# Performance of an Astrophysical Radiation Hydrodynamics Code under Scalable Vector Extension Optimization

Dennis C. Smolarski

Department of Mathematics & Computer Science

Santa Clara University

Santa Clara, USA

dsmolarski@scu.edu

F. Douglas Swesty, Alan C. Calder

Department of Physics and Astronomy

Stony Brook University

Stony Brook, USA

{douglas.swesty, alan.calder}@stonybrook.edu

Abstract—We present results of a performance study of an astrophysical radiation hydrodynamics code, V2D, on the Armbased A64FX processor developed by Fujitsu. The code solves sparse linear systems, a task for which the A64FX architecture should be well suited. We performed the performance analysis study on Ookami, an Apollo 80 platform utilizing the A64FX processor. We explored several compilers and performance analysis packages and found the code did not perform as expected under scalable vector extension optimization, suggesting that a "deeper dive" into analyzing the code is worthwhile. However, a simple driver program that exercised basic sparse linear algebra routines used by V2D did show significant speedup with the use of the scalable vector extension optimization. We present the initial results from the study which used V2D on a relatively simple test problem that emphasized the repeated solution of sparse linear systems.

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

#### I. INTRODUCTION

## A. Astrophysical Radiation Transport

Many astrophysical simulations require modeling the flow of some form of radiation, either photons or neutrinos, through gas. Modeling the flow of radiation requires the parallel, implicit solution of a large, sparse, set of coupled linear equations that describe the time evolution of the radiation energy density across a spectrum of energies. In this paper we investigate the computational performance of one such simulation code, V2D [1], which models the flow of radiation in the multigroup flux-limited diffusion approximation. V2D uses a parallelized Krylov subspace algorithm to solve the linear system of equations arising from the finite-difference discretization of the underlying equations that describe the diffusive evolution of the radiation energy density.

## B. The Ookami Platform

Ookami [2] is a test bed supported by the United States National Science Foundation (NSF). The platform is an HPE Apollo 80 with 174 A64FX Fujitsu compute nodes, each with 32GB high-bandwidth memory and a 512GB SSD. The A64FX processors consist of four core memory groups each

with 12 cores, 64KB L1 cache, and 8MB L2 cache shared between the cores and runs at 1.8 GHz. The processor uses the Armv8.2–A Scalable Vector Extension (SVE) SIMD instruction set with 512 bit vector implementation. This allows for vector lengths anywhere from 128–2048 bits and enables vector length agnostic (VLA) programming. Ookami has an Infiniband HDR100 fat tree interconnect with 200 gigabit switches, and a high-performance Lustre file system provides about 800 TB storage.

Ookami was the first open machine outside of Japan featuring the A64FX processor, and the aim of the Ookami project is to provide researchers with access to this state-of-the-art scientific computing technology in order to explore it and demonstrate its potential. The code, V2D, is one of the application codes being ported and tuned for the machine. More details on the system and the project can be found in [3], [4]. Ookami is presently administered by Stony Brook University and the University at Buffalo, but in October 2022 Ookami will be an XSEDE level 2 service provider [5].

## C. The V2D Code

The V2D code uses finite-difference algorithms to solve the equations of Eulerian hydrodynamics and multi-species fluxlimited diffusive radiation transport in two spatial dimensions. It was designed primarily for the purpose of simulating core collapse supernovae but has a wider applicability to many radiation-hydrodynamic problems. Details related to the underlying numerical methods can be found in [1]. Written in Fortran-95, V2D employs MPI for domain-decomposed parallelism and HDF5 for parallel input and output. The linear system solver uses a restructured version of the BiCGSTAB [6] algorithm, which gangs inner products to reduce the number of parallel global reduction operations required per iteration of the BiCGSTAB solver. Preconditioning of the linear system is accomplished using a sparse approximate inverse preconditioner [7]. Because of its prohibitive size, the sparse linear system matrix is never stored and the Krylov subspace methods are implemented in matrix-free form by application of a finite-difference operator to column vectors that are stored

as Fortran arrays defined with the same spatial shape as the 2D grid. This strategy also avoids the costly packing/unpacking of data into some form of sparse matrix storage each time a linear system must be solved. The V2D code has been generically written to allow various coordinate systems and the x1 and x2 spatial directions are always considered to be orthogonal. The problem is domain decomposed using a Cartesian 2-D spatial tile decomposition that is controlled by adjustable runtime parameters NPRX1 and NPRX2 that control the tiles in the x1 and x2 directions, respectively. Thus the process topology may be varied to better apportion the load among processors. Finally, we note that the calculations tested here were performed in double precision arithmetic.

