On Using Linux Kernel Huge Pages with FLASH, an Astrophysical Simulation Code

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Abstract—We present efforts at improving the performance of FLASH, a multi-scale, multi-physics simulation code principally for astrophysical applications, by using huge pages on Ookami, an HPE Apollo 80 A64FX platform. FLASH is written principally in modern Fortran and makes use of the PARAMESH library to manage a block-structured adaptive mesh. We explored options for enabling the use of huge pages with several compilers, but we were only able to successfully use huge pages when compiling with the Fujitsu compiler. The use of huge pages substantially reduced the number of translation lookaside buffer misses, but overall performance gains were marginal.

Index Terms—high-performance computing, computer architecture, exascale, astrophysics

I. INTRODUCTION

A. Ookami

Ookami is a development platform featuring Fujitsu A64FX processors that is supported by the United States National Science Foundation and hosted by Stony Brook University with additional support from the University at Buffalo [1]. The project is meant to provide open access to this new hardware, and beginning in October, 2022, Ookami will be an XSEDE level 2 service provider [2].

Ookami, an HPE Apollo 80, has 174 A64FX Fujitsu compute nodes, each with 32GB high-bandwidth memory (HBM) and a 512GB SSD for the OS. Ookami’s 700 series A64FX processors consist of four core memory groups each with 12 cores, 64KB L1 cache, and 8MB L2 cache shared between the cores and run at 1.8 GHz. These processors use the ARMv8.2–A Scalable Vector Extension (SVE) SIMD instruction set with a 512 bit vector implementation, allowing for vector lengths anywhere from 128–2048 bits (in 128 bit increments) and enabling vector length agnostic programming [3]. Ookami has an Infiniband HDR100 fat tree interconnect with 200 gigabit switches, and a high-performance Lustre file system provides about 800 TB storage.

The expectation is that the A64FX processors will provide high performance and reliability for applications with common programming models, particularly memory-intensive applications, while maintaining a good performance to power ratio. Ookami allows users with a variety of applications to explore the A64FX architecture, and various codes are being ported to and performance tested on the machine including our application code, FLASH (described below) [4].

B. Thermonuclear Supernovae

Our science application is in nuclear astrophysics, specifically thermonuclear (Type Ia) supernovae. These events are thought to occur when a compact star known as a white dwarf composed principally of carbon and oxygen explodes via a thermonuclear runaway, but are incompletely understood despite their widely-accepted use as distance indicators for cosmological studies [5], [6]. Our goal is to model these events to explore systematic effects on the brightness [7], and our present study explores one subclass of dim events, Type Ia supernovae, that are thought to be produced by a pure deflagration (subsonic burning front) occurring in a special “hybrid” white dwarf [8], [9].

Thermonuclear supernovae are challenging to model because in addition to including a host of physics, e.g. hydrodynamics, self-gravity, and the material equation of state (EOS) for the degenerate electron/positron plasma of the core of the white dwarf star, models must address the vast disparity of the scales between the white dwarf radius (∼10^9 cm) and the width of the laminar nuclear flame at high densities (< 1 cm). We employ adaptive mesh refinement (AMR), but even with many orders of AMR it is not possible to resolve the physical flame in a whole-star simulation. Thus we also employ a model flame to capture the burning on sub-grid scales.

C. The FLASH Code

The FLASH code is a scientific simulation software package for addressing multi-scale, multi-physics applications [10], [11]. FLASH was originally developed at the Flash Center at the University of Chicago, supported by the Department of Energy’s Accelerated Strategic Computing Initiative (ASCI) [12] to address astrophysical problems involving thermonuclear flashes, stellar explosions powered by a thermonuclear runaway occurring on the surface or in the interiors of compact stars. FLASH continues to be developed for astrophysics [13], high-energy-density physics [14], and more general problems as FLASH-X, a new code derived from FLASH with a completely new infrastructure, being funded by the U.S. Department of Energy’s Exascale Computing Project [15].

As part of ASCI, the Flash Center was allowed access to unclassified versions or partitions of the state of the art supercomputers installed at the US National Laboratories [16],
establishing a history of use on advanced platforms. FLASH won the SC2000 Gordon Bell Prize, Special Category, for AMR simulations of reactive flow that achieved 238 GFlops on 6420 processors of ASCI Red at the Los Alamos National Laboratory [17], simulated weakly compressible stirred-turbulence at an unprecedented resolution on the IBM BG/L machine commissioned at the Lawrence Livermore National Laboratory in 2005 [18], [19], and served as a formal acceptance test for both Intrepid, an IBM BG/P, and MIRA, an IBM BG/Q machine, at the Argonne Leadership Computing Facility [20].

