

HPCToolkit: Performance Analysis of GPU-accelerated Kokkos Applications on NVIDIA GPUs

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Current Funding for HPCToolkit

- Government
 - Lawrence Livermore National Laboratory Subcontract B658833
 - DOE Software Tools Ecosystem Project UT-Battelle Subcontract CW54422
 - Argonne National Laboratory Subcontract 4F-60094
- Corporate
 - Advanced Micro Devices
 - TotalEnergies EP Research & Technology USA, LLC.

A Hands-on Example for the Tutorial: ArborX

A library written in Kokkos that provides performance portable algorithms for geometric search

% git clone https://github.com/hpctoolkit/hpctoolkit-tutorial-examples % cd hpctoolkit-tutorial-examples/examples/gpu/arborx % source setup/perlmutter.sh % make all # downloads, builds, measures, and analyzes two executions % make view % make view-pc

Note: precomputed databases available on Perlmutter at /global/cfs/cdirs/m3977/data/arborx



Outline

- Introduction to HPCToolkit performance tools
 - Overview of HPCToolkit components and their workflow
 - HPCToolkit's graphical user interfaces
- Analyzing the performance of GPU-accelerated codes with HPCToolkit
 - GAMESS
 - ArborX
 - LAMMPS at Exascale
- Coming attractions
- Troubleshooting



Rice University's HPCToolkit Performance Tools

Measure and analyze performance of CPU and GPU-accelerated applications

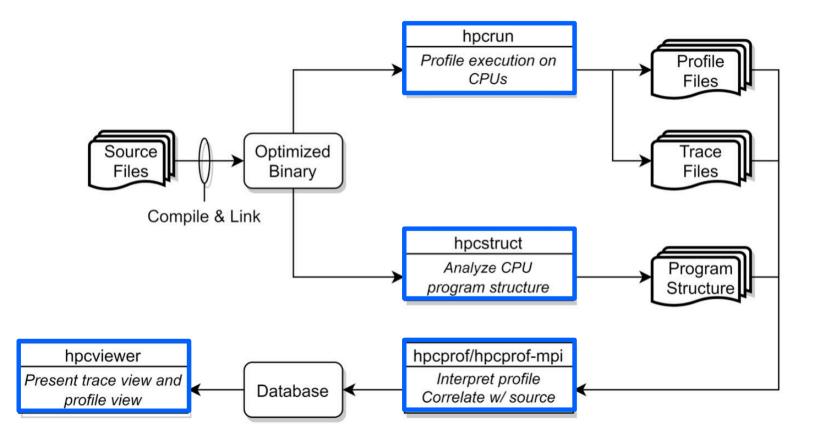
- Easy: profile unmodified application binaries
- Fast: low-overhead measurement
- Informative: understand where an application spends its time and why
 - call path profiles associate metrics with application source code contexts
 - optional hierarchical traces to understand execution dynamics
- Broad audience
 - application developers
 - framework developers
 - runtime and tool developers
- Measures complex programs on a broad range of platforms
 - CPU: x86_64, Power, ARM
 - GPU: NVIDIA, AMD, Intel

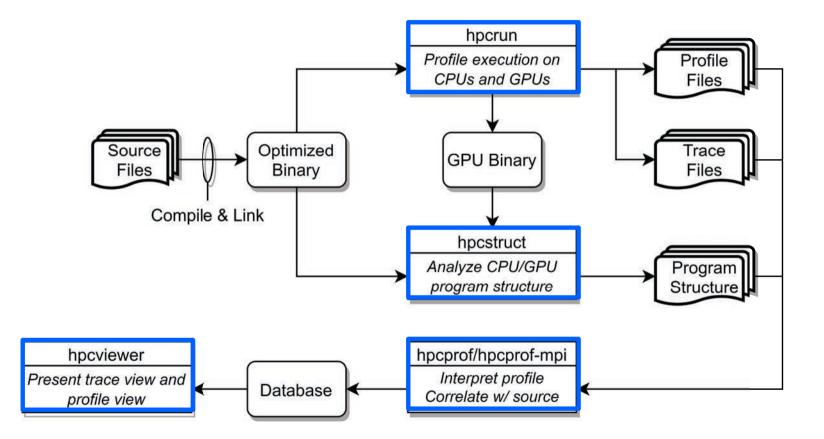


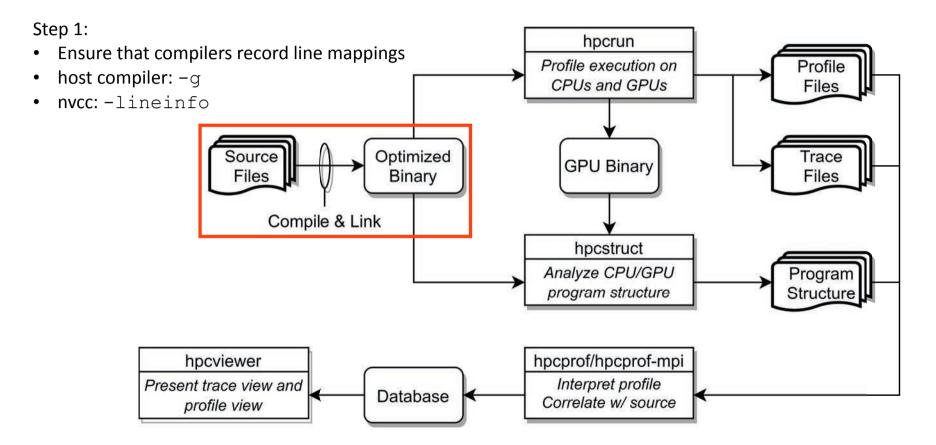
How does HPCToolkit Differ from NVIDIA's Tools?

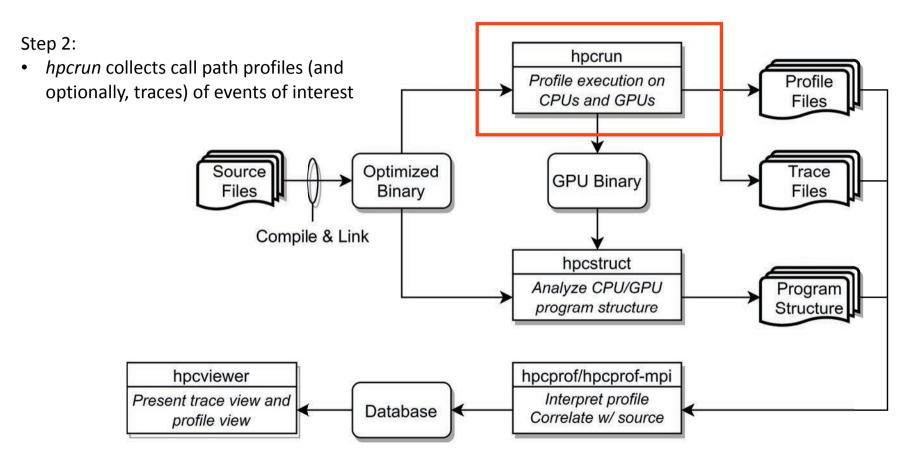
- NVIDIA NSight Systems
 - tracing of CPU and GPU streams
 - analyze traces when you open them with the GUI
 - long running traces are huge and thus extremely slow to analyze, limiting scalability
 - designed for measurement and analysis within a node
- NVIDIA NSight Compute
 - detailed measurement of kernels with counters and execution replay
 - very slow measurement
 - flat display of measurements within GPU kernels
- HPCToolkit
 - supports more scalable tracing than Nsight Systems
 - measure exascale executions across many GPUs and nodes
 - scalable, parallel post-mortem analysis vs. non-scalable in-GUI analysis
 - detailed reconstruction of estimates for calling context profiles within GPU kernels

HPCToolkit's Workflow for CPU Applications







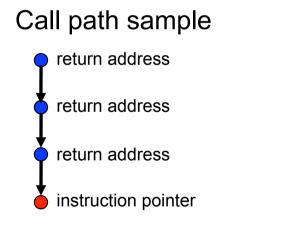


Measurement of CPU and GPU-accelerated Applications

- Sampling using Linux timers and hardware counter overflows on the CPU
- Callbacks when GPU operations are launched and (sometimes) completed
- Event stream for GPU operations; PC Samples (NVIDIA)
- Binary instrumentation of GPU kernels on Intel GPUs for fine-grain measurement

Call Stack Unwinding to Attribute Costs in Context

- Unwind when timer or hardware counter overflows
 - measurement overhead proportional to sampling frequency rather than call frequency
- Unwind to capture context for events such as GPU kernel launches



