Understanding Power and Energy Utilization in Large Scale Production Physics Simulation Codes

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Abstract

Power is an often-cited reason for moving to advanced architectures on the path to Exascale computing. This is due to the practical concern of delivering enough power to successfully site and operate these machines, as well as concerns over energy usage while running large simulations. Since accurate power measurements can be difficult to obtain, processor thermal design power (TDP) is a possible surrogate due to its simplicity and availability. However, TDP is not indicative of typical power usage while running simulations. Using commodity and advance technology systems at Lawrence Livermore National Laboratory (LLNL) and Sandia National Laboratory, we performed a series of experiments to measure power and energy usage in running simulation codes. These experiments indicate that large scale LLNL simulation codes are significantly more efficient than a simple processor TDP model might suggest.

Keywords HPC · energy · power

1 Introduction

Power and energy usage needs of a supercomputer are important factors in siting and operating costs and on its environmental impact. Exascale machines will require tens of megawatts to operate and the facilities hosting them are undergoing costly renovations to accommodate their power needs. Given these high costs, it is important to understand the relative power consumption of various processor options for different workloads.

One approach to lower power usage is through the use of accelerators. Many TOP500 systems today use GPUs for both performance benefits and lower power consumption. For FLOP heavy workloads that are similar to the LinPACK benchmark, they provide clear performance per watt advantages as is evidenced by the top machines on recent Green500 lists [1].

While studies looking at real applications abound, and there are numerous comparisons between various systems, most only focus on the processor component of power and energy rather than full system power. In addition, some look at the impact of code optimization on power and energy usage at the processor level. However, there is still much uncovered ground. In this paper we investigate the following areas not covered in other studies:

- Holistic power measurements that include switches, power supply losses and processors that show where all the power goes in running HPC applications.
- The relationship between TDP and measured power usage. We show that system TDP often means significantly more power is provisioned, even for LinPACK, compared with what is needed to run the system in production.
• Cross platform energy breakdowns and comparisons and energy/performance tradeoffs.

In addition, we cover some old ground with new large production simulation codes as we look at the effects of code optimization on power and energy. Our overall results show that processor TDP is a poor proxy for system power/energy usage. Other components may dominate usage, and processor power is often significantly less than the stated peak for many real HPC workloads.

The rest of this article is organized as follows: We conclude this section with a discussion on using processor TDP as a surrogate for understanding application power usage and with a literature review of related work. We continue in Sections 2 and 3 with overviews of the different platforms, our strategies for measuring power and the different production simulation codes and test problems. In Sections 4 and 5, we examine relationships between performance and optimizations on GPU-based platforms and establish metrics for energy breakeven points for a cross platform comparison. We provide concluding remarks in Section 6.

1.1 Processor thermal design power as a surrogate

Thermal design power (TDP) is the maximum amount of heat that a component is designed to generate. It is included in the standard specification for many computer components, including processors. Due to simplicity and accessibility, it may be tempting to use a processor’s TDP as a surrogate for power usage in cross platform evaluations, where the node TDP is not readily available. Using this single number can make it easy to make performance targets for energy breakeven. If one processor’s TDP is two times higher than that of another, the second processor merely needs to run two times faster to be equally energy efficient. Such a simplified analysis would ignore differences in overall node design or assume that the whole node’s TDP is dominated by the processor, which is not necessarily true. It should also be noted that the TOP500 list does not list TDP of any machine, but instead the actual power used when running the LinPACK benchmark.

1.2 Related work

Several studies have been published examining GPU/CPU power consumption. For example, Abe et al. [2] examine GPU performance compared to CPU performance. They show that GPUs have a significantly higher performance per watt across the Intel and NVIDIA roadmaps covering a 6-year time frame from 2006 through 2012. They also show that GPU power usage can be significantly reduced by 28% while only reducing performance by 1%, further increasing energy efficiency.