FLASH uses AMR to address problems with a wide range of physical and temporal scales. The current release of FLASH (version 4.6.2) implements AMR using the PARAMESH library [21], [22], which uses a block-structured mesh. FLASH is parallelized primarily through MPI, although some solvers have been modified to take advantage of threaded approaches to parallelization [20] and development continues toward a more general design for better allowing threading [23], [24].

The PARAMESH library manages a block-structured adaptive mesh, with the data typically in $16 \times 16 \times 16$ zone blocks ($16 \times 16$ in 2-d). The principal data container unk stores variables such as density, temperature, pressure, etc., in the form unk(nvar, il_bnd, iu_bnd, jl_bnd, ju_bnd, kl_bnd, ku_bnd, maxblocks) where nvar is the number of variables, il_bnd:ju_bnd, kl_bnd:ku_bnd are the x, y, and z zone limits, and maxblocks is the number of blocks. PARAMESH is thus designed for loops using data from blocks, and there is a stride in memory for addressing variables in different zones or blocks. This feature motivated our interest in investigating the use of huge pages as a way of improving performance.

The modified version of FLASH we use for supernova simulations utilizes an advection-diffusion-reaction (ADR) scheme [25] that propagates reaction progress variables to model the stages of the sub-grid-scale flame. Flame speeds are from the tabulated results of previous calculations [26], [27] and also include enhancement to the burning rate from unresolved buoyancy and background turbulence [28]–[30]. Finally we note that the FLASH simulations use double precision arithmetic.

II. PORTING AND PROFILING FLASH

Our efforts at porting FLASH to Ookami began with identifying the prerequisites for running our supernova application, e.g. compilers, MPI, and HDF5, and ensuring these were available. We initially explored the GCC 10.3.0, Cray 10.0.3, and Arm 21.0 compilers with MVAPICH 2.3.5 and OpenMPI 4.0.5. This effort showed that FLASH ran “right out of the box” with these and scaled reasonably well with no tuning. As different combinations of compilers and MPI implementations have been shown to produce large performance differences for the same code, we were interested to see if this trend persisted with our supernova problem. We found that the ARM compiler produced an executable that ran almost 2.5 times slower than those created with the Cray and GCC compilers; the runtime differences between the latter were negligible. However, the same executable compiled using GCC 10.2.0 with MVAPICH 2.3.5 on Intel Xeon E5-2683v3 CPUs ran three times quicker than the fastest runs on Ookami. It is important to note that this runtime comparison was done before tuning our code to use the A64FX’s main features, including use of SVE instructions and HBM, so accordingly this is where we turned to next.

To see where our code could most benefit from use of these features, we began our investigation into the performance of FLASH on Ookami by profiling with Arm MAP [31]. Our scientific investigation of Type Ia supernova is currently performing suites of 2-d simulations that allow for a relatively inexpensive exploration of both the Ookami platform and the parameter space of the astrophysics problem. Our MAP study indicated that FLASH spent considerable time in the routines for the EOS. Accordingly, we decided to analyze that part of the code while running 2-d supernova simulations.

The next step was to investigate use of SVE, but taking advantage of SVE proved difficult and we found that considerable modification will be required to vectorize our version of FLASH. The problem is the vast scope and branching of the main loops in the EOS routines that prevents using SVE.

Accordingly, in an effort to identify other issues to address to boost performance we instrumented the code with the Performance Application Programming Interface (PAPI) [32], and we describe this process in detail below. The finding of that analysis was that the number of data translation lookaside buffer (DTLB) misses were exceptionally high, so we focused on the use of huge pages in memory as the next avenue of investigation, which is the main topic of the paper. A full report on our exploration with scaling results and details of our attempt to utilize the A64FX’s SVE instructions and NUMA architecture may be found in [33].

The 2-d supernova problem with the EOS was the obvious choice for our investigation into the use of huge pages. Eventually, however, we will run full 3-d simulations of supernovae, so to test the principal component of 3-d simulations, the hydrodynamics routines, we settled on also investigating a pure hydrodynamics simulation, the Sedov explosion problem [34], one of the standard test problems provided with FLASH.

For the two problems, we instrumented the code to record the performance of the routines of interest, the EOS routines in the supernova case and the hydrodynamics routines in the Sedov case. Thus in this work we report on two tests dubbed “EOS” and “3-d Hydro” because those were the parts of the code we instrumented for performance measurements. Details of both the EOS and the Sedov explosion problem may be found in the original FLASH paper [10]. The EOS test ran a 2-d supernova simulation for 50 time steps and the 3-d Hydro test ran a Sedov explosion simulation for 200 time steps.

