Programmable accelerators have become commonplace in modern computing systems. Advances in programming models and the availability of unprecedented amounts of data have created a space for massively parallel accelerators capable of maintaining context for thousands of concurrent threads resident on-chip. These threads are grouped and interleaved on a cycle-by-cycle basis among several massively parallel computing cores. One path for the design of future supercomputers relies on an ability to model the performance of these massively parallel cores at scale.

The SST framework has been proven to scale up to run simulations containing tens of thousands of nodes. A previous report described the initial integration of the open-source, execution-driven GPU simulator, GPGPU-Sim, into the SST framework. This report discusses the results of the integration and how to use the new GPU component in SST. It also provides examples of what it can be used to analyze and a correlation study showing how closely the execution matches that of a Nvidia V100 GPU when running kernels and mini-apps.

### **A** Introduction

As the architectures of high-performance computing (HPC) evolves, there is a growing need to understand and quantify the performance and design benefits of emerging technologies. To complicate the design space, the rise of General-Purpose Graphics Processing Units (GPGPUs) and other compute accelerators, which are needed to handle the growing demands of compute-heavy workloads, have become a necessary component in both high-performance supercomputers and datacenter-scale systems. That the first exascale machines will leverage the massively parallel compute capabilities of GPUs [10, 11, 13] is indicative of the growing necessity of acceleratorbased node architectures to obtain high compute throughputs. As the software stack and programming model of GPUs and their peer accelerators continue to improve, there is every indication that this trend of accelerator integration will continue, leading to a diverse ecosystem of technologies. GPUs are likely to continue to play a role as discrete accelerators or integrated as a part of an SOC. As a result, architects who wish to study the design of large-scale systems will need to evaluate system and software designs using a GPU model. However, the focus of all publicly available cycle-level simulators (e.g. GPGPU-Sim [3]) to date has been on single-node performance. In order to truly study the problem at scale, and to permit larger workloads to be evaluated, a parallelizable, multi-node GPU simulator is necessary.

The Structural Simulation Toolkit (SST) [12] is a parallel discrete event-driven simulation framework that provides an infrastructure capable of modeling a variety of high performance computing systems at many different scales. Currently used by a wide variety of government agencies and computer manufacturers to design and simulate HPC architectures, and, supported by a Python and C++ code base with a large array of customization options, SST offers the HPC community powerful, highly customizable, tools to create and integrate models for evaluating current and future HPC node architectures and interconnect networks. What has been lacking, up to this point, has been a method to integrate accelerators into a node model in SST. This report builds upon previous work [9], providing more details on our efforts to integrate an open-source GPGPU simulator, GPGPU-Sim, into SST. This integration effort will provide SST users the ability to run GPGPU-based simulations using the Balar GPU component and will serve as a model for future accelerator integration studies.

# **B** Balar Components

### **B.1 GPU** Scheduler

The first step in integrating GPGPU-Sim into SST is to handle the interaction with an SST CPU component. Since GPUs today function solely as co-processors, functionally executing GPU-enabled binaries requires the CPU to initialize and launch kernels of work to the GPU. In our model, the GPU is constructed out of two discrete SST components – a scheduler and a SM block [2]. When CUDA functions are called from the CPU component, they are intercepted and translated into messages that are sent over SST links to the GPU (along with the associated parameters). Table 1 enumerates the CUDA API calls currently intercepted and sent to the GPU elements. These calls are enough to enable the execution of a number of CUDA SDK kernels, DoE proxy apps as well as a collection of Kokkos Unit tests. Table 8 lists the number of Kokkos unit tests that pass with our current implementation of SST-GPU, which is about 60%. There is ongoing work with the PTX parser to increase the number of running kernels.