Price et al. [3] investigate the performance per watt on GPUs. They specifically catalog the effect of temperature and supply voltage showing that performance per watt can be increased by 37-48% over default settings by lowering supply voltage and increasing clock frequency while maintaining low die temperatures.

Enos et al. [4] develop a hardware methodology for measuring and comparing performance per watt for specific applications for both CPU and GPU implementations. They show that for the same workload, performance per watt can be improved by running the same application after porting to the GPU.

Patel et al. [5] explore the power characteristics of typical HPC jobs during the approach to the Exascale era. As HPC systems become increasingly power constrained, they show that a data-driven approach to HPC application power characteristics can be used to make more effective use of HPC systems.

Kamil et al. [6] show that High Performance Linpack (HPL) is a useful proxy for compute intensive kernels in multiple HPC workloads for the purpose of predicting power consumption, while it is not a useful proxy for projecting application performance. They describe the increasing need to establish practical methods for measuring application power usage in-situ to understand behavior in a post Dennard scaling era.

We extend these works with methods for collecting power and energy data on some production applications of interest, which are our large simulation codes, which can be run during normal production runs on the Sierra supercomputer. We show that the energy to solution advantage for GPU enabled applications is significant over CPU-only solutions. We also show that GPU TDP is not a valid proxy for power usage on these production applications due to the significant and variable differences between GPU TDP and GPU average power for these production applications.

2 Overview of computing platforms

In this work we study power and energy usage on three computing platforms from Lawrence Livermore National Laboratory (LLNL), a commodity system (CTS-1), Magma, and Sierra. As a fourth platform, we exercise Astra, an
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Figure 1: Computing platforms used in this work. The commodity based platform (CTS-1) serves as our baseline for comparisons.

Arm-based supercomputer at Sandia National Laboratory (SNL). Figure 1 provides a comparison of reported LinPACK FLOP rates, memory bandwidth performance with a stream benchmark, and processor TDP per node. Throughout the table the commodity platform (CTS-1) serves as our baseline for comparisons. Notably the CTS-1 processors have the smallest TDP, while graphics processing units have the highest.

2.1 Measuring power on Sierra

The Sierra system has multiple touchpoints for the measurement of both power and energy. Each 360-node section of the system is equipped with a wall plate power meter with 1 second time resolution. The system also has node-level power measurement capabilities provided by the IBM Witherspoon compute node. This node-level power measurement is integrated over the course of a compute job and recorded by the IBM Cluster System Management (CSM) software and stored as a job energy value in a database. The scale of Sierra meant that 360 node runs would be too large for some of the measurements in this work. As a result, we installed an additional wall plate power management system on the switch components of one rack and over the course of large test runs we were able to determine the typical switch power usage to be 15 watts per node and the power supply and other losses to be 15 percent when comparing power data computed from CSM database energy values to the 360 node wall plate values. The collected power data does not attempt to account for a percentage of the top-level switch power.

2.2 Measuring power on CTS-1 and Magma

Our CTS-1 and Magma systems use rack-level power rectifiers and DC power distribution within the rack. As a result, power for this system may be measured at the rack level. The system software does not provide any correlation between power and job data, so dedicated runs were performed using whole compute racks in the machine and the power data was collected with the help of system staff. The data from these power rectifiers includes switch power and power supply losses within the rack but does not attempt to account for a percentage of the top-level switch power, allowing for a direct comparison against our other systems. The rectifier power data was collected every minute through the runs in order to determine an energy value for the run.

