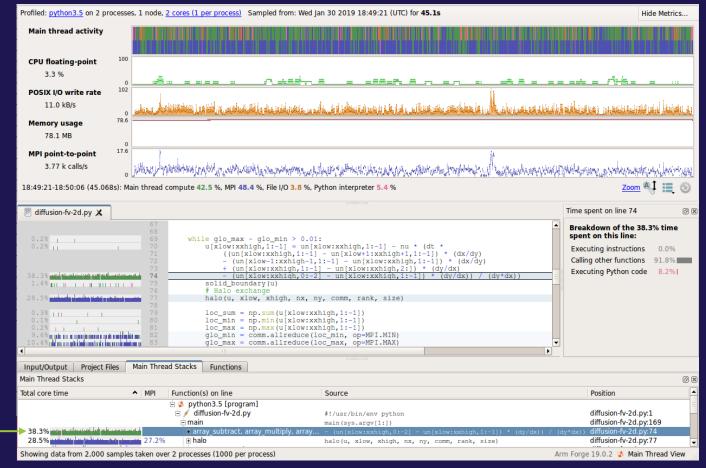
#### Works with MPI4PY

• 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))	<b>^</b>
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

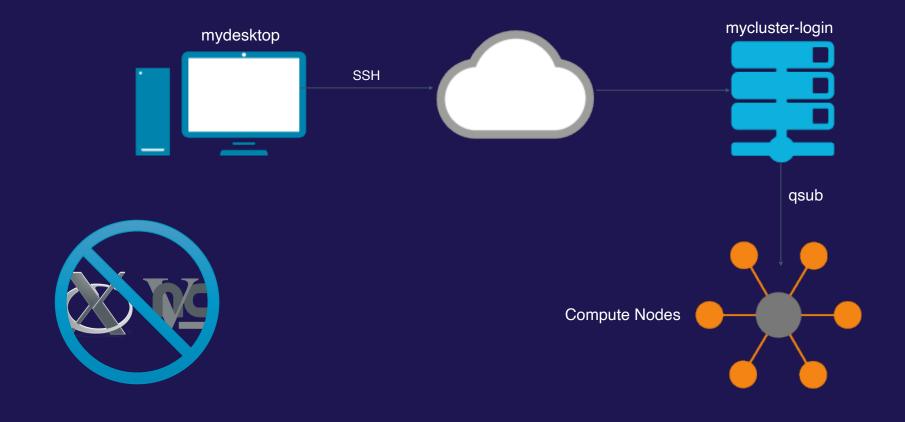


Forge userguide



# 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>