Our instrumentation of FLASH with PAPI began by identifying a subset of PAPI events that can characterize overall performance — use of SVE measured as SVE instructions and hardware cycles, and the number of hardware cycles, and we tested the use of PAPI to monitor these quantities with several simple example programs.

Following the Object Oriented Programming in Fortran
2003 lesson, “Tutorial OOP(III): Constructors and Destructors” by Danny Vanpoucke, we began instrumenting FLASH by constructing a Fortran object to interface with the PAPI routines [35]. We used a Fortran module to initialize the object and allocate member variables, call the PAPI begin function, and finalize by calling the PAPI end function and deallocate the variables. The object also used another Fortran module to store an identifier for the region of the code that was instrumented. Using the Fortran block construct allows avoiding the Fortran requirement that declarations be made before any executable statements and instantiating the performance object at any point in a routine.

This module worked with the GNU compiler version 11.2.0 and worked (with a slight modification) with the Cray compiler version 10.0.3 (both SVE and non-SVE versions). Unfortunately, however, this module did not work with the Fujitsu compiler version 4.5. The issue was with calling the finalizer, and we attribute the problem to the compiler having not reliably implemented initializers and finalizers of the Fortran standard [36], [37]. So we fell back to just “hard coding” the PAPI calls to work with all compilers we tested.

FLASH also has internal timers, and we noted those results as a consistency check on our PAPI instrumentation. The timers record the elapsed time for the simulation, and we record these below in addition to the PAPI results. We also report the SVE results from PAPI although the code was not vectorized and these results are not critical for this study. At some point recalling these “un-tuned” results may useful.

III. TESTING USE OF HUGE PAGES

At the time we performed our investigation, the operating system on Ookami was CentOS 8.1 with kernel 4.18.0-147.el8.aarch64, which allowed huge pages for memory access. On its own, the kernel should invoke transparent huge pages, an abstraction layer that automates most aspects of creating, managing, and using huge pages [38], when it processes a file greater than 2 Gb. In this case, the kernel does most of the work, though one can alter that with the hugetlb utility of the hugetlbfs filesystem of Linux [39] with commands of the form hugetlb --shm --thp ... and LD_PRELOAD=libhugetlbfs.so ... for any compiler and with the XOS_MMM_L_HPAGE_TYPE environment variable for the Fujitsu compiler. While the documentation mentions that acceptable values are none or hugetlbfs, [40] mentions another possible value thp for the variable on Fugaku and is accepted by the FX700 processor as well.

Huge pages can also be invoked via mechanisms such as the hugeadm tool of the libhugetlbfs library [41] and as part of our exploration we configured two nodes of Ookami for using these tools (described below).

We monitored the use of huge pages by looking at system variables in /proc/meminfo that would have values if the huge pages were in use, AnonHugePages, ShmemHugePages, HugePages_Total, HugePages_Free, HugePages_Rsvd, HugePages_Surp, Hugepagessize, Hugetlb. Our tests consisted of running the instrumented code with and without huge pages, while monitoring the values of the variables in /proc/meminfo to ensure that huge pages were in use when expected.

Our investigation into huge pages also involved modifications to Ookami. We installed the Fujitsu compiler and also modified the system on two Ookami nodes [42]–[44]. The modifications to the two nodes include:

- Installation of the Fujitsu compiler, which required kernel boot time parameters to be set.
  - Kernel boot parameters set: hugepagesizez=2M
  
- Setting kernel parameter in /etc/sysctl.d/98-fujitsucompilersettings.conf
  kernel.perf_event_paranoid=1

- Installation of the package libhugetlbfs-utils, specifically the tool: hugeadm for configuring the hugepage environment.
  - Specialized UNIX group created for empowered end user use: ‘hugetlb_shm_group’ and added members.
  - Allowed enabling and disabling transparent huge pages by changing settings in the file /sys/kernel/mm/transparent_huge-page/enabled.
    - Enable transparent huge pages by setting the file contents to “always” madvise never” (command: echo always > /sys/kernel/mm/transparent_huge-page/enabled.
    - Disable transparent huge pages by setting the file contents to “always madvise [never]” (command: echo never > /sys/kernel/mm/transparent_huge-page/enabled.

IV. FLASH RESULTS

Our first test was compiling FLASH with the GNU compiler to demonstrate it was able to use huge pages. Try as we might, however, we were not able to use huge pages when compiling with the GNU compiler. We tried many variations of explicitly using the hugetlb tools, explicit linking the hugetlbfs library, and using the modified nodes, to no avail.