2.3 Measuring power on Astra

The Astra supercomputer provides power and energy measurement capabilities at the processor, node, chassis, rack, and full system levels [7]. At the processor level, the Marvell ThunderX2 Arm processors used in the system provide extensive on-die voltage, power, frequency, and temperature measurements on a per-core basis. These measurements can be accessed in-band by users by instrumenting their code using the PowerAPI [8] or by using vendor supplied tools. At the node and chassis levels, the HPE Apollo 70 server architecture provides out-of-band interfaces for measuring per-node power usage and a range of environmental sensors. At the rack level, the power distribution unit
(PDU) in each rack provides a convenient location for measuring the total energy consumed by all the equipment in the rack, including the compute nodes, network switches, and other ancillary components. Lastly, at the full system-level, the 480VAC overhead bus bars and 208VAC PDUs that together supply power to the system include measurement capabilities that can be used to calculate the system’s total power and energy usage.

### 2.3.1 Tradeoffs of the different measurement points

Each of the available power measurement points has different accuracy, precision, sampling frequency, and user interface characteristics that must be carefully considered when designing experiments and interpreting results. For example, the system’s health monitoring infrastructure collects node-level power measurements via out-of-band interfaces that do not affect application performance, however the measurements obtained are low precision and low fidelity (e.g., quantized to multiples of 8 watts with 1/min sampling). This is appropriate for system monitoring activities, but it may not be appropriate for performing detailed application power usage experiments. In contrast, the rack-level PDUs provide billing grade energy measurements based on high internal sampling rates and ±1% overall accuracy. This provides high-quality aggregate rack-level measurements, but it is not possible to resolve the energy used by individual compute nodes.

### 2.3.2 Experimental method, what is presented in this paper

The Astra results presented in this paper were gathered using rack-level energy measurements since this was the most closely comparable result to the experiments performed on the other systems. Each of the workloads was configured to run on either one or two full racks (72 or 144 compute nodes) and to execute for several hours of runtime. The jobs were run on a dedicated reservation of two compute racks that was pre-screened to ensure that all nodes were available and operating correctly. As each job ran, the job ID was noted so that the job’s start time, end time, and node list could be looked up from the batch scheduler logs. This information was used to retrieve the corresponding rack-level energy measurements from the system monitoring database, resulting in a series of 1/min timestamped energy measurements covering the job’s entire execution window. The low sampling rate does not induce significant error due to the long runtimes (e.g., a 3-hour job with 1/min energy sampling results in < 1% error). The job’s total energy consumption can be calculated by subtracting the first measurement from the last, resulting in the total Joules consumed, or a power vs. time plot can be generated by examining the energy and timestamp deltas between adjacent measurements.

### 3 Overview of tested simulation codes

For many large scale LLNL simulation codes, running efficiently on Sierra required major code refactoring such as porting computational kernels and revisiting memory management strategies. Abstraction layers such as RAJA [9] and memory resource managers such as Umpire [10] were utilized to simplify the porting process while enabling a single source code for different computing platforms. Expertise from developers and domain scientists was required to ensure correctness and performance. Many of the LLNL codes which have successfully ported to GPUs have realized major speedups compared to existing CPU-based computing platforms [9, 11].

In this paper, we showcase three such codes written in C++: Ares, MARBL and Imp, which we describe in Sections 3.1, 3.2 and 3.3, respectively. To run on GPUs, Ares and MARBL use RAJA and Umpire while Imp uses Umpire and a custom portability layer to enable the same capabilities as RAJA. In all our experiments all three codes were executed with MPI-only parallelism on CPU based platforms, utilizing one MPI per processor core. For the GPU platforms, we employed 1 MPI rank per GPU and used the CUDA backend of our abstraction layer for offloading to the device. We begin with a cross platform study using all three codes, then follow with a study on the impact code optimizations have on power and energy on Sierra using the Ares and MARBL codes. As Ares has established GPU capabilities, we present experiments with various optimizations. Additionally, we were able to align the refactoring of MARBL for GPUs to this study enabling us to present data capturing power and energy usage as kernels are ported and optimized.

#### 3.1 Ares

Ares is a massively parallel, multi-dimensional, multi-physics simulation code [12]. Its capabilities include Arbitrary Lagrangian-Eulerian (ALE) hydrodynamics with Adaptive Mesh Refinement (AMR), radiation diffusion and transport, 3T plasma physics and high explosive modeling. It has been used to model many different types of experiments, such as inertial confinement fusion (ICF), pulsed power and high explosives.