#### II. THE SVE OPTIMIZATION STUDY

## A. The V2D Radiation Test Problem

The test diffusive radiation transport problem that we consider in this paper involves the diffusion of a 2-D Gaussian pulse of radiation [1] and does not involve hydrodynamic evolution. This particular test problem was chosen for this study because the principal computational effort is expended in the solution of a large, sparse, memory-bandwidth-limited linear system that describes the time evolution of the radiation distribution. Solving this system should be a task for which the Ookami architecture is ideally suited. The linear system, as described below, consists of  $x1 \times x2 \times 2$  coupled linear equations, where the spatial dimensions are x1 = 200 and  $x^2 = 100$  zones respectively, and the number of radiation species is 2. We wish to emphasize that this is a small test problem that we have chosen for a study of performance under SVE optimization. In the work in this paper we make only limited use of the parallel capability of V2D when we vary the process topology to adjust the problem size on each processor.

While the aforementioned linear system is sparse, it has a regular structure. If the matrix corresponding to this system were actually stored, with a dictionary ordering it would form a banded matrix with five bands. A portion of what the sparsity pattern for this matrix would look like is depicted in Fig. 1. The figure only depicts the upper left  $400 \times 400$  block of the complete  $40,000 \times 40,000$  matrix. On either side of the diagonal are two adjacent diagonals with two outlying diagonals spaced farther from the diagonal. The x1 parameter indicates the distance of the two outlying diagonals from the center diagonal.

The Krylov subspace algorithms employed by V2D require only matrix-vector multiplication operations (hereafter Matvec), and not the matrix itself. Because the matrix would arise from a second-order spatial finite-difference scheme for the diffusion operator, we instead evaluate the Matvec operations by applying the diffusion operator in finite-difference form to a vector to form a new resultant vector. For each element of the vector there are relatively few floating-point operations needed to evaluate the Matvec operation and thus the Matvec operations are memory bandwidth limited.

The Krylov subspace algorithm we employ for the linear system solution is the BiCGSTAB algorithm [6]. BiCGSTAB

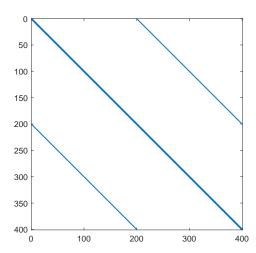


Fig. 1. The sparsity pattern of matrices used in the V2D code.

is an extension of the Conjugate Gradient (CG) method (which is designed for a symmetric linear system of the form Ax = b, where A would represent the system matrix) to those cases where the system matrix A is non-symmetric. The time evolution of the radiation energy density in this test problem involves many repeated solutions of linear systems, one for each timestep, thus causing the computational cost of the simulation to be dominated by the sparse matrix operations employed by the BiCGSTAB algorithm.

### B. Compilers and SVE Optimization

Our first task was to identify the prerequisites of V2D, e.g., MPI [8], [9] and HDF5 [10], and determine how those are accessed and configured on Ookami. We then tested combinations of compilers and MPI implementations. As a sample of results, those presented below indicate test runs using the GNU (ver. 11.1.0), Fujitsu (ver. 4.5), and Cray (ver 21.03) compilers. Some compilers allowed the use of either MVAPICH [11] or OpenMPI [12] and others only provided one option for MPI.

#### C. Performance Monitoring

We compared the CPU times of simulations compiled with different compilers, both with and without SVE optimization. Because the craypat performance tool will only work with the Cray compiler, the Linux perf stat command of the Linux kernel performance monitor, with the -e duration\_time and -e cpu-cycles flags, was used to measure the time of the simulations for the different compilers. This command measures the entire CPU time of the process. Each configuration (of the total number of processors used and the process topology in the x1- and x2- directions, determining how the linear system was partitioned) was run several times to confirm the timing results.

In addition, for the fastest versions of the executable, produced by the Cray compiler, the TAU software (developed

TABLE I TIMES BY COMPILER

$N_p$	Direction		Times by Compiler (seconds)			
	NX1	NX2	GNU	Fujitsu	Cray	Cray
					(opt)	(no-opt)
1	1	1	363.91	252.31	181.26	262.57
10	10	1	43.85	31.76	24.20	32.35
20	20	1	26.80	19.79	16.78	20.66
20	10	2	25.74	19.66	15.73	19.93
20	5	4	25.42	18.85	15.39	19.79
25	25	1	24.62	17.24	15.65	
40	40	1	25.30	13.97	19.12	
40	20	2	22.88	12.96	17.37	
40	10	4	21.91	13.04	17.16	
50	50	1	30.10	13.05	25.56	
50	25	2	29.26	12.09	24.07	
50	10	5	27.55	11.40	23.51	

at the University of Oregon [13]) was also used to verify the times recorded from the runs. TAU's ParaProf visualization tool also enabled us to see which routines contributed most to the total time without the need to add additional routine calls in the software.

#### D. Results for SVE Optimization of V2D

Table I summarizes the results of using three different compilers on Ookami to produce a V2D executable that solves a linear system consisting of  $x1 \times x2 \times 2$  equations, where x1=200 and x2=100. The test problem time-evolves the radiation energy density for 100 time steps. Each time step requires the solution of three unique  $x_1 \times x_2 \times 2$  linear systems via the BiCGSTAB algorithm. Thus this test problem establishes performance results for the solution of 300 linear systems. As noted above, the times were clocked using the Linux perf stat performance analysis command, which was used to measure the duration of the execution, giving values in seconds.

