Exploring the SW4 Synthetic Seismic Performance of the ARCH Rockfish Cluster

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For seismic research, high-performance computing enables us to perform earthquake simulations at higher source frequencies and lower minimum shear-wave velocity parameters than on desktop or laptop systems, delivering higher-accuracy seismic ground motion estimates. We initially computed 27 low-resolution, low-frequency (<0.6 Hz) 3D shaking models using SW4 2.01 software and a MacBook Pro. Eleven high-resolution scenarios were computed using the ARCH Rockfish supercomputing cluster located at the Johns Hopkins High Performance Computing Center. We compared low-resolution MacBook Pro simulations to both low- and high-resolution Rockfish simulations and analyzed Rockfish's overall performance using SW4. We found that low-resolution simulations were slightly faster on Rockfish. We achieved high efficiency for the high-resolution simulations on Rockfish; for all configurations tested, efficiency was above 99%. High-resolution scenarios on Rockfish show a substantial improvement in detail, with prominent basin-edge amplifications. Notably, in high-resolution scenarios we see wave resonance within the narrow Wainuiomata Valley, an effect not visible in the low-resolution models. Scenarios built using Rockfish showed a wide variety of performance, highly dependent on Slurm job directive values. With just a portion of our CPU allocation, we were able to successfully compute a non-ergodic set of Wellington shaking scenarios valid from 0.2 to 1.5 Hz. These scenarios will provide the city with basin-amplification maps and spectra. Results enable increased accuracy for seismic analysis, improving seismic hazard estimates and preparedness for expected seismic events within the Wellington region. This work also provides a starting point for any subsequent seismology research that may choose to utilize high-performance computing.

CCS CONCEPTS • Parallel algorithms • Modeling and simulation • Earth and atmospheric sciences

Additional Keywords and Phrases: high-performance computing, seismic modeling, parallel performance analysis, ground motion simulation

1 INTRODUCTION

Instead of traditionally relying only on data recorded during large earthquakes, SW4 software allows scientists to predict earthquake effects for cities lacking sufficient recordings through 3-D seismic modeling. Although New Zealand's capital city of Wellington has abundant recordings of strong earthquakes, almost all the recorded sources are at distances and directions that are not expected to be representative of larger quakes in the future that could do the most damage- a shortcoming termed an ergodic assumption. Modeling the city's response to a non-ergodic, more representative distribution of synthetic events using SW4 will help the city improve earthquake resilience. SW4 was created by N. Anders Petersson and Bjorn Sjögreen of Lawrence Livermore National Laboratory and is distributed by the Computational Infrastructure for Geodynamics [5]. SW4 is a fourth-order finite difference code which uses a distributed memory programming model. The software is mostly written in C++ and numerical computations are implemented in Fortran-77 [6]. Using SW4, we analyzed how seismic waves travel through soft sediments in the Wellington, New Zealand basins by performing simulations using an array of quakes and three alternative earth-structure and velocity models.

2 EARTHQUAKE SCENARIOS

To investigate possible ground motions in the Wellington basins, we performed simulations of a M3.3 event with three 3D velocity models: one which contrasts an older geologically-based GNS Science basin model having a maximum sediment thickness under the City Centre of 250 m [1], a second that included newly developed gravity-based model by Stronach and Stern with a maximum thickness of 540 m under the city [8], and a 1D model without basin data [4]. Our initial simulations were performed utilizing a MacBook Pro with a 2020 1.4 GHz Quad-Core Intel Core i5 and 8 GB of RAM running on macOS Monterey. Due to hardware limitations, simulations were built with an increased minimum shear-wave velocity paired with lower frequencies, and each run took around 3 hours. Despite these limitations, our research was successful in indicating that the adjustments of sedimentary basin thickness under the city of Wellington made by Stronach and Stern produce a substantial difference in how seismic waves travel compared to the older GNS Science model, providing a clear basis for a continuing study of earthquake basin effects within Wellington [4].