For the cross-platform comparison study, Ares used a 3D multi-material ALE hydrodynamics problem that contained 103 million zones and ran for 25,000 cycles.
For the optimization study, Ares used an ALE hydrodynamics problem that modeled a Rayleigh-Taylor mixing layer in a convergent geometry. It was a $4\pi$, 3D simulation which contained 23.8 million zones and ran for 10,380 cycles.

### 3.2 MARBL

MARBL is a new multi-physics simulation code at LLNL [13]. Some of its key capabilities include multi-material radiation hydrodynamics in both an Eulerian and an Arbitrary Lagrangian-Eulerian (ALE) framework for applications in inertial confinement fusion (ICF), pulsed power and equation of state/material strength experiments. MARBL builds on modular physics and computer science packages such as Axom [14], MFEM [15], RAJA [9], and Umpire [10]. A distinct feature of this code is its design choice of employing high-order numerical methods. In this study we exercise the high-order finite element multi-material ALE package to perform our power and energy studies.

As a test problem for a cross platform comparison, we choose the three-dimensional multi-material triple-point problem. For the CPU based platforms (CTS-1, Magma, and Astra), the problem was configured with a mesh consisting of 462 million quadrature points and was executed for 500 cycles. For the GPU based platform, Sierra, the problem was scaled to a mesh with 3.7 billion quadrature points and 5000 cycles. The discrepancy in problem size stemmed from the large run-time differences between the platforms and the requirement of running the code long enough in order to measure power and energy usage.

Additionally, we were able to align this study with MARBL’s GPU modernization effort [11], which allowed us to track the effects of incrementally offloading and optimizing kernels on power and energy usage. For this study we exercised a three-dimensional shaped charge problem on a node of Sierra (4 NVIDIA V100’s) for 1000 cycles.

### 3.3 Imp

Imp is a new implicit Monte Carlo (IMC) thermal radiative transfer simulation code [16] which implements the standard IMC algorithm for time- and frequency-dependent x-ray radiative transfer as defined by Fleck and Cummins [17]. Imp is used to model thermal radiative transfer for ICF and high energy density experiments. Some general features of Imp include photon sources, effective photon scattering, thermal photon emission, photon opacities, and source tilting. Imp supports multiple mesh geometries and implements multiple parallel algorithms including MPI, OpenMP, and GPU parallelism.

The test problem used for the energy study is a half-hohlraum, a simplified 2D hohlraum simulation modeling thermal radiative transfer in a geometry motivated by laser-driven radiation-hydrodynamics experiments. This is further defined in Yee et al. [18].

### 4 Cross platform energy and power analysis

To better understand how power and energy usage varies across the different platforms, we consider several approaches. One approach is to consider energy usage with respect to speedups, and the second is to compare throughput. Using the Ares code, we performed a strong scaling study on a multi-material ALE hydrodynamics problem; while MARBL examined energy required per a unit of work for a multi-material ALE hydro problem, and Imp was used to measure energy required per unit of work for a 2D hohlraum simulation.

Since LinPACK corresponds to exceptionally heavy computational workloads we believe the idle power and LinPACK can serve as lower and upper respectively bounds for scientific simulation codes. Table 1 compares processor TDP, idle power, and LinPACK power usage as reported from the TOP500 list.

| Platform       | Processor TDP | Power usage (idle) | Power usage (LinPACK) |
|----------------|---------------|--------------------|-----------------------|
| CTS-1          | 240           | 86                 | 450                   |
| Magma          | 700           | 161                | 1,365                 |
| Astra          | 360           | 240                | 460                   |
| Sierra         | 1,580         | 500                | 1,721                 |
| Sierra (GPUs only) | 1,200       | 162                | not measured          |
In our studies we are able to measure energy in terms of joules, which we simplify in terms of Kilowatt-hours (1 kWh = 3.6 \cdot 10^6 J). Conversion to watts per node is given by
\[
\text{watts per node} = \frac{\text{joules}}{\text{seconds} \times \text{nodes}}.
\]