Table 1: Intercepted CUDA API Calls Forwarded to GPU Model

cudaRegisterFatBinary
$_{}$ cudaRegisterFunction
cudaMalloc
cudaMemcpy
cudaConfigureCall
cudaSetupArgument
cudaFree
cudaLaunch
cudaGetLastError
$_{}$ cuda $RegisterVar$
cudaOccupancyMaxActiveBlocksPerMultiprocessorWithFlags

Aside from the basic functional model provided by GPU-SST, an initial performance model has also been developed. Figure 1 details the overall architecture. A CPU component (Ariel in the initial implementation) is connected via SST links to 2 GPU components: the SMs, which implement the timing and functional model for the GPU cores, and a centralized kernel and CTA scheduler (GPUSched). When CUDA calls are intercepted from the CPU, messages are sent to both the SMs and the GPU scheduler. Messages related to memory copies and other information necessary to populate the GPU functional model are sent directly to the SMs element, since the functional model for executing the GPU kernels lives inside the SMs element. Calls related to enqueuing kernels for execution are sent to the GPU scheduler element, which co-ordinates the launching of CTAs on the SMs, e.g. cudaConfigureCall and cudaLaunch.

As CTAs complete on the SMs, messages are sent back to the GPU scheduler element, which pushes new work to the SMs from enqueued kernels as needed. Memory copies from the CPU to GPU address space are handled on a configurable page-size granularity, similar to how conventional CUDA unified memory handles the transfer of data from CPU to GPU memories.

The centralized GPU scheduler receives kernel launch commands from the CPU, then issues CTA launch commands to the SMs. The scheduler also receives notifications from the SMs when

Table 2: Functionally Passing Kokkos Unit Tests

w in	CDCDI C	CDCDL C: /CCT
Kernel Name abs_double	GPGPU-Sim OK	GPGPU-Sim/SST OK
abs_mv_double	OK	OK
asum_double	OK	OK
axpby_double	OK	OK
axpby_mv_double axpy_double	OK OK	OK OK
axpy_uouble axpy_mv_double	OK OK	OK
dot_double	OK	OK
dot_mv_double	OK	OK
mult_double	OK	OK
mult_mv_double nrm1_double	OK OK	OK OK
nrm1_mv_double	OK	OK
nrm2_double	OK	OK
nrm2_mv_double	OK	OK
nrm2_squared_double nrm2_squared_mv_double	OK OK	OK OK
nrminf_double	FAILED	PREVIOUS FAILED
nrminf_mv_double	FAILED	PREVIOUS FAILED
reciprocal_double	FAILED	PREVIOUS FAILED
reciprocal_mv_double	FAILED	PREVIOUS FAILED
scal_double scal_mv_double	OK OK	OK OK
sum_double	OK	OK
sum_mv_double	OK	OK
update_double	OK	OK
update_mv_double gemv_double	OK FAILED	OK PREVIOUS FAILED
gemm_double	FAILED	PREVIOUS FAILED
sparse_spgemm_double_int_int_TestExecSpace	FAILED	PREVIOUS FAILED
sparse_spadd_double_int_int_TestExecSpace		PREVIOUS FAILED
sparse_gauss_seidel_double_int_int_TestExecSpace		PREVIOUS FAILED
sparse_block_gauss_seidel_double_int_int_TestExecSpace sparse_crsmatrix_double_int_int_TestExecSpace		PREVIOUS FAILED PREVIOUS FAILED
sparse_blkcrsmatrix_double_int_int_TestExecSpace		PREVIOUS FAILED
sparse_replaceSumIntoLonger_double_int_int_TestExecSpace	NOT PARSED	PREVIOUS FAILED
sparse_replaceSumInto_double_int_int_TestExecSpace		PREVIOUS FAILED
sparse_graph_color_double_int_int_TestExecSpace sparse_graph_color_d2_double_int_int_TestExecSpace	FAILED	PREVIOUS FAILED PREVIOUS FAILED
common_ArithTraits		PREVIOUS FAILED
common_set_bit_count	FAILED	PREVIOUS FAILED
common_ffs	OK	OK
batched_scalar_serial_set_double_double batched_scalar_serial_scale_double_double	OK OK	FAILED OK
batched_scalar_serial_gemm_nt_nt_double_double	OK	OK
batched_scalar_serial_gemm_t_nt_double_double	OK	OK
batched_scalar_serial_gemm_nt_t_double_double	OK	OK
batched_scalar_serial_gemm_t_t_double_double batched_scalar_serial_trsm_l_l_nt_u_double_double	OK OK	OK OK
batched_scalar_serial_trsm_l_l_nt_n_double_double	FAILED	PREVIOUS FAILED
batched_scalar_serial_trsm_l_u_nt_u_double_double	OK	OK
batched_scalar_serial_trsm_l_u_nt_n_double_double	FAILED	PREVIOUS FAILED
batched_scalar_serial_trsm_r_u_nt_u_double_double	OK FAILED	OK PREVIOUS FAILED
batched_scalar_serial_trsm_r_u_nt_n_double_double batched_scalar_serial_lu_double	OK	FAILED
batched_scalar_serial_gemv_nt_double_double	OK	OK
batched_scalar_serial_gemv_t_double_double	OK	OK
batched_scalar_serial_trsv_l_nt_u_double_double batched_scalar_serial_trsv_l_nt_n_double_double	OK FAILED	FAILED PREVIOUS FAILED
batched_scalar_serial_trsv_u_nt_u_double_double	OK	FAILED
batched_scalar_serial_trsv_u_nt_n_double_double	FAILED	PREVIOUS FAILED
batched_scalar_team_set_double_double	OK	FAILED
batched_scalar_team_scale_double_double	OK OK	OK OK
batched_scalar_team_gemm_nt_nt_double_double batched_scalar_team_gemm_t_nt_double_double	OK	OK
batched_scalar_team_gemm_nt_t_double_double	OK	OK
batched_scalar_team_gemm_t_t_double_double	OK	OK
batched_scalar_team_trsm_l_l_nt_u_double_double	OK EAH ED	OK
batched_scalar_team_trsm_l_l_nt_n_double_double batched_scalar_team_trsm_l_u_nt_u_double_double	FAILED OK	PREVIOUS FAILED OK
batched_scalar_team_trsm_l_u_nt_n_double_double	FAILED	PREVIOUS FAILED
batched_scalar_team_trsm_r_u_nt_u_double_double	OK	OK
batched_scalar_team_trsm_r_u_nt_n_double_double	FAILED	PREVIOUS FAILED
batched_scalar_team_lu_double batched_scalar_team_gemv_nt_double_double	OK OK	FAILED OK
batched_scalar_team_gemv_t_double_double	OK	OK