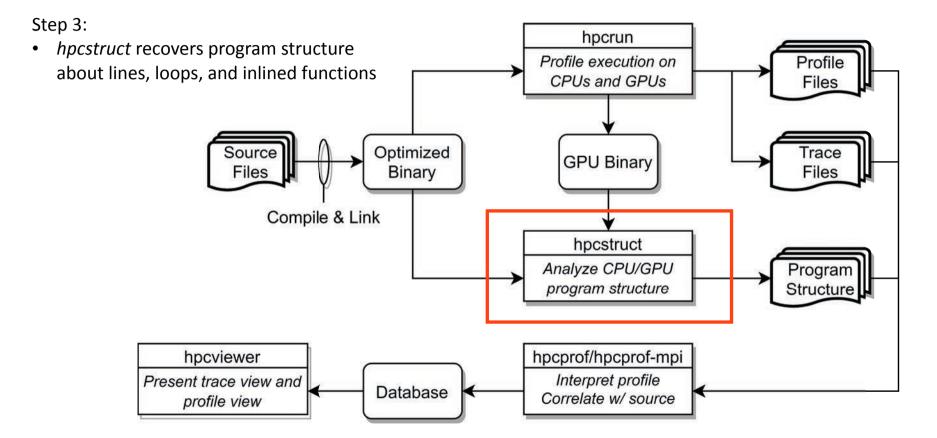
Calling context tree

hpcrun: Measure CPU and/or GPU activity

- GPU profiling
 - hpcrun -e gpu=xxx <app>
- GPU instrumentation (Intel GPU only)
 - hpcrun -e gpu=level0,inst=count,latency <app>
- GPU PC sampling (NVIDIA GPU only)
 - hpcrun -e gpu=nvidia,pc <app>
- CPU and GPU Tracing (in addition to profiling)
 - hpcrun -e CPUTIME -e gpu=xxx -t <app>
- Use hpcrun with job launchers
 - srun -n 1 -G 1 hpcrun -e gpu=xxx <app>



xxx ∈ {nvidia,amd,opencl,level0}



hpcstruct: Analyze CPU and GPU Binaries Using Multiple Threads

• Usage

hpcstruct [--gpucfg yes] <measurement-directory>

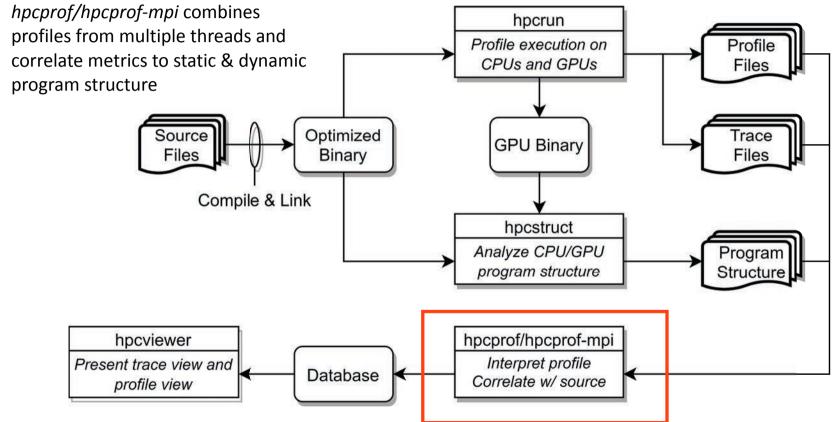
- What it does
 - Recover program structure information
 - Files, functions, inlined templates or functions, loops, source lines
 - In parallel, analyze all CPU and GPU binaries that were measured by HPCToolkit
 - -default: use size(CPU set)/2 threads
 - -analyze large application binaries with 16 threads
 - -analyze multiple small application binaries concurrently with 2 threads each
 - Cache binary analysis results for reuse when analyzing other executions

NOTE: --gpucfg yes needed only for analysis of GPU binaries for interpreting PC samples on NVIDIA GPUs



Step 4:

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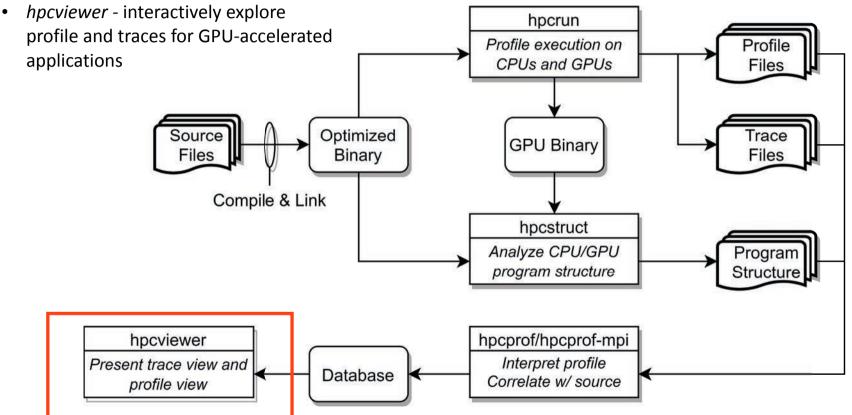


hpcprof/hpcprof-mpi: Associate Measurements with Program Structure

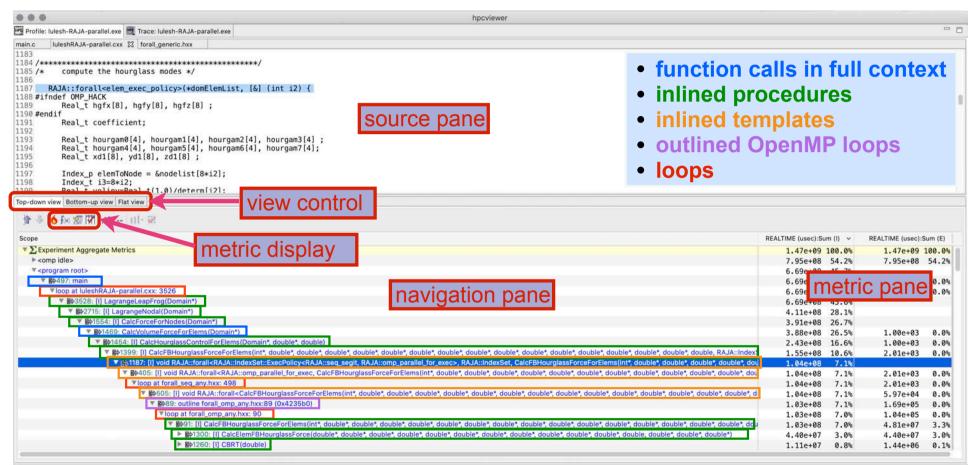
- Analyze data from modest executions with multithreading hpcprof <measurement-directory>
- Analyze data from large executions with distributed-memory parallelism + multithreading srun -N 2 -n 2 -c 126 hpcprof-mpi <measurement-directory>



Step 4:



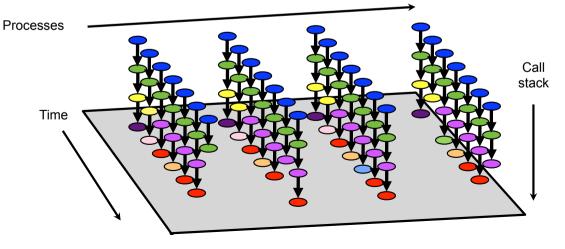
Code-centric Analysis with hpcviewer





Understanding Temporal Behavior

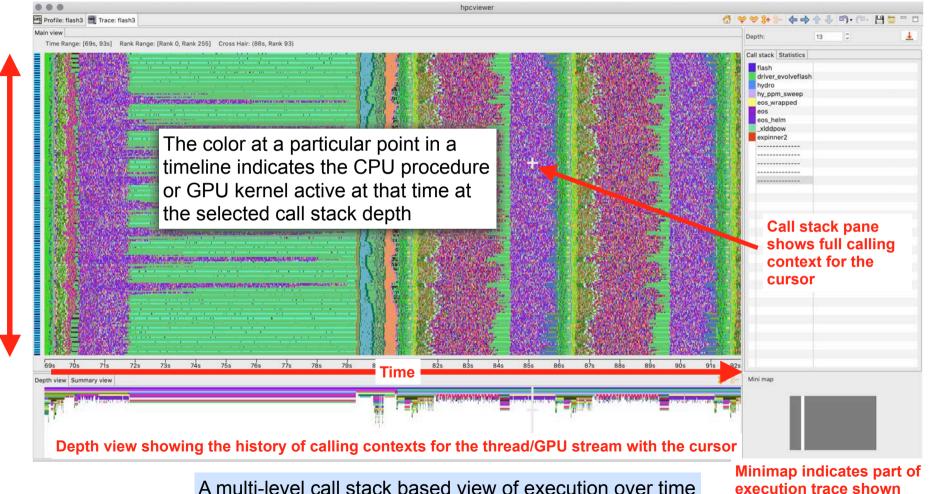
- Profiling compresses out the temporal dimension
 - Temporal patterns, e.g. serial sections and dynamic load imbalance are invisible in profiles
- What can we do? Trace call path samples
 - N times per second, take a call path sample of each thread
 - Organize the samples for each thread along a time line
 - View how the execution evolves left to right
 - What do we view? assign each procedure a color; view a depth slice of an execution