All the compilers available on Ookami are able to make use of the SVE capabilities of the architecture. In the trials listed in Table I, the SVE and optimization features were used, but we also turned off the SVE and other optimization features on some of the Cray trials for comparison purposes.

In Table I the values in the  $N_p$  column refer to the total number of processors used for a run, with the values in the "Direction" NX1 column indicating the number of domain decomposition tiles in the x1 direction and similarly for the values in the NX2 column. Thus the product of the two values equals the total number of processors requested. The column labeled Cray (opt) indicates results obtained with an executable compiled both with both -03 optimization and SVE optimization enabled. The last column, labeled "Cray (no-opt)", used an executable compiled with the Cray compiler without either the -03 optimization or SVE optimization enabled.

## E. Timing analysis

The timing information in Table I reveals that the Cray and Fujitsu compilers produced substantially faster code than the GNU compiler. The Cray compiler also produced slightly faster code than the Fujitsu compiler when using 25 or fewer processors.

The various trials using the Cray compiler with and without SVE optimization reveal a reduction in CPU time with the use of SVE optimization. Using PAPI analysis calls, we noted speedup using SVE optimization in the routines that applied the preconditioner to the system matrix, as well as when using the dot product, vector addition, and combined vector scaling/addition routines.

When using a single processor, the majority of time was spent in the matrix-vector multiplications, approximately 141 seconds out of 181, with preconditioning taking about 14 additional seconds. We also make use of Arm's MAP performance analysis tool, which indicated that the three calls to the BiCGSTAB routine each took approximately 31-33% of the total time using a single processor.

When using 20 processors, in a  $5 \times 4$  configuration, approximately 7.5 seconds out of 15 were spent in the matrix-vector multiplications at maximum per processor, with preconditioning taking about 0.8 seconds at maximum. As to be expected with multiple processors, a significant amount of time was taken by MPI calls.

Increasing the number of processors will decrease the amount of time needed for the matrix-vector products, but there is a point, varying with each compiler, at which the increased time needed for inter-processor communication via MPI calls does not lead to further overall reduction in time. The variations exhibited in Table I between different compilers can be attributed to the machine architecture used for vector multiplications as well as the different ways the compilers optimize the code.

These results were qualitatively as expected—optimization with SVE produced a speedup. But the magnitudes of the speedups observed with the Cray compiler were smaller than what we expected for memory-bound linear system operations. We attributed this to the overall complexity of the multi-physics V2D code. V2D was designed with abstracted operators for linear algebra, but calls to these operators are interspersed with calls to other physics routines and a simulation exercises more than just the operators. Further analysis is certainly needed.

#### F. Timing V2D matrix operations using PAPI

Because the use of SVE optimization did not produce the speedup in V2D that we had hoped for, we therefore wrote a simple single-processor driver program that exercised the actual V2D routines that are utilized in the BiCGSTAB solver without the added complications of the other V2D code. With this driver program we then examined the CPU time utilized for repeated computation of the linear algebra routines, both with and without the SVE optimization enabled. We used a linear system with 1000 equations and repeated operations 100,000 times. The CPU times spent in the linear-algebra routines were obtained both from checking the hardware clock

TABLE II LINEAR ALGEBRA ROUTINES TIMES

PAPI times (seconds)								
Routine	No-SVE	SVE	SVE/No-SVE					
MATVEC	599	96	0.16					
DPROD	132	24.3	0.18					
DAXPY	206	53.8	0.26					
DSCAL	153	47.7	0.31					
DDAXPY	296	65	0.22					

and by using PAPI software timers, but the differences between the two were insignificant.

As Table II indicates, when these V2D sparse linear-algebra routines were exercised using the driver program, a significant speedup was realized with SVE optimization. Overall, the use of SVE (with the Cray compiler) reduced the time spent in these routines to approximately between 16% and 31% of the time needed without SVE. (The times are given in seconds in the following table.) MATVEC = Matrix Vector Product; DPROD = Dot Product; DAXPY = computation of  $a \cdot x + y$ ; DSCAL = computation of  $c - d \cdot y$ ; DDAXPY = computation of  $a \cdot x + b \cdot y + z$ .

## III. CONCLUSIONS AND FUTURE WORK

The principal conclusion, which in hindsight we realize is fairly obvious, is that a complex multi-physics code, even though it is dominated by memory bandwidth-limited sparse linear algebra computations, will not necessarily demonstrate the speedup expected with the use of SVE optimization. However, testing just the memory bandwidth-limited sparse linear algebra routines did reveal that they were able to undergo significant speedup with SVE optimization. Because V2D relies on these same routines for its implementation of the BiCGSTAB algorithm, we need to do further work to understand what is limiting the overall V2D code performance. Future work will entail more detailed instrumentation of the code to delineate the origins of the performance bottleneck.

As also noted, the times recorded when using the Fujitsu compiler with more than 25 nodes were less than times recorded with the Cray compiler. Further investigation with a larger problem and more nodes comparing the Fujitsu and Cray compilers is warranted, along with the use of other compilers, such as Clang [14].

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