In this work we are interested in quantifying a required speedup in order to reach an energy breakeven even point. As we are taking actual energy measurements, we define the power ratio as:
\[
\text{PowerRatio}_{\text{energy breakeven}} = \frac{\text{Measured Power on Sys 1}}{\text{Measured Power on Sys 2}}.
\]

The power ratio informs us of the required speedup needed between platforms to reach an energy breakeven point.

### 4.1 Ares

We performed a strong scaling study of a multi-material ALE hydrodynamics problem across all platforms studied, which was constrained by node counts needed to get accurate power and energy data and the results are in Table 2.

The range of power usage across all runs are summarized in Figure 2. The power usage on each platform for this problem remains in a narrow band, relative to the spread of idle power and LinPACK. It is also apparent that the processor TDP is not generally indicative of actual usage. The only clear commonality that can be seen in this data is that the CTS-1 and Magma platforms have similar TDP to actual usage ratios, which have similar node designs.

On every platform with multiple runs, the runs with the fewest number of nodes is consistently the most energy efficient and offer the highest throughput of work. Ares does not strong scale perfectly, so as the resources increase, the time does not decrease proportionally. Although there is also a reduction in power per node as the code is strong scaled, it does not reduce enough to offset the increased number of nodes used.

One common metric for comparing platforms is to use a node-to-node comparison. Due to limitations in the energy measuring methodology (as discussed in Section 2), there aren’t exact node count matches across platforms. For comparing Sierra to Astra, the closest available is Sierra’s 80 node run with Astra’s 72 node run. Comparing those two data points shows that Sierra has a 3.3x speedup over Astra and that it is 1.4x more energy efficient. The ratio of node power at these points is 2.15, which suggests that the speedup needed to reach breakeven on a GPU for this problem is only 2.15. It should also be noted that at this point, the Sierra runs are strong scaled and less energy efficient than its other runs.

For the same metric on the CPU platforms, Astra’s 72 node run and CTS-1’s 62 node run are the closest. For those runs, there is a 1.3x speedup on Astra and Astra is 1.13x more energy efficient. The ratio of the power between the two runs is 1.04, so the gain in efficiency is almost entirely from the faster runtime on Astra.

Another way to compare platforms is to look at equivalent node counts to get the same answer in the same amount of time. Using this lens, the runs with the closest duration are Sierra’s 5 node run with Astra’s 72 node run and Sierra’s 10 node run with Astra’s 144 node run. In these cases, Sierra is about 5.5x more energy efficient than Astra for running the same problem in the same amount of time. The ratio of node power between these runs is between 2.6 and 2.7, which is more than offset by the 14x difference in nodes being used.

Table 2: Energy and time measurements gathered from the various platforms with Ares, running the same problem, strong scaled across nodes.

| Nodes | Duration (s) | Total Energy (kWh) | Avg. Watts Per Node |
|-------|--------------|---------------------|--------------------|
| CTS-1 | 62           | 28,424              | 167.56             | 342.28             |
| Magma | 48           | 17,094              | 212.41             | 931.96             |
| Astra | 72           | 20,851              | 148.37             | 356.71             |
|       | 144          | 12,705              | 181.28             | 355.7              |
| Sierra| 5            | 19,755              | 26.53              | 967.23             |
|       | 10           | 13,106              | 32.71              | 898.52             |
|       | 20           | 8,967               | 42.5               | 853.23             |
|       | 40           | 6,979               | 63.3               | 816.3              |
|       | 80           | 6,240               | 106.5              | 768.05             |
4.2 MARBL

MARBL’s cross platform study compares energy and power usage across the smallest number of nodes necessary for the highest fidelity energy and power estimates. For the CPU based platforms, CTS-1, Magma, and Sierra, the node counts were 62, 48, and 72 respectively. Prior to understanding the correction factor for Sierra, 360 nodes were required to achieve the highest fidelity measurements.