Time-centric Analysis with hpcviewer

GPU streams

MPI ranks, OpenMP Threads,



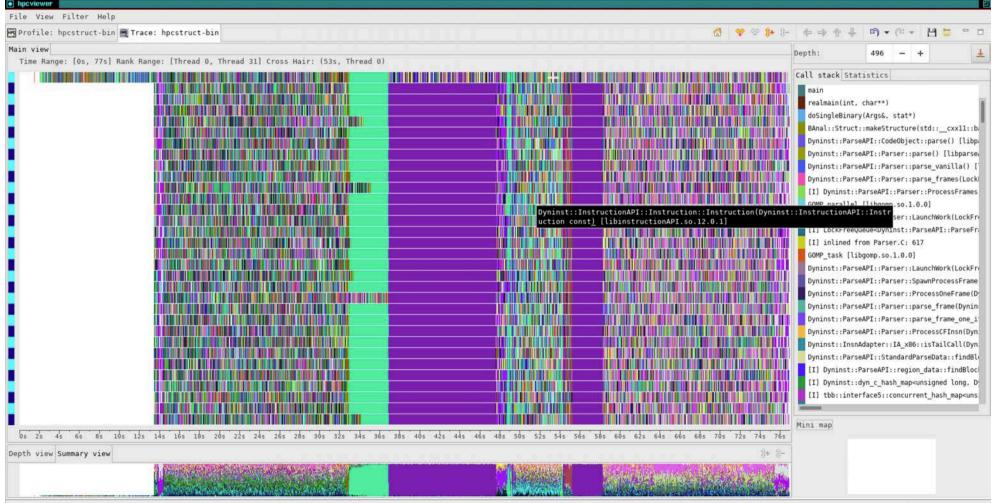
A multi-level call stack based view of execution over time

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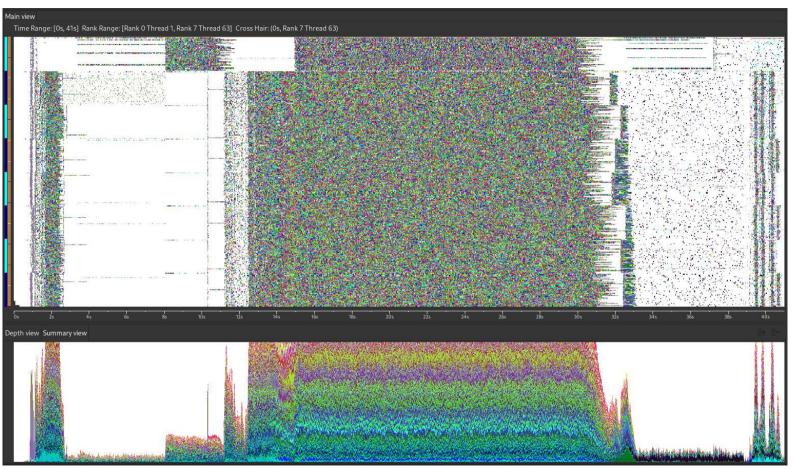
Summary of ECP Developments

- Measurement
 - profile and trace GPU-accelerated applications on AMD, Intel, and NVIDIA GPUs
 - source-level measurement of Python frameworks, e.g. Pytorch
 - record measurement data in sparse formats: benefits GPU-accelerated programs with many metrics
 - implement of OMPT performance tools interface in AMD OpenMP and LLVM
- Binary analysis
 - binary analysis of AMD, Intel, NVIDIA GPU binaries
 - parallel analysis of application binaries to speed recovery of program structure
- Performance analysis and attribution
 - MPI + OpenMP highly parallel analysis of measurement data at exascale
 - sparse representations observed to reduce performance analysis results by > 1000x
 - detailed attribution of PC samples to rich calling contexts within GPU kernels
- Presentation
 - interactive display profiles and terabytes of traces from exascale executions

hpcstruct Example: Analyze 7.7GB TensorFlow library (170MB text) in 77s



Analyze 38.1GB data for 2K MPI ranks + 2K GPUs using 1K threads in 41s





Case Studies

- GAMESS (OpenMP)
- ArborX (Kokkos)
- LAMMPS (Kokkos) at exascale

Case Study: GAMESS

- General Atomic and Molecular Electronic Structure System (GAMESS)
 - general *ab initio* quantum chemistry package
- Calculates the energies, structures, and properties of a wide range of chemical systems
- Experiments
 - GPU-accelerated nodes at a prior Perlmutter hackathon
 - Single node with 4 GPUs
 - Five nodes with 20 GPUs

Perlmutter node at a glance

AMD Milan CPU 4 NVIDIA A100 GPUs 256 GB memory



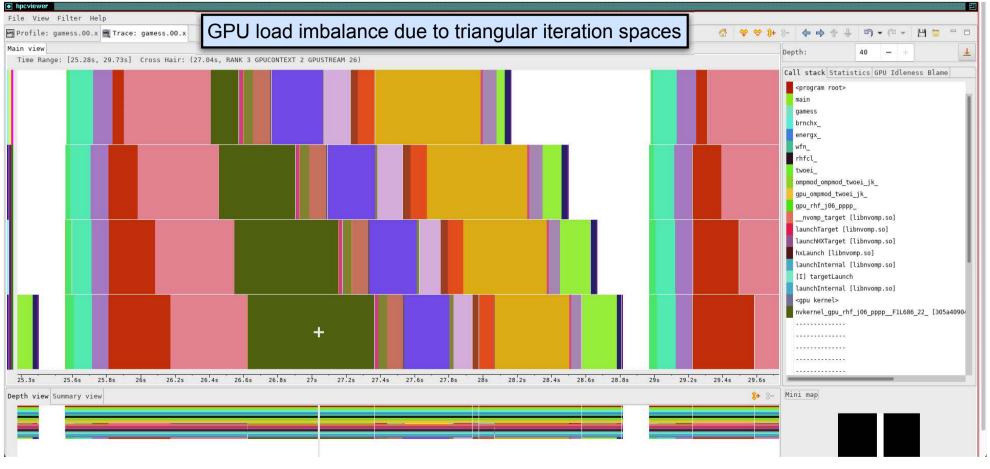
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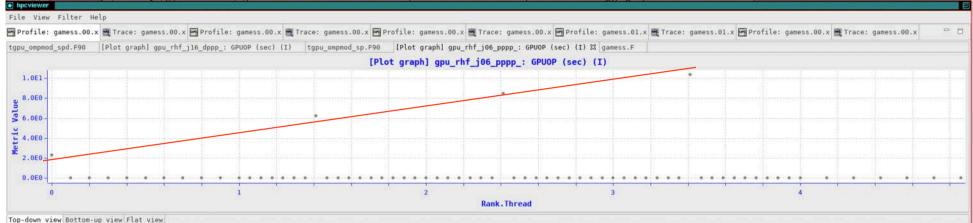


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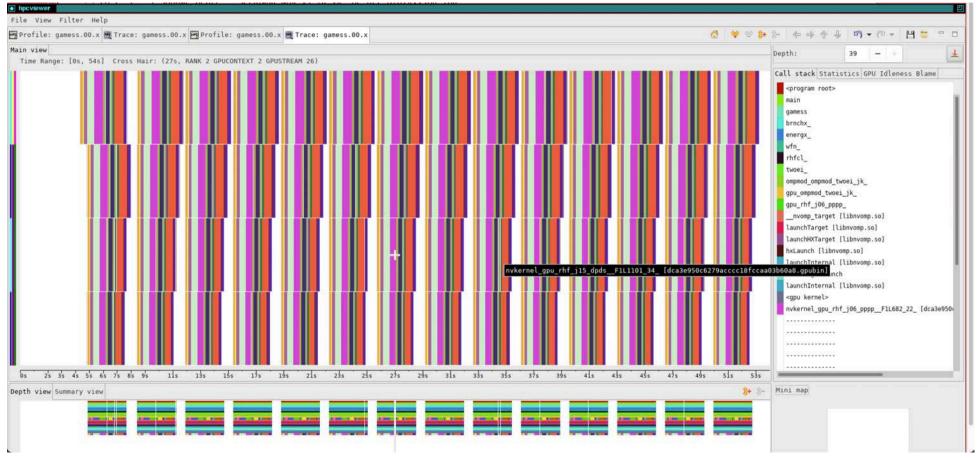