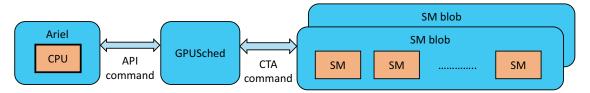


Figure 1: SST Element architecture for kernel/CTA scheduler and SMs components

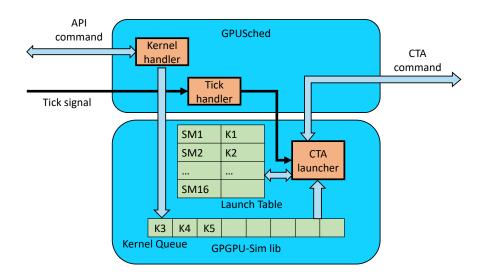


Figure 2: Centralized GPU Scheduler component

the CTAs finish. The reception of kernel launch and CTA complete notifications are independent, therefore we designed a different handler for each type of message. Figure 2 shows the design of the centralized kernel and CTA Scheduler. The kernel handler listens to calls from a CPU component and pushes kernel launch information to the kernel queue when it receives kernel configure and launch commands. The SM map table contains CTA slots for each of the SMs, which is reserved when launching a CTA and released when a message indicating that a CTA has finished is received from the SMs. The scheduler clock ticks trigger CTA launches to SMs, when space is available and there is a pending kernel. On every tick, the scheduler issues a CTA launch command for currently unfinished kernels if any CTA slot is available or tries to fetch a new kernel launch from kernel queue. The CTA handler also waits for SMs to reply the CTA finish message, so that CTA slots in the SM map table may be freed.