Our starting point for the cross-platform analysis begins with understanding watts used for the simulation and the total runtime. Table 3 reports the rate at which energy is consumed, while Figure 3 compares application power rates with other known values.

Table 3: Watts used in MARBL for 3D Triple point problem

| Platform | Nodes | Duration (s) | Avg. Watts Per Node | Ratio of Watts used relative to CTS-1 |
|----------|-------|--------------|---------------------|---------------------------------------|
| CTS-1    | 62    | 2,217        | 314                 | 1x                                    |
| Magma    | 48    | 1,024        | 842                 | 2.68x                                 |
| Astra    | 72    | 1,266        | 351                 | 1.12x                                 |
| Sierra   | 360   | 1,581        | 958                 | 3.05x                                 |
To compare across platforms, we introduce the concept of a “CTS-1 work unit”. We define the CTS-1 work unit as total number of quadrature points × cycles. Table 4 presents our observed energy usage along with throughput with comparisons to the CTS-1 platform. After normalization, our findings show that relative to CTS-1 performance, the GPU platform Sierra delivers a clear advantage in terms of improved energy efficiency (6.35x more efficient) and throughput (19.37x). We also find that although Magma does utilize an energy quantity like the CTS-1 platform, it can deliver an almost three-fold throughput performance (2.78x). Lastly, we find that Astra can provide reduced energy usage (1.34x improvement to CTS-1) for a 1.5x throughput improvement.

### Table 4: Cross platform study for MARBL using the 3D Triple point problem

| Platform | Nodes | Quadrature points | Cycles | Total Energy (kWh) | Throughput per kWh | Energy efficiency relative to CTS-1 | Throughput improvement relative to CTS-1 |
|----------|-------|------------------|--------|--------------------|-------------------|------------------------------------|------------------------------------------|
| CTS-1    | 62    | 4.68 \cdot 10^8  | 500    | 12.02              | 1.92 \cdot 10^{10} | 1x                                 | 1x                                       |
| Magma    | 48    | 4.62 \cdot 10^8  | 500    | 11.49              | 2.01 \cdot 10^{10} | 1.04x                              | 2.78x                                    |
| Astra    | 72    | 4.62 \cdot 10^8  | 500    | 8.91               | 2.59 \cdot 10^{10} | 1.34x                              | 1.5x                                    |
| Sierra   | 360   | 3.7 \cdot 10^9   | 5,000  | 151.5              | 1.22 \cdot 10^{11} | 6.35x                              | 19.37x                                   |

### 4.3 Imp

The Imp simulations were designed such that each run would take 60 to 80 minutes on each of three platforms: CTS-1, Magma, and Sierra. Like the MARBL cross platform study, runs were designed to compare energy and power usage across the smallest number of nodes necessary to gather the data.

Refer to Table 5 for a cross platform comparison of the watts/node used by Imp. Figure 4 compares the application power rates with other known values.

To perform the comparison, we defined a work unit as the processing of 1e8 computational particles. We measured the amount of work units completed, the seconds to solution, and the energy consumed. After normalization, we see that relative to CTS-1 performance, the Sierra GPU is 2.33x more efficient. Also, Sierra provided 6.94x the throughput for the 2D hohlraum simulation (see Table 6 for details).