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GAMESS improved



All CPU threads and GPU streams

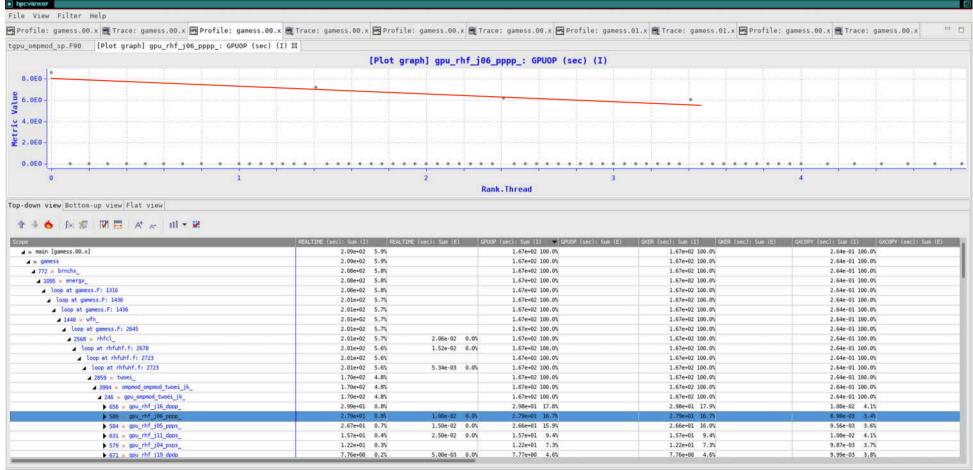


GAMESS improved



GAMESS improved

All GPU streams: 2 iterations



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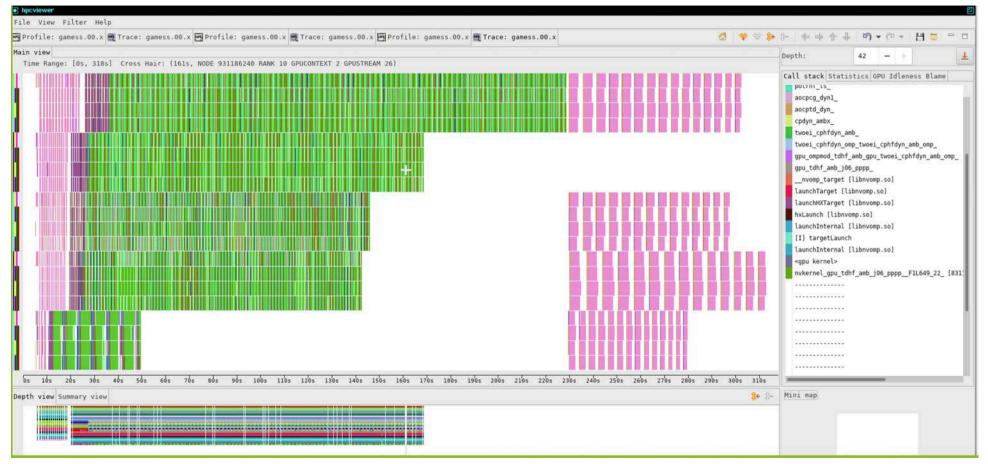
GAMESS improved

Time-centric Analysis: GAMESS 5 nodes, 40 ranks, 20 GPUs on Perlmutter

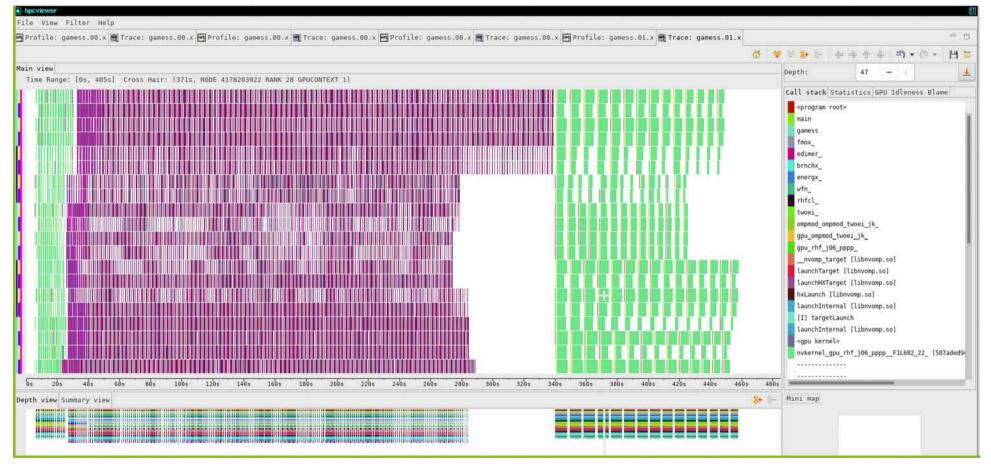
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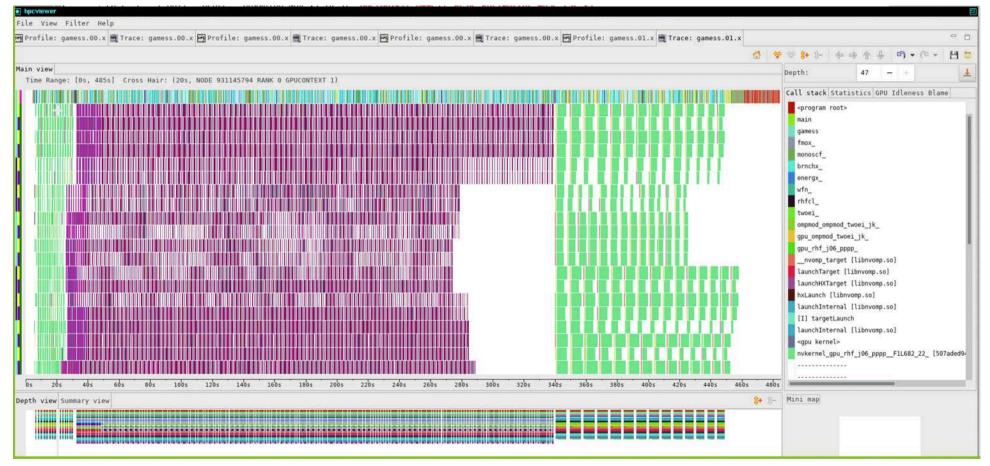
GAMESS improved