### **B.2** SM Blobs

To support the GPGPU-Sim functional model, a number of the simulator's overloaded CUDA Runtime API calls were updated. A number of functions that originally assumed the application and simulator were within same address space now support them being decoupled. Initialization functions, such as \_\_ cudaRegisterFatBinary, now take paths to the original application to obtain the PTX assembly of CUDA kernels.

Supporting the functional model of GPGPU-Sim also requires transferring values from the

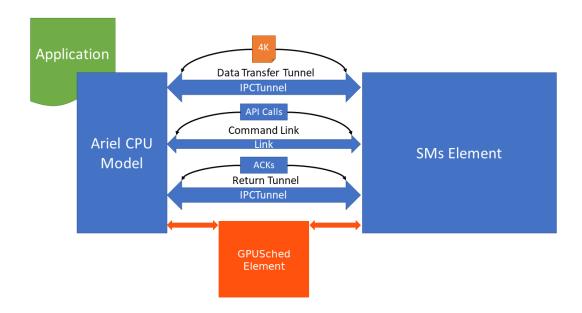


Figure 3: SST Link and IPCTunnels for functional model support

CPU application to the GPU memory system. This is solved by leveraging the inter-process communication tunnel framework from SST-Core, as shown in 3. Chunks of memory are transferred from the CPU application to the GPU memory system at the granularity of a page (4KiB). The transfer of pages is a blocking operation, therefore all stores to the GPU memory system must be completed before another page is transferred or another API call is processed.

To model GPU performance, the memory system of the public GPGPU-Sim is completely removed. Instead, all accesses to GPU memory are sent though SST links to the MemHierarchy interface. As Figure 4 shows, a multi-level cache hierarchy is simulated with the shared L2 sliced between different memory partitions, each with its own memory controller. Several backend timing models have been configured and tested, including SimpleMem, SimpleDRAM, Timing-DRAM, and CramSim [6]; CramSim will be used to model the HBM stacks in the more detailed performance models. We have created an initial model for the GPU system similar to that found in an Nvidia Volta. The configuration for the GPU, CramSim and Network components is shown in Listing 1.