To further investigate, we wrote two simple Fortran test programs, one statically allocating memory for a 2-d array and one dynamically allocating memory for a 2-d array, and then just repeated calculating sums over the arrays. As expected, the program with the dynamically allocated array was able to use huge pages with the GNU compiler while the statically allocated array version could not. This behavior is expected because transparent huge pages only maps anonymous memory regions such as heap and stack space [38].

In normal usage, FLASH is compiled with specific values of the block sizes, e.g. 16 × 16 × 16, for the variables in the data container unk and changing any of those requires re-compiling the code. PARAMESH also has a library mode that
is designed to allow use of it as a pre-compiled library so that the block sizes may be set at run time. Our interpretation was that FLASH using PARAMESH with the block sizes set at compile time was statically allocating the array unk. Investigation showed that this was not the case, however, and unk was dynamically allocated even when PARAMESH was not in library mode. Apparently at some point the FLASH or PARAMESH developers switched to dynamic allocation to avoid difficulties with statically allocating large arrays [45].

We subsequently found that FLASH did not also use huge pages with the Cray compiler. Why FLASH does not use huge pages with the GNU and Cray compilers remains a mystery, unfortunately. We did find success with the Fujitsu compiler as FLASH naturally used huge pages and use of huge pages had to be explicitly turned off via the -Knolargepage flag for compiling and linking. Accordingly we have a performance comparison only for the Fujitsu compiler.

Tables I and II present results for the EOS and 3-d Hydro problem, respectively. Shown are results for the five PAPI performance measures and the elapsed time from the FLASH timer for simulations run with and without huge pages.

**Table I**

**Results with the Fujitsu Compiler for the EOS Problem**

| Measure                  | Without HPs | With HPs |
|--------------------------|-------------|----------|
| Hardware (cycles)        | 1.25 × 10^12 | 1.17 × 10^12 |
| Time (s)                 | 6.97 × 10^3  | 6.52 × 10^3  |
| SVE Instructions/cycle   | 0.47        | 0.51     |
| Memory (Gbytes/s)        | 4.19        | 4.45     |
| DTLB misses (1/s)        | 2.34 × 10^6  | 1.10 × 10^7  |
| FLASH Timer (s)          | 339.032     | 333.150  |

**Table II**

**Results with the Fujitsu Compiler for the 3-d Hydro Problem**

| Measure                  | Without HPs | With HPs |
|--------------------------|-------------|----------|
| Hardware (cycles)        | 1.21 × 10^12 | 1.20 × 10^12 |
| Time (s)                 | 6.70 × 10^4  | 6.69 × 10^4  |
| SVE Instructions/cycle   | 0.11        | 0.11     |
| Memory (Gbytes/s)        | 10.10       | 10.09     |
| DTLB misses (1/s)        | 2.42 × 10^7  | 7.83 × 10^7  |
| FLASH Timer (s)          | 1203.616    | 1176.312  |

Figure 1 compares the results with and without use of huge pages for the two simulations. Shown is a bar chart with the ratio of each performance measure using huge pages to the measure without use of huge pages for the two test simulations. All measures but DTLB misses are close to one, showing little effect when using huge pages. The low ratios for DTLB misses (0.047 and 0.324 for the EOS and 3-d Hydro tests, respectively) show that use of huge pages drastically reduces these misses. The near unity ratios for the times, however, show the reduction of DTLB misses did not significantly improve the performance for either problem.

**V. SUMMARY AND CONCLUSIONS**

We found that the FLASH code was only able to use huge pages when compiled with the Fujitsu compiler. The reason executables compiled with the GNU and Cray compilers did not use huge pages remains a mystery. A small test program that dynamically allocated memory was able to use huge pages when compiled with the GNU and Cray compilers (in addition to the Fujitsu compiler) as expected. The main data containers in FLASH are dynamically allocated, so our first proposed explanation of the problem, static allocation of arrays in FLASH, does not explain the behavior.

We found that when using huge pages, simulations that exercised physics modules in FLASH known to have significant computational expense showed a dramatic reduction in DTLB misses. This reduction, however, did not significantly improve the performance of these simulations. Further investigation is needed to understand why.

Installing the Fujitsu compiler on Ookami required installing packages for huge pages. While we modified two nodes of Ookami to enable huge pages, the unmodified nodes also readily used huge pages upon installing the Fujitsu compiler and did not demonstrate different behavior from modified nodes. We suspect the modifications were either unnecessary or redundant with the installation of the Fujitsu compiler.

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