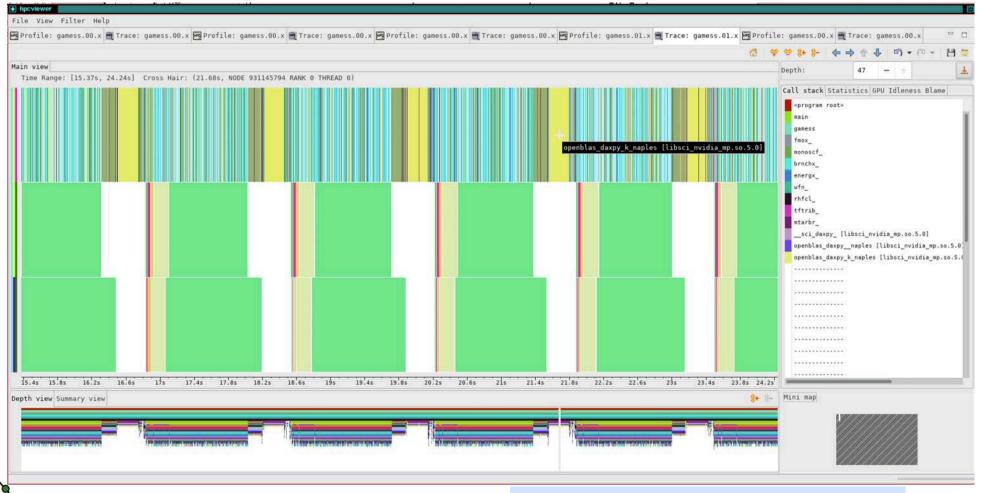




GAMESS improved with better manual distribution of work in input



GAMESS improved adding Rank 0 Thread 0 to GPU streams



1 CPU Stream, 2 GPU Streams: 6 Iterations

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1067 (* 1068 (*FUNCTION - TO MULTIPLY SYMMETRIC MATRIX A	
1069 C* TIMES RECTANGULAR MATRIX B AND GET RECTANGULAR MATRIX AB 1070 C*	
1071 (*PARAMETERS 1072 (* A - THE INPUT REAL SYMMETRIC MATRIX OF ORDER NA	
1073 (* STORED IN SYMMETRIC STOAGE MODE. 1074 (* 8 - THE INPUT REAL NA BY ME RECTANGULAR MATRIX	
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1079 C* INCA - ADDRESS DIFFERENCE OF TWO ADJACENT ELEMENTS OF A	
1081 INC=INCA 1082 C	
1083 C PROCESS DIAGONAL ELEMENTS OF INPUT MATRIX A 1084 C	
1085 IJ=1-INC 1086 DO 120 I=1.NA	
1087 IJ=IJ=IJ=IINC 1088 AIJ=A(IJ)	
1089 DO 110 K=1,MB 1090 AB(I,K)=AIJ*B(I,K)	
1091 110 CONTINUE 1092 120 CONTINUE 1093 IF(NA.EQ.1) RETURN	
1094 C 1095 C PROCESS OFF-DIAGONAL ELEMENTS OF INPUT MATRIX A	
1095 C IDENTIFICATION AND ELEMENTS OF INFOLMENT A	
1098 DO 150 I=2,NA 1099 IJ=IJ+INC	
1100 INI-T-1 1101 D0 140 -14. INI	
1102 IJ=IJ+INC 1103 AIJ=A(IJ)	
1104 IF(AIJ.E0.ZER0) GO TO 140 1105 CALL DAXPY(MB.AIJ.B(T.I.).NA.AB().1).NAB)	
1106 CALL DAXPY(MB,AIJ,B(J,1),NA,AB(I,1),NAB) 1107 140 CONTINUE	
1108 150 CONTINUE 1109 RETURN	
1110 END	
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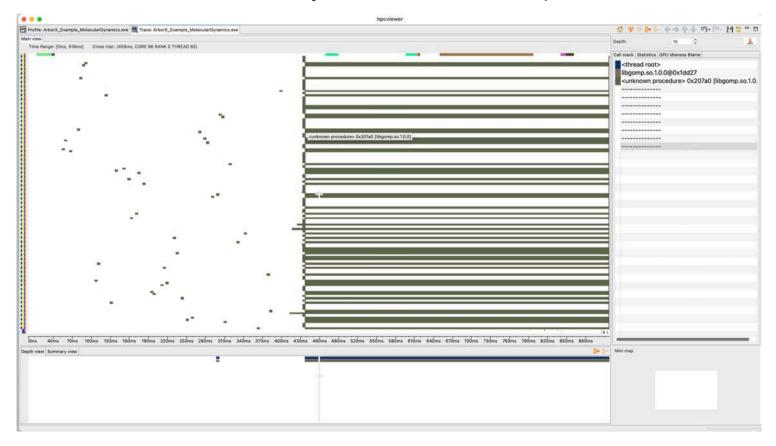
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편 Profile: gamess.00.x 🗮 mthlib.f 🛙	Trace: gamess.00.x 🖻 Profile: gamess.00.x 🗮 Trace: gamess.00.x 🖻 Profile: gamess.00.x 🗮 Trace: gamess.00.x 🖻 Profile: gamess.01.x	80
1096 C		
1097	IJ=1-INC	
1098	DO 150 I=2,NA	
1099	IJ=IJ+INC	
1100	IM1=I-1	
1101	DO 140 J=1,IM1	
1102	IJ=IJ+INC	
1103	AIJ=A(IJ)	
1104	IF(AIJ.EQ.ZERO) GO TO 140	
1105	CALL DAXPY(MB,AIJ,B(I,1),NA,AB(J,1),NAB)	
1106	CALL DAXPY(MB,AIJ,B(J,1),NA,AB(I,1),NAB)	
1107 1	40 CONTINUE	
1108 1	50 CONTINUE	
1109	RETURN	
1110	END	
Top-down view Bottom-up vi	iew Flat view	

Case Study: ArborX

• A library written in Kokkos that provides performance portable algorithms for geometric search

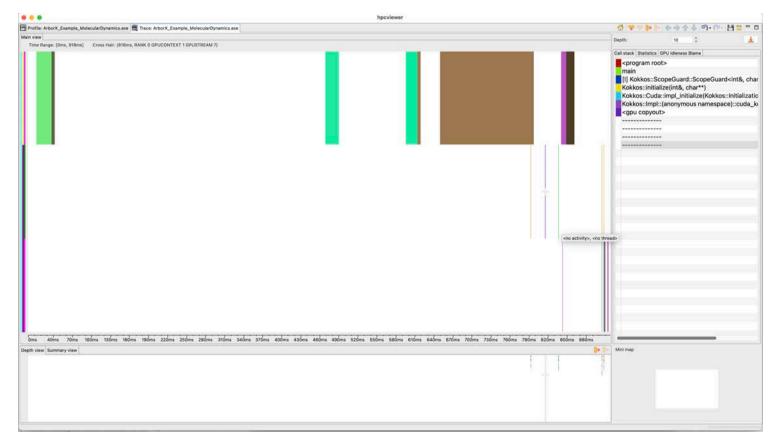
ArborX Trace: Lots of irrelevant CPU Trace Lines for Idle Threads

• Solution: Filter out trace lines with very small numbers of samples



ArborX Trace: Filter to Focus on Relevant CPU and GPU Traces

• Use Filter→Filter Ranks: select Rank 0 and GPU trace lines



ArborX Trace: PC sampling of ArborX

	hpcviewer	
Profile: Arbor	rX_Example_MolecularDynamics.exe 🗮 Trace: ArborX_Example_MolecularDynamics.exe 🚾 Profile: ArborX_Example_MolecularDynamics.exe	- 0
ArborX_DetailsT	freeTraversal.hpp X	
101 i	<pre>int node = HappyTreeFriends::getRoot(bvh); // start with root</pre>	
102 d		
103 {		
104	if (HappyTreeFriends::isLeaf(bvh, node))	
105		
106	if (predicate(HappyTreeFriends::getIndexable(_bvh, node)) &&	
107	invoke callback and check early exit(
108	_callback, predicate, HappyTreeFriends::getValue(_bvh, node)))	
109	return;	
110	<pre>node = HappyTreeFriends::getRope(_bvh, node);</pre>	
111	}	
112	else	
111 112 113	{	
114	node =	
115	<pre>(predicate(HappyTreeFriends::getInternalBoundingVolume(_bvh, node))</pre>	
116	<pre>? HappyTreeFriends::getLeftChild(_bvh, node)</pre>	
117	· HannuTrooEcionderrootDono(hub nodo));	

Scope	GINS: Sum (I) GINS: Sum (E)	GINS:STL_ANY: S	Sum (I)	GINS:STL_ANY: Sun	1 (E)	GINS:STL_IFET: S	Sum (I)	GINS:STL_IFET: Sun	n (E)	GINS:STL_IDEP: S	Sum
497 » ArborX::Details::TreeTraversal <arborx::boundingvolumehiera< p=""></arborx::boundingvolumehiera<>	1.39e+07	47.8%		1.27e+07	48.7%			2.20e+06	54.7%			3.22e+06	4
4 63 » Kokkos::parallel_for <kokkos::rangepolicy<kokkos::cuda, arb<="" p=""></kokkos::rangepolicy<kokkos::cuda,>	1.39e+07	47.8%		1.27e+07	48.7%			2.20e+06	54.7%	6		3.22e+06	4
4 144 » Kokkos::Impl::ParallelFor <arborx::details::treetraversal<ar< p=""></arborx::details::treetraversal<ar<>	1.39e+07	47.8%		1.27e+07	48.7%			2.20e+06	54.7%	6		3.22e+06	4
4 108 » [I] Kokkos::Impl::CudaParallelLaunch <kokkos::impl::parallel< p=""></kokkos::impl::parallel<>	1.39e+07	47.8%		1.27e+07	48.7%			2.20e+06	54.7%	5		3.22e+06	4
4 717 » [I] Kokkos::Impl::CudaParallelLaunchImpl <kokkos::impl::p< p=""></kokkos::impl::p<>	1.39e+07	47.8%		1.27e+07	48.7%			2.20e+06	54.7%	6		3.22e+06	4
4 678 » [I] Kokkos::Impl::CudaParallelLaunchKernelInvoker <kokk< p=""></kokk<>	1.39e+07	47.8%		1.27e+07	48.7%			2.20e+06	54.7%	5		3.22e+06	4
4 368 » [I] cuda_parallel_launch_local_memory <kokkos::impl::< p=""></kokkos::impl::<>	1.39e+07	47.8%		1.27e+07	48.7%			2.20e+06	54.7%	5		3.22e+06	4
# 86 » [I]wrapperdevice_stub_cuda_parallel_launch_loca	1.39e+07	47.8%		1.27e+07	48.7%			2.20e+06	54.7%	5		3.22e+06	4
406 » _ZL592_device_stub_ZN6Kokkos4Impl33cuda_pa	1.39e+07	47.8%		1.27e+07	48.7%			2.20e+06	54.7%	5		3.22e+06	4
403 » [I] cudaLaunchKernel <char></char>	1.39e+07	47.8%		1.27e+07	48.7%			2.20e+06	54.7%	i .		3.22e+06	4
✓ 216 » <gpu kernel=""></gpu>	1.39e+07	47.8%		1.27e+07	48.7%			2.20e+06	54.7%	5		3.22e+06	4
Kokkos::Impl::cuda_parallel_launch_local_memory <ko< p=""></ko<>	1.39e+07	47.8% 4.10e+03	0.0%	1.27e+07	48.7%	4.10e+03	0.0%	2.20e+06	54.7%	5		3.22e+06	4
# 87 » [I] Kokkos::Impl::ParallelFor <arborx::details::treetr< p=""></arborx::details::treetr<>	1.39e+07	47.8% 2.05e+04	0.1%	1.27e+07	48.7%	2.05e+04	0.1%	2.20e+06	54.7%	8.19e+03	0.2%	3.21e+06	4
Ioop at Kokkos_Cuda_Parallel_Range.hpp: 77	1.39e+07	47.8% 2.05e+04	0.1%	1.27e+07	48.7%	2.05e+04	0.1%	2.20e+06	54.7%	8.19e+03	0.2%	3.21e+06	4
4 80 » [I] Kokkos::Impl::ParallelFor <arbloop at="" kokkos_cuda_pa<="" p=""></arbloop>	allel_Range.hpp: 77	47.7%		1.27e+07	48.6%			2.19e+06	54.5%	6		3.20e+06	4
4 63 » [I] ArborX::Details::TreeTraversal <arborx::boun< p=""></arborx::boun<>	1.39e+07	47.7%		1.27e+07	48.6%			2.19e+06	54.5%	6		3.20e+06	4
Ioop at ArborX_DetailsTreeTraversal.hpp: 95	1.38e+07	47.3%		1.26e+07	48.2%			2.18e+06	54.4%	5		3.13e+06	4
4 95 » [I] ArborX::Details::TreeTraversal <arborx::bo< p=""></arborx::bo<>	1.37e+07	46.9% 1.81e+06	6.2%	1.25e+07	47.9%	1.69e+06	6.5%	2.11e+06	52.6%	4.92e+05	12.2%	3.13e+06	4
107 » [I] ArborX::Details::invoke_callback_and_ch	4.06e+06	13.9%		3.96e+06	15.2%			1.06e+05	2.7%	5		4.22e+05	-
115 » [I] ArborX::Intersects <arborx::sphere>::op</arborx::sphere>	3.59e+06	12.3%		3.16e+06	12.1%			4.84e+05	12.1%	5		1.02e+06	1
		· ··										~	