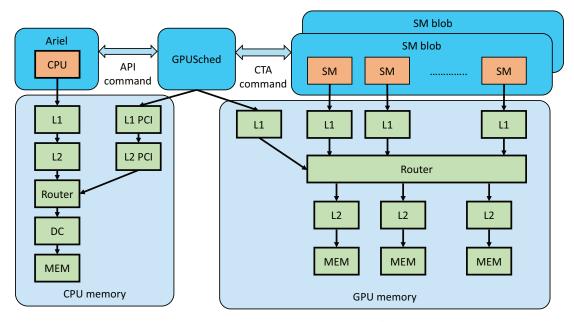


Figure 4: Timing and memory model for SMs component

### Listing 1: Sample SST-GPGPU Configuration

### [CPU]

clock: 2660MHz
num\_cores: 1

application: ariel
max\_reqs\_cycle: 3

### [ariel]

executable: ./vectorAdd

gpu\_enabled: 1

#### [Memory]

clock: 200MHz

network\_bw: 96GB/s
capacity: 16384MiB

### [Network]

latency: 300ps
bandwidth: 96GB/s
flit\_size: 8B

### [GPU]

clock: 1200MHz
gpu\_cores: 80
gpu\_l2\_parts: 32

gpu\_l2\_capacity: 192KiB
gpu\_cpu\_latency: 23840ps
gpu\_cpu\_bandwidth: 16GB/s

### [GPUMemory]

clock: 1GHz

network\_bw: 32GB/s
capacity: 16384MiB
memControllers: 2

hbmStacks: 4 hbmChan: 4 hbmRows: 16384

#### [GPUNetwork]

latency: 750ps

bandwidth: 4800GB/s linkbandwidth: 37.5GB/s

flit\_size: 40B

### **C** Evaluation

#### C.1 Correlation

A validation sweep was run using two kernels and a mini-app. The three applications were run using an SST model that approximates a Nvidia V100 attached to a CPU. The simulation parameters are shown in Table 3. The overall kernel runtime was compared with the results of running the three applications through nvprof on Sandia's Waterman testbed, which is comprised of IBM Power9 CPUs and Nvidia Volta GPUs. Table 4 shows the total number cycles that each application took on the SST-GPU model and on the native V100. Note that this is only cycles where a kernel was running and does not include host execution time. There are challenges isolating the cause of the performance gaps. This is one of the largest, if not the largest, node simulation that has been run with 139 unique components and 906 links (the statistics output contains nearly 20k unique entries). The complex model interactions and scale make it difficult to pinpoint where models are lacking in detail or are incorrect. Turning on debug for even a small run can produce multi-terabyte output files. That being said, the authors do have some intuition into why there are gaps and how to close them.

Table 3: CPU/V100 Model Parameters

(~)	CDII
(4)	UPU

Clock	2660MHz
DDR Clock	2666
DDR Capactiy	16384MiB
Mesh Frequency	800MHz
Mesh Input Ports	1
Mesh Output Ports	1
Data Link Latency	23840ps
Command Link Latency	23840ps

(b) GPU

Clock	1312MHz
SMs	84
L2 Slices	32
L2 Capactiy	192KiB per slice
HBM Capacity	16384MiB
HBM Stacks	4
Crossbar Frequency	1200MHz
Crossbar Input Ports	2
Crossbar Output Ports	1

Table 4: SST-GPGPU Correlation

	P9/V100	SST-GPGPU	Error
vectorAdd	5271	5751	9.09
lud	494519	605685	22.48
lulesh	12454750	11896477	4.48

### **C.2** Vector Addition

The vectorAdd application is from the Cuda SDK with error checking removed. It implements element by element vector addition using an array with 163840 elements.

vectorAdd contains a single kernel with a single invocation that, essentially, streams through memory performing integer operations. It was expected that this would have a higher correlation, but the fact that there are so many memory dependencies and memory operations make the results highly dependent on the model for the backing store. A number of models were tried and flaws were found in all of them. With the exception of Cramsim, all of the models are derived from simple DRAM models and are unable to accurately replicate the behavior of HBM. It is believed that there is an issue in the memory controller that Cramsim uses and that when this is solved, it will serve as a good model for HBM2. However, the timingDRAM model clearly provides enough detail for kernels that are not bottle-necked by memory bandwidth.

### **C.3** LU Decomposition

The lud application is from the Rodinia benchmark suite [4][5] and implements the LU decomposition algorithm to solve a set of linear equations using a 256x256 element matrix.

The lud application from Rodinia contains 3 kernels with 46 total kernel launches. lud has the worst correlation. The perimeter and diagonal kernels occupy the majority of the compute time – diagonal has 16 invocations and consumes 63% of the time; perimeter has 15 invocations and consumes 22% of the time; internal has 15 invocations and consumes 14% of the time. perimeter and diagonal spend 50% and 80% of their time inactive, respectively, due to the number of divergences. Given that LULESH has a much greater diversity of instructions, including FP64, and the previously reported issues determining control flow, it's unlikely that the problem lies in the ALU models and more likely that the issues stem from how the GPU model handles divergences or complex issues exposed by the differences in using PTX verses SASS.

### C.4 LULESH

LULESH is one of the most widely used mini-applications developed by the US Department of Energy. The code was originally developed by Lawrence Livermore National Laboratory to represent challenging hydrodynamics algorithms that are performed over unstructured meshes [7][8]. Such algorithms are common in many high-performance computing centers and are particularly prevalent within the NNSA laboratories. In the original LULESH specification, the authors state that such algorithms routinely count in the top ten application codes in terms of CPU hours utilized [7].

The unstructured nature of LULESH presents challenges for the design of memory subsystems, not least because operands are gathered from a fairly limited locale but are done so sparsely. This makes efficient streaming and vectorization of the data operations difficult and places additional pressure on the memory subsystem (typically the L2 caches) to provide operands quickly.