### Table 5: Watts used by Imp for 2D hohlraum simulation

| Platform | Nodes | Work units | Duration (s) | Avg. Watts Per Node | Ratio of Watts used relative to CTS-1 |
|----------|-------|------------|--------------|---------------------|---------------------------------------|
| CTS-1    | 62    | 9.9        | 3,947        | 340                 | 1x                                    |
| Magma    | 48    | 25.3       | 4,590        | 901                 | 2.65x                                 |
| Sierra   | 48    | 51.2       | 3,798        | 1,012               | 2.98x                                 |

### Table 6: Cross platform study of 2D hohlraum simulation

| Platform | Nodes | Work units | Duration (s) | Total Energy (kWh) | Throughput (kWh per work unit) | Energy efficiency relative to CTS-1 | Throughput improvement relative to CTS-1 |
|----------|-------|------------|--------------|--------------------|-------------------------------|------------------------------------|------------------------------------------|
| CTS-1    | 62    | 9.9        | 3,947        | 23.12              | 2.33                          | 1x                                 | 1x                                       |
| Magma    | 48    | 25.3       | 4,590        | 55.14              | 2.18                          | 1.06x                              | 2.81x                                    |
| Sierra   | 48    | 51.2       | 3,798        | 51.25              | 1                             | 2.33x                              | 6.94x                                   |

### 5 Optimization impact on power and energy on Sierra

#### 5.1 Ares

To study the effects of optimization on power and energy on Sierra, we tested two optimizations. The first was to run the code asynchronously as long as possible, where the unoptimized version would synchronize after every kernel.
Figure 4: Imp power requirements (dark bar) relative to machine idle (lower whisker) and LinPACK (upper whisker) power rates. Power ratio refers to the necessary speed up to break even in terms of energy usage compared to the CTS-1 machine. Light colored bars corresponds to processor TDP for a given platform.

The second was to perform kernel fusion on packing and unpacking kernels that are used to pack MPI communication buffers. These are very small kernels that are kernel launch bound due to the small amount of data being moved per kernel. This optimization is focused on improving strong scaling behavior. The results of the tests running with and without all optimizations are presented in Figure 5 (and the data is presented in Table 7). As an additional baseline, the code was also run utilizing only the CPU cores on the platform. For these CPU only runs, we subtracted out the idle GPU power from Table 1 to have a fairer comparison.

As noted in the cross-platform section, we see that the energy consumption increases as we strong scale the problem under all problem configurations. We also see that as we optimize the code, the strong scaling inefficiencies lessen, which yields significantly lower energy usage at the highest node counts.

When we look at the data across the optimizations, we see that the optimizations all decrease the runtime of the problem and generally reduce the overall energy consumption of the total run, except for the kernel fusion optimization at 1 or 2 nodes, where they had little effect. There is a trend in the data that as more optimizations are added, the power increases. This is due to the optimizations eliminating gaps in between kernels, due to kernel launch overheads, which keeps the GPU from idling, and thus does more work in a shorter amount of time. Although the power is increasing, the runtime of the problems are decreasing faster, which leads to an overall gain in energy efficiency.

This data can also be used to discuss the energy breakeven point between using the CPU and the GPU. Most simplistically, the ratio of the power used between two runs can be used to determine how much faster the code needs to run to have the same energy consumption. In comparing all the GPU runs to the CPU runs, that ratio ranges between 1.15 and 1.42, depending on which node count is used. Comparing the 16 node unoptimized run to the CPU only run confirms this, as their energy usage is almost equal with only being 1.13x faster. For every other comparison, the GPUs are clearly far more energy efficient than using CPUs alone.

Another feature of the data to note is that although the vast majority of the compute and memory bandwidth are being used by the GPU, the GPUs only account for 35-45% of the overall energy consumption of the node. This reinforces that it is important to consider an entire architecture’s node design when looking at energy efficiency, rather than just the compute units alone.