Key Metrics Available for GPU Kernels

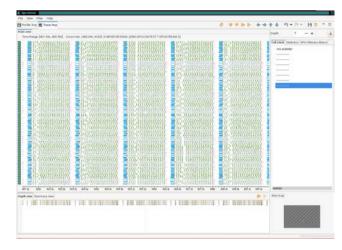
- GPUOP: GPU operation time (kernel launch, copies, etc.)
- GXCOPY:* GPU copies of various kinds
- GKER: GPU kernel time
- GKER:FGP_ACT: fine grain parallelism actual (number of threads used)
- GKER:FGP_MAX: maximum possible fine-grain parallelism (number of threads possible)
- GKER:BLK_THR: threads per block
- GKER:BLK_SM: block shared memory
- GKER:OCC_THR: theoretical thread occupancy



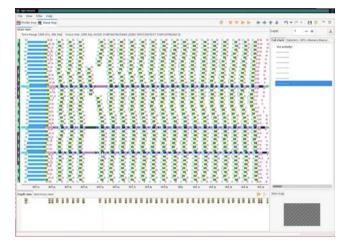
What Metrics Are Available for GPU Kernels with PC Sample

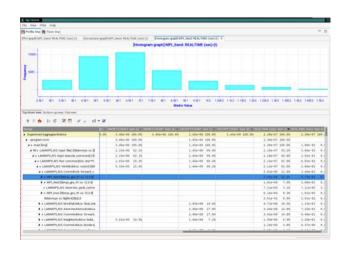
- GINS: GPU instructions
- GINS:STL_ANY: GPU instruction stalls for any reason
- GINS:STL_IFET: GPU instruction stalls for instruction fetch
- GINS:STL_GMEM: GPU instruction stalls for global memory
- GINS:STL_CMEM: GPU instruction stalls for constant memory
- GINS:STL_IDEP: GPU instruction stalls for instruction dependences
- GINS:STL_PIPE: GPU instruction pipeline stalls
- GINS:STL_MTHR: GPU instruction stalls for memory throttling
- GSAMP:EXP: expected number of samples
- GSAMP:TOT: total number of samples recorded
- GSAMP:UTIL: GPU utilization = (PC samples expected) / (PC samples total)