For this experiment, the problem size was set to 22 with 50 iterations, leading to an application that contains 26 kernels with 1400 total invocations. The top three kernels, in terms of execution time, provided a good mix of operations, shown in Table 5. The diversity of operations in lulesh, compared to the other too applications, obfuscates the areas where the simulation is lacking, leading to higher correlation with the V100 target platform.

It's clear that a more detailed study is needed to isolate the weaknesses in the models.

#### C.5 Kokkos

The functional correctness of the model was validated using the unit tests from the Kokkos Kernels suite [14]. The unit tests were compiled using the parameters in Table 6. The target node architecture was assumed to be an Intel Broadwell attached to an NVIDIA Pascal GPUs. This target architecture was chosen based on hardware availability, specifically Sandia's Doom cluster, which

Table 5: LULESH Instruction Count Percentages (nyprof)

	FP32	FP64	INT	CTRL	L/S	MISC	INACTIVE
CalcFBHourglassForceForElems	1	10	11	10	12	31	23
CalcPressureForElems	5	17	27	2	19	16	15
CalcHourglassControlForElems	0	25	21	3	38	9	1

is based on the CTS-1 procurement. The SST model is derived from Figure ?? using the model parameters in Table'7 to represent an NVIDIA P100 SXM2 [1].

Table 6: Kokkos Build Parameters

KOKKOSKERNELS_SCALARS=double
KOKKOSKERNELS_LAYOUTS=left
KOKKOSKERNELS_ORDINALS=int
KOKKOSKERNELS_OFFSETS=int
KOKKOSKERNELS_DEVICES=Cuda,Serial
KOKKOS_ARCH=BDW,Pascal60

Table 7: Broadwell/P100 Model Parameters

(a) CPU

Clock	1200MHz
DDR Clock	2400
DDR Capactiy	16384MiB
Mesh Frequency	800MHz
Mesh Input Ports	1
Mesh Output Ports	1
Data Link Latency	23840ps
Command Link Latency	23840ps

(b) GPU

Clock	1328MHz
SMs	56
L2 Slices	8
L2 Capactiy	512KiB per slice
HBM Capacity	16384MiB
HBM Stacks	4
Crossbar Frequency	1000MHz
Crossbar Input Ports	2
Crossbar Output Ports	1

Table 8 shows the Kokkos Kernels unit tests that were run. With the current implementation of SST-GPU, 54 out of 89 tests run to completion and pass. The passing tests are highlighted in green. Of the remaining tests, all but the yellow tests fail in both SST-GPGPU and GPGPU-Sim. The tests in pink fail because the PTX parser cannot locate a post-dominator. This can happen when the control flow is too complex for the parser and a path from the point of divergence to a convergence point for all of the threads cannot be found. There are plans to work with the Kokkos Kernels developers to find a solution. The tests in purple fail because of a bug in the parser that creates an empty file, which should contain the PTX for the kernel, but the simulator crashes when it attempts to read from it. Neither the SST developers nor the GPGPU-Sim developers have been able to locate the problem. The tests in red fail because the problem size is overflowing the address space. Both teams are actively engaged on a fix for this. The two remaining tests, in yellow, run

to completion and pass in GPGPU-Sim but have run for more than 10 days without completion in Balar. It is believed that they would complete successfully if given more run time.