5.2 MARBL

To better understand the impact on power and energy on Sierra, we tracked power and energy usage on Sierra during MARBL’s GPU porting effort. From inception, MARBL strictly used MPI for parallelism; thus, to run on GPU platforms would require refactoring. We began tracking energy usage on Sierra shortly after reaching the performance breakeven point between CPU and GPU runs, i.e. where we had comparable runtimes when running the same problem on a CTS-1 node and on a Sierra node and utilizing the GPUs. We present our energy usage from May through October 2020 when exercising the shaped charge problem on a Sierra node. In general, we find that performance optimizations can affect power usage differently. Figure 6(a) illustrates that although not all optimizations led to increased power, there was a general downwards trend in total runtime. Total energy usage can be shown to decrease as the runtime performance of the code improves as shown in Figures 6(b).
Figure 5: Comparing the affects of several optimizations on Ares runtime (a), energy (b) and average power (c) in a strong scaling study.
6 Conclusion

In this work we have presented a methodology based on actual computing system energy measurements for understanding power and energy consumption of production level scientific simulation codes. Using our methodology, we performed studies using LLNL’s Ares, MARBL, and Imp codes. We found that it is imperative to perform energy measurements, as using a surrogate such as processor TDP may overestimate power usage when running scientific applications.

Additionally, we introduce the notion of the required speedup for an energy breakeven point between platforms. Based on our experiments, we have found that Ares, MARBL, and Imp require 2-3x speedups on Sierra over a CTS-1 platform (node-to-node comparison) to reach the breakeven point between platforms. In practice, however these codes achieve much greater speedups on a GPU based system compared to the CTS-1 platform thereby requiring less energy to run on the GPU platform. For these problems Sierra was able to provide an energy savings of 2.33x for the Imp code, 6.35x for MARBL, and 1.6-5x for Ares over the CTS-1 platform.

Our studies also suggest that faster execution time tends to result in improved energy efficiency, but often with greater power usage. Figure 7 illustrates the different power ranges for the applications comparing in addition to the idle and LinPACK power rates. Finally, higher throughput correlates with higher energy efficiency.
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|                  | Sierra Energy with Optimizations (kWh) |                  | Sierra GPU Energy with Optimizations (kWh) |                  | Sierra Average Watts per Node |                  | Sierra Duration (seconds) |
|------------------|----------------------------------------|------------------|--------------------------------------------|------------------|-------------------------------|------------------|--------------------------|
|                  | Unopt | Async opt | Fusion opt | Full opt | CPU only | Unopt | Async opt | Fusion opt | Full opt | CPU only | Unopt | Async opt | Fusion opt | Full opt | CPU only | Unopt | Async opt | Fusion opt | Full opt | CPU only | Unopt | Async opt | Fusion opt | Full opt | CPU only |
| 1 node            | 1.80  | 1.77      | 1.92      | 1.80    | X        | 0.84  | 0.81      | 0.86      | 0.81    | X        | 756   | 779      | 817      | 793     | X        | 8572  | 8179     | 8463     | 8162    | X        |
| 2 nodes           | 2.14  | 2.00      | 2.15      | 1.98    | 6.92     | 0.92  | 0.87      | 0.91      | 0.85    | X        | 777   | 795      | 801      | 795     | 591      | 4977  | 4523     | 4839     | 4491    | 21084    |
| 4 nodes           | 2.86  | 2.41      | 2.72      | 2.45    | 7.26     | 1.18  | 1.02      | 1.10      | 1.03    | X        | 768   | 758      | 773      | 782     | 395      | 3349  | 2859     | 3172     | 2819    | 10977    |
| 8 nodes           | 4.14  | 3.35      | 3.63      | 3.23    | 7.17     | 1.45  | 1.30      | 1.32      | 1.28    | X        | 685   | 736      | 683      | 750     | 587      | 2720  | 2051     | 2388     | 1941    | 5491     |
| 16 nodes          | 7.70  | 5.50      | 6.22      | 4.76    | 7.50     | 2.57  | 1.90      | 2.11      | 1.70    | X        | 660   | 684      | 666      | 675     | 572      | 2625  | 1807     | 2104     | 1587    | 2968     |

Table 7: Ares optimizations

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A Ares optimization data

Table 7 lists the data from the charts in Figure 5.

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