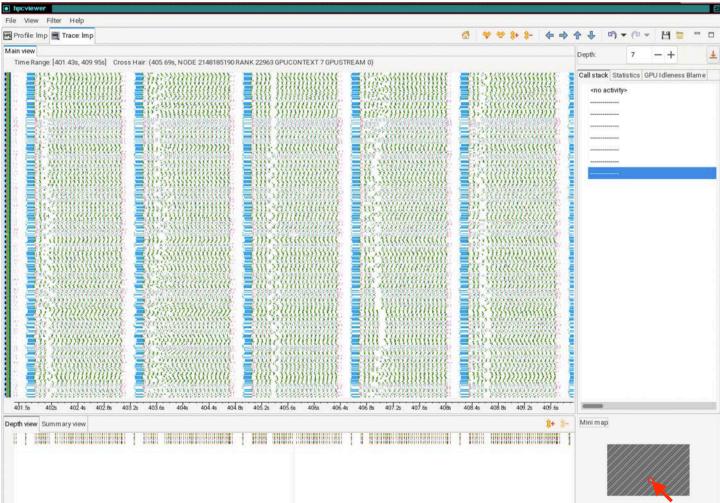


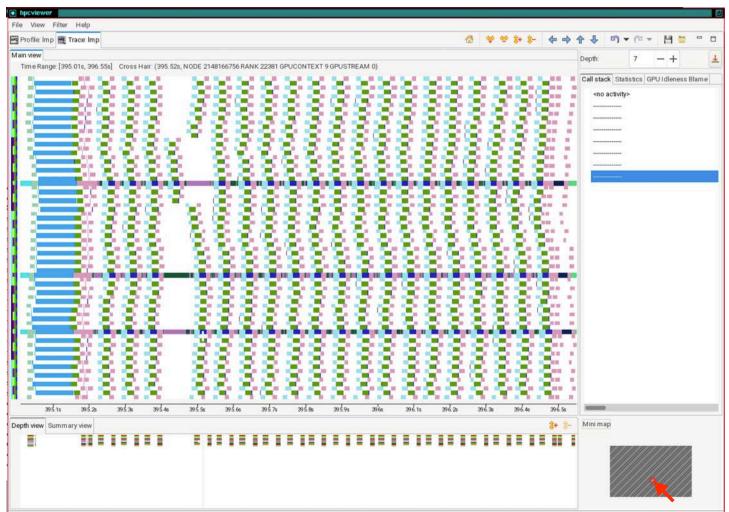
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Experiment-Approprie Metrics	3.44	1.454-00 100.00	3,484+85 100.00	1.454-05 154.05	1.456-09 109.00	1.304-57 108.84	2,364-57	101
Comment Aggregate Matters oprogram math								101.
		1,454-55 158.85		1.450-00 100.00		2.304-87 208.8%		
sprogten moto		1.45e-00 100.00 1.45e-05 100.00		1.45e+00 100.00 1.45e+00 100.00		2.30e-87 200.89 2.30e-87 200.89	2.30x-51	
oprogram met- oprogram met- oprogram met-		1.454-56 338.85 1.454-56 338.85 1.454-55 338.85		1,454-00 100,00 1,454-00 100,00 1,454-00 100,00		2.304-87 200.05 2.304-87 200.05 2.804-87 200.05	2,300-61	8. 8.
sprigter not- s = man(Brg) s = st = (AMMPS_NT transfer Hel)(Manneger in t)		1,454-00 100.00 3,454-05 100.00 8,454-05 100.00 2,154-05 82.10		1.450+00 100.00 1.450+00 100.00 1.450+00 100.00 1.450+00 00.00		1.30e-57 200.05 2.30e-57 200.05 2.30e-57 200.05 2.30e-57 200.05 2.50e-57 95.25	2,300-01 1,300-02 5,600-02	8. 8.
groupser moto was long was (Anthr?S,N1 input Be() Silamoups as if et (ANMAPS,N1 input second, commant())		1.45e+00 100.00 3.45e+00 100.00 8.46e+05 100.00 2.15e+06 82.15 2.15e+06 82.15		1.45e+09 100.08 1.45e+09 100.08 1.45e+09 100.09 1.45e+09 09.09 1.45e+09 09.09		2.354-87 200.89 2.354-87 200.89 2.254-87 200.99 2.254-87 200.99 2.554-87 95.29 2.554-87 94.93	2,388-87 1,398-42 5,488-42 2,434-41	8.1 8.1 8.1 8.1
Grogisti nob small (high mail mail		1.49e-96 100.00 3.49e-95 190.00 2.49e-95 190.00 2.35e-95 52.00 2.35e-95 52.00 1.41e-95 29.90		1,45+05 100,05 1,45+05 100,05 1,45+05 100,05 1,45+05 10,05 1,45+05 99,05 1,44+05 99,05		2.30x-87 200.00 2.30x-87 200.00 2.30x-87 200.00 3.50x-87 95.30 3.30x-87 95.00 3.30x-87 93.00 3.10x-97 92.00 5.60x-90 21.00	2,388+87 1,588+42 5,888+82 2,878+82 6,828+82 2,868+82 3,458+82 3,458+82	8. 8. 8. 8. 8.
compare motion constraining		1.49e-96 100.00 3.49e-95 190.00 2.49e-95 190.00 2.35e-95 52.00 2.35e-95 52.00 1.41e-95 29.90		1,45+05 100,05 1,45+05 100,05 1,45+05 100,05 1,45+05 10,05 1,45+05 99,05 1,44+05 99,05		2,30+47 (20,40 2,30+47 (20,40 2,30+47 (20,40 2,50+47 (20,40 2,50+47 (20,40 2,50+47 (20,40 1,50+47 (20,40 1,50+47 (20,40 1,50+46 (20,40)	2,386-87 1,000-02 5,686-02 2,020-02 0,420-02 2,000-02 2,000-02 0,000-	8.0 8.0 8.0 8.0 8.0 8.0 8.0 8.0 8.0 8.0
		1.49e-96 100.00 3.49e-95 190.00 2.49e-95 190.00 2.35e-95 52.00 2.35e-95 52.00 1.41e-95 29.90		1,45+05 100,05 1,45+05 100,05 1,45+05 100,05 1,45+05 10,05 1,45+05 99,05 1,44+05 99,05		2.36+97 200.00 2.35+97 200.00 2.35+97 200.00 2.35+97 90.00 2.35+97 90.00 2.35+97 90.00 2.35+97 90.00 2.35+97 90.00 2.35+98 21.00 5.55+98 19.00 1.45+98 7.00	2,306-07 1,00+42 5,66-42 2,52+47 4,62+42 2,564-42 2,564-42 4,616-42 1,564-42 1,564-42	8.0 8.0 8.0 8.0 8.0 8.0 8.0
- sprogart non- - synogart non- -		1.49e-96 100.00 3.49e-95 190.00 2.49e-95 190.00 2.35e-95 52.00 2.35e-95 52.00 1.41e-95 29.90		1,45+05 100,05 1,45+05 100,05 1,45+05 100,05 1,45+05 10,05 1,45+05 90,05 1,44+05 90,05		1. Meetr 100, m 2. Meetr 100, m 3. Meetr 100, m	2,348-82 1,358-42 5,488-7 2,528-42 2,528-42 2,548-42 3,548-52 3,548-5	8.1 8.1 8.1 8.1 8.1 8.1 8.1 8.1
 grapper solution strate Update (1) (1) (1) (1) (1) (1) (1) (1) (1) (1)		1.49e-96 100.00 3.49e-95 190.00 2.49e-95 190.00 2.35e-95 52.00 2.35e-95 52.00 1.41e-95 29.90		1,45+05 100,05 1,45+05 100,05 1,45+05 100,05 1,45+05 10,05 1,45+05 90,05 1,44+05 90,05		2.36-47 109.00 2.30-47 109.00 2.30-47 109.00 2.30-47 109.00 2.30-47 59.00 2.46-47 59.00 2.46-47 59.00 2.46-47 59.00 1.45-40 21.00 1.45-40 7.00 1.45-40 9.10 1.45-40 9.10	2.384-87 1.984-42 5.644-42 3.454-42 3.454-42 3.454-42 3.454-42 3.454-42 3.454-42 3.454-42 1.514-42 1.514-42	
		1.49e-96 100.00 3.49e-95 190.00 2.49e-95 190.00 2.35e-95 52.00 2.35e-95 52.00 1.41e-95 29.90		1,458+99 199,99 1,458+99 199,99 1,458+99 199,99 1,458+99 99,99 1,458+99 99,99 1,448+99 99,28		2. March? 100. 8% 2. Jones P. 100. 8% 3. Jones P. 100. 8%	2,388-87 1,398-42 5,688-42 2,598-42 2,598-42 2,598-42 3,598-42 8,798-42 1,518-42 1,518-42 2,518-	
groups non- second se		1.49e-96 100.00 3.49e-95 190.00 2.49e-95 190.00 2.35e-95 52.00 2.35e-95 52.00 1.41e-95 29.90		1.456+09 100.09 1.456+09 100.09 1.456+09 100.09 1.456+09 99.09 1.446+09 99.20 1.446+09 99.20 1.446+09 99.20		2. Masself 100.89 3. Masself 100.89	2.384-83 1.984-82 3.484-82 2.494-82 2.494-82 2.494-82 3.494-82 3.494-82 3.494-82 3.494-82 3.494-82 1.114-82 1.114-82 1.114-82 1.114-82	
		1.49e-96 100.00 3.49e-95 190.00 2.49e-95 190.00 2.35e-95 52.00 2.35e-95 52.00 1.41e-95 29.90		1.489+09 109.09 1.459+09 109.09 1.459+09 109.09 1.459+09 09.09 1.449+09 09.00 1.449+09 09.20 2.459+08 19.00 2.459+08 19.00		2.366-07 200.00 2.366-07 200.00 2.366-07 200.00 2.366-07 200.00 2.366-07 94.00 2.366-07 94.00 3.366-07 94.00 3.366-07 94.00 3.366-07 94.00 3.366-07 94.00 3.366-07 94.00 3.366-07 94.00 3.466-08 9.00 3.466-08 9.00 3.466-08 9.00 3.466-08 9.00 3.466-08 9.00 3.466-08 9.00 3.466-08 14.00 3.466-08 14.00	2,300-02 5,400-02 2,420-02 2,420-02 2,420-02 2,450-02 3,450-02 3,450-02 3,450-02 3,450-02 3,450-02 3,410-02 2,410-02 3,410-02 2,410-02 3,4	
		1.48e+96 109.49 1.46e+96 109.49 1.46e+46 109.49 2.15e+86 42.49 1.51e+86 42.49 5.35e+85 13.46 5.35e+85 13.46		1.456+09 100.09 1.456+09 100.09 1.456+09 100.09 1.456+09 99.09 1.446+09 99.20 1.446+09 99.20 1.446+09 99.20		2. Masself 100.89 3. Masself 100.89	2.384-83 1.984-82 3.484-82 2.494-82 2.494-82 2.494-82 3.494-82 3.494-82 3.494-82 3.494-82 3.494-82 1.114-82 1.114-82 1.114-82 1.114-82	
		1.49e-96 100.00 3.49e-95 190.00 2.49e-95 190.00 2.35e-95 52.00 2.35e-95 52.00 1.41e-95 29.90		1.489+09 109.09 1.459+09 109.09 1.459+09 109.09 1.459+09 09.09 1.449+09 09.00 1.449+09 09.20 2.459+08 19.00 2.459+08 19.00		2.364-97 (20.87) 2.364-97 (20.97) 2.364-97 (20.97) 2.364-97 (20.97) 2.364-97 (20.97) 2.364-97 (20.97) 2.344-97 (20	2,384-42 1,884-42 2,484-42 3,424-43 3,424-43 3,424-43 3,484-43 3,484-43 3,484-43 1,124-43 1,124-43 1,124-43 1,124-43 1,124-43 2,484-43 1,124-43 1,124-43 2,284-41 2,284-41 2,284-41 2,284-43 2,294-43 2,294-43 2,294-43 2,294-43 2,294-43 2,294-43 2,294-43 2,294-43 2,294-	
		1.48e+96 100.49 1.46e+96 100.49 1.46e+46 100.49 2.15e+86 42.19 1.51e+86 42.19 5.35e+85 13.40 5.35e+85 13.40		L.48e+86 199.08 L.45e+9 29.08 L.45e+9 29.08 L.45e+9 29.08 L.45e+99 99.09 L.45e+99 99.09 L.45e+99 99.20 L.45e+99 99.20 L.45e+98 19.20 L.45e+88 17.00		2.366-07 208.39 2.366-07 208.39 2.366-07 208.79 2.366-07 208.79 2.366-07 208.79 2.366-07 30.70 2.366-07 30.70 3.367 3.367 3.367 3.367 3.367 3.377 3.367 3.367 3.3777 3.3777 3.3777 3.3777 3.3777 3.3777 3.3777 3.3777 3.3777 3.3777 3.3777 3.37777 3.37777 3.37777 3.37777 3.377777 3.377777 3.37777777777	2.398-42 3.498-42 3.498-42 3.498-42 3.498-42 3.498-42 3.498-42 3.498-42 3.498-42 3.498-42 3.498-42 3.418-	