Table 8: Kokkos Kernels Unit Test Results

1	abs_double
2	abs_mv_double
3	asum double
4	axpby_double
5	axpby_mv_double
6	axpy_double
7	axpy_mv_double
8	dot_double
9	dot_mv_double
10	mult_double
11	mult_mv_double
12	nrm1_double
13	nrm1_mv_double
14	nrm2_double
15	nrm2_mv_double
16	nrm2_squared_double
17	nrm2_squared_mv_double
18	nrminf_double
19	nrminf_mv_double
20	reciprocal_double
21	reciprocal_mv_double
22	scal_double
23	scal_mv_double
24	sum_double
25	sum_mv_double
26	update_double
27	update_mv_double
28	gemv_double
29	gemm_double
30	sparse_spgemm_double_int_int_TestExecSpace
31	sparse_spadd_double_int_int_TestExecSpace
32	sparse_gauss_seidel_double_int_int_TestExecSpace
33	sparse_block_gauss_seidel_double_int_int_TestExecSpace
34	sparse_crsmatrix_double_int_int_TestExecSpace
35	sparse_blkcrsmatrix_double_int_int_TestExecSpace
36	sparse_replaceSumIntoLonger_double_int_int_TestExecSpace
37	sparse_replaceSumInto_double_int_int_TestExecSpace
38	graph_graph_color_double_int_int_TestExecSpace
39	graph_graph_color_deterministic_double_int_int_TestExecSpace
40	graph_graph_color_d2_double_int_int_TestExecSpace common_ArithTraits
41	
42	common_set_bit_count
43	common_ffs
44	batched_scalar_serial_set_double_double
45	batched_scalar_serial_scale_double_double

46	batched_scalar_serial_gemm_nt_nt_double_double
47	
48	
49	batched_scalar_serial_gemm_t_t_double_double
50	
51	batched_scalar_serial_trsm_l_l_nt_n_double_double
52	batched_scalar_serial_trsm_l_u_nt_u_double_double
53	
54	batched_scalar_serial_trsm_r_u_nt_u_double_double
55	batched_scalar_serial_trsm_r_u_nt_n_double_double
56	batched_scalar_serial_trsm_l_l_t_u_double_double
57	batched_scalar_serial_trsm_l_l_t_n_double_double
58	batched_scalar_serial_trsm_l_u_t_u_double_double
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-	
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88	
88	
89	batched_scalar_team_solvelu_double

### C.6 Lulesh

A parameter sweep was performed using LULESH, described in Section C.4. The device clock was varied from 500MHz to 1312MHz to 1800MHz. The memory clock was varied from 877MHz to 1200MHz to 1600MHz. Figure 5 shows the results, where lower runtime time is better.

As expected, changing the frequency of the backing store has little effect on LULESH for this problem size because it is not memory bandwidth bound. The most improvement is seen at the low

device clock frequency, but at this frequency the speedup is still small at 1.04x. However, increasing the frequency of the SMs does improve the performance noticeably. Going from 500MHz to 1312MHz shows a 2.5x speedup; going from 1312MHz to 1800MHz shows a further 1.3x speedup.

Although this was a small study, one can imagine being able to run a more complete parameter sweep over any of the Balar parameters.

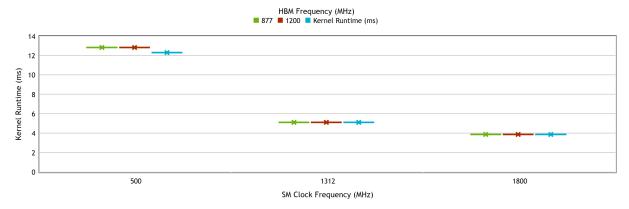


Figure 5: GPU Parameter Sweep Using LULESH (Baseline was 1312MHz/877MHz)

### C.7 Parallel Simulation Performance

**Fixme:** @Mengchi - put the new performance data and discussion in here. Make sure to run it through Grammarly and I will vett it too.

## **D** Conclusion

This report described the final integration of phase one of the SST-GPU project. Functional validation against the Kokkos Kernels unit tests shows that the GPU component can successfully run more than 60% of the tests with a path to reach a coverage of greater than 90%. Correlation with the Waterman V100 testbed is excellent, showing 4-22% error in the runtime for the applications considered. The next phase of the project will focus on further disaggregating the GPU to enable truly scaled GPU performance in a multi-process MPI simulation.

# Acknowledgment

We would like to thank Gwen Voskuilen for her help with memHierarchy and recommendations on debugging problems with the NIC and interconnect. We would also like to thank Arun Rodrigues and Scott Hemmert for their support and help in defining the scope of the project.

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