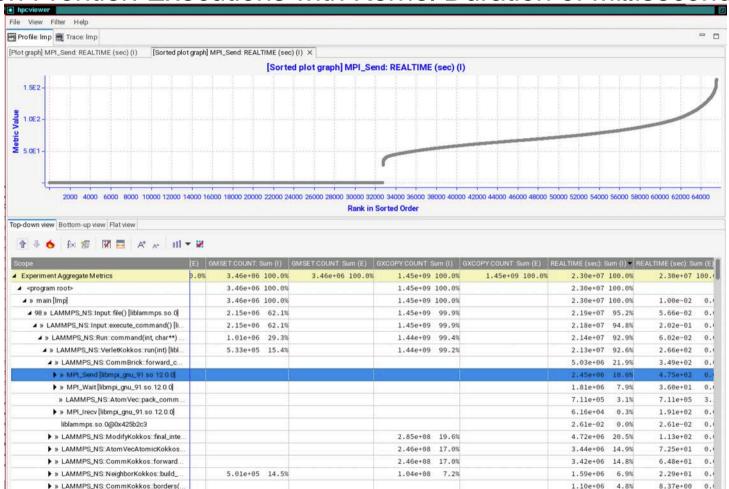








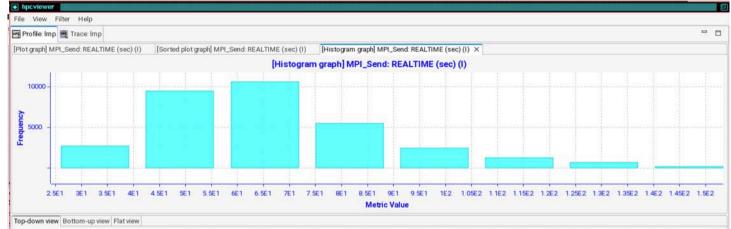




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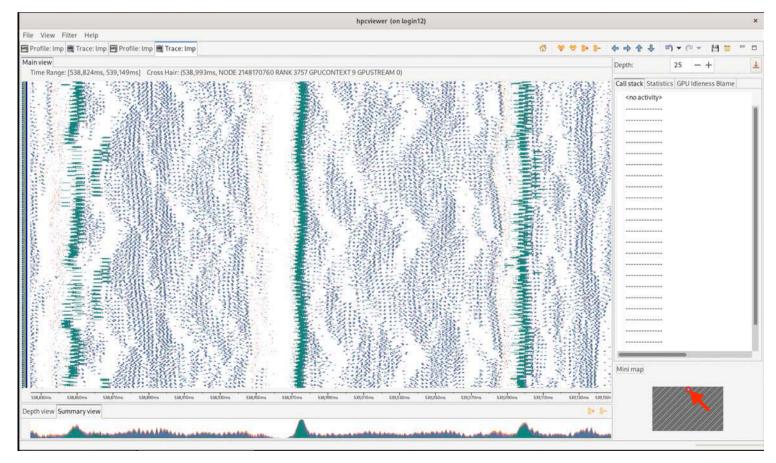


- 11 - 2 - 11 - 2

				GXCOPY:COUNT: Sum (I)	GXCOPY:COUNT: Sum (E)	REALTIME (sec): Sum (I)	REALTIME (sec): Sur	m (E)
 Experiment Aggregate Metrics 	9.0%	3.46e+06 100.0%	3.46e+06 100.0%	1.45e+09 100.0%	1.45e+09 100.0%	2.30e+07 100.0%	2.30e+07 1	100.
<pre> <program root=""></program></pre>		3.46e+06 100.0%		1.45e+09 100.0%		2.30e+07 100.0%		
◢ » main [lmp]		3.46e+06 100.0%		1.45e+09 100.0%		2.30e+07 100.0%	1.00e-02	θ.
▲ 98 » LAMMPS_NS.Input.file() [liblammps.so.0]		2.15e+06 62.1%		1.45e+09 99.9%		2.19e+07 95.2%	5.66e-02	θ.
 LAMMPS_NS Input execute_command() [li 		2.15e+06 62.1%		1.45e+09 99.9%		2.18e+07 94.8%	2.02e-01	0.0
▲ » LAMMPS_NS::Run::command(int, char**)		1.01e+06 29.3%		1.44e+09 99.49		2.14e+07 92.9%	6.02e-02	θ.
▲ » LAMMPS_NS::VerletKokkos::run(int) [libl		5.33e+05 15.4%		1.44e+09 99.2%		2.13e+07 92.6%	2.66e+02	θ.
A » LAMMPS_NS:CommBrick:forward_c						5.03e+06 21.9%	3.49e+02	0.1
MPI_Send [libmpi_gnu_91 so 12.0.0]						2.45e+06 10.6%	4:75e+02	θ.)
MPI_Wait [libmpi_gnu_91.so.12.0.0]						1.81e+06 7.9%	3.60e+01	0.1
» LAMMPS_NS_AtomVec_pack_comm						7.11e+05 3.1%	7.11e+05	3.
MPI_Irecv [libmpi_gnu_91 so 12.0.0]						6.16e+04 0.3%	1.91e+02	0.1
liblammps.so.0@0x425b2c3						2.61e-02 0.0%	2.61e-02	θ.
LAMMPS_NS:ModifyKokkos::final_inte				2.85e+08 19.6%		4.72e+06 20.5%	1.13e+02	0.1
LAMMPS_NS:AtomVecAtomicKokkos				2.46e+08 17.0%		3.44e+06 14.9%	7.25e+01	0.1
» LAMMPS_NS:CommKokkos: forward				2.46e+08 17.0%		3.42e+06 14.8%	6.48e+01	0.1
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K				1 20-107 0.00		0.07-10F 0.FM	0.1000	0

LAMMPS on Frontier: 8K nodes, 64K MPI ranks + 64K GPU tiles

Kernel duration of microseconds



LAMMPS on Frontier: 8K nodes, 64K MPI ranks + GPU times

Kernel duration of microseconds

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Coming Attractions

- Developing comprehensive support for NVTX/ROCTX/Caliper/Kokkos Labels
- Support for instruction-level measurement and attribution on AMD and Intel GPUs
- New GUI support for analysis of remote data
- Python-based interface for analysis of performance results

Troubleshooting: Only GPU kernel Name

• Need to measure with PC sampling to measure within GPU kernels

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  81 driver():
  82 }
  83
  84 template <class DriverType>
  85 global static void cuda parallel launch local memory(
  86 const DriverType driver) {
  87 driver():
  88 }
  89
  90 template <class DriverType, unsigned int maxTperB, unsigned int minBperSM>
  91_global___launch_bounds__(
  92
           maxTperB,
  93
          minBperSM) static void cuda_parallel_launch_local_memory(const DriverType
  94
                                                                                                         driver) +
  95 driver();
  96 }
  07
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                        * % Kokkos::Impl::cuda parallel launch local memory<Kokkos::Impl::ParallelFor<ArborX::Details::TreeTraversal<Ar.</p>
                           Kokkos Cuda KernelLaunch.hpp: 85
         182 » ArborX::BoundingVolumeHierarchy<Kokkos::CudaSpace, ArborX::PairValueIndex<ArborX::Box, unsigned int>, ArborX::D...
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         209 » ArborX::Details::KokkosExt::exclusive_scan<Kokkos::Cuda, Kokkos::View<int*, Kokkos::CudaSpace>, Kokkos::View
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Troubleshooting: No GPU source code lines with PC sampling

• If you don't see source code with PC sampling on NVIDIA GPUs: compile with "-lineinfo" option

	hpcviewer								
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okkos_Cuda_KernelLaunch.hpp Kokkos_Parallel.hpp ArborX_DetailsTreeTraversal.hpp X									
61 else									
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54 Kokkos::RangePolicy <executionspace, fulltree="">(</executionspace,>									
<pre>65 space, 0, predicates.size()),</pre>									
56 *this);									
67 } 68 }									
69									
70 KOKKOS_FUNCTION TreeTraversal(BVH const &bvh, Callback const &callback)									
71 : _bvh{bvh} 72 , callback{callback}									
72 , _callback{callback} 73 {}									
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75 struct OneLeafTree									
76 {};									
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Troubleshooting: Compiling ArborX with GPU Line Map Info

- ArborX cmake isn't set up to include GPU line mappings
- Force the compiler to record GPU line mappings
- % cmake _DARBORX_ENABLE_EXAMPLES=true \

-DCMAKE_INSTALL_PREFIX=`pwd`/../install \

-DCMAKE_CXX_COMPILER=g++ \

-DCMAKE_BUILD_TYPE=RelWithDebInfo \

-DCMAKE_CXX_FLAGS_RELWITHDEBINFO="-O2 -g -DNDEBUG -lineinfo"



HPCToolkit Resources

- Documentation
 - User manual
 - http://hpctoolkit.org/manual/HPCToolkit-users-manual.pdf
 - Tutorial videos
 - http://hpctoolkit.org/training.html
 - recorded demo of GPU analysis of Quicksilver: https://youtu.be/vixa3hGDuGg
 - recorded tutorial presentation including demo with GPU analysis of GAMESS: https://vimeo.com/781264043
 - Cheat sheet
 - https://gitlab.com/hpctoolkit/hpctoolkit/-/wikis/home
- Software
 - Download hpcviewer GUI binaries for your laptop, desktop, cluster, or supercomputer
 - OS: Linux, Windows, MacOS
 - Processors: x86_64, aarch64, ppc64le
 - http://hpctoolkit.org/download.html
 - Install HPCToolkit on your Linux desktop, cluster, or supercomputer using Spack
 - http://hpctoolkit.org/software-instructions.html