Using SW4 software with supercomputing drastically improves productivity, expands modeling capability, and advances the field of seismic research by enabling scientists to increase source frequencies and lower minimum shear-wave velocities, thus creating more accurate scenarios. Rockfish is a shared advanced research computing facility housed at the Maryland Advanced Research and Computing Center (ARCH). We explored performance of the ARCH Rockfish supercomputing cluster for our high-resolution scenarios. We were awarded an initial project resource allocation through ACCESS of 20,000 core-hours on the Rockfish "defq" partition. After several successfully run scenarios with the "defq" partition, we were awarded an additional 100,000 core-hours on the "bigmem" partition for large-memory high-resolution scenarios.

partition	available nodes	min/max time (h)	max cores-per-node	max memory-per-node
defq	667	1/72	48	192 GB
bigmem	22	1/48	48	1,537 GB

Table 1: Partition Maximum and Minimum Values

3 SCALING ANALYSIS

An initial strong scaling analysis was performed to estimate optimal values for job sizes. Cluster queue time was not incorporated into the scaling analysis. When conducting a scaling analysis, we analyze the number of nodes, the number of tasks-per-node requested, the CPU parallel efficiency, and the speed-up ratio of each test scenario. Equation 1 [7], used for CPU parallel efficiency is calculated by dividing the serial execution time (t_s) by the parallel time (t_p) multiplied by the total number of tasks (n). Equation 2 [3], used for speed-up ratio is calculated by dividing serial execution time (t_s) by parallel time (t_p):

$$\text{CPU parallel efficiency} = \frac{t_s}{(t_p \cdot n)} \quad (1) \qquad\qquad \text{Speed-up ratio} = \frac{t_s}{t_p} \quad (2)$$

We selected a representative scenario for our scaling analysis seen in Figure 1. This scenario had parameters of 0.6 Hz maximum source frequency, 350 m/s minimum shear-wave velocity and was run for only 116 timesteps (two seconds of simulated time). The timesteps, or image slice parameter, is how often SW4 writes an image to disk, showing the particle-velocity field. We found excellent efficiency, 98.9%, up to 16 tasks. After 16 tasks, efficiency begins to drop to 82%, and again to 72%. Although using the maximum limit of tasks-per-node (48) is fastest at 43 seconds, it is not the most efficient use of allocation.

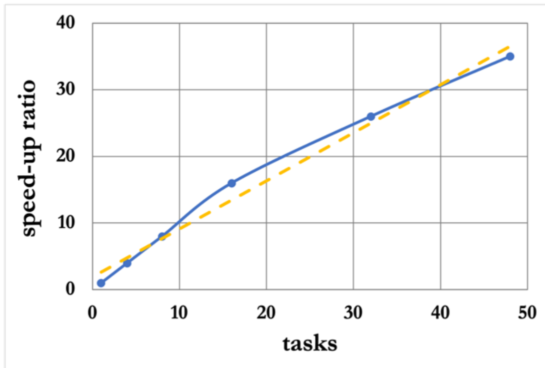


Figure 1: Strong scaling analysis shows a linear increase in speed-up ratio when doubling tasks. Linear performance is seen in dashed yellow.

4 SCENARIO SIMULATIONS

For our second series of runs, we adjusted parameters for source frequency and grid spacing. We used maximum source frequency values of 0.6 Hz, 1.2 Hz, and 1.5 Hz, and grid spacing values of 100 m, 50 m, 40 m, and 20 m. All computational grids represented 21 km east-west length, 17 km north-south width, and 15 km depth. For the computation grid with 100 m spacing these extents lead to a grid node count of about 6.0 million; at 20 m spacing the count is about 0.69 billion (Table 3). Nominally, total memory usage by SW4 runs about 25 bytes per grid node, suggesting our low-resolution runs used about 0.15 Gb. Our highest-resolution runs would have used on the order of 17 Gb. To account for the increase in computation cost needed for these simulations, tasks-per-node were increased from 16 to the node maximum, 48. We first performed low-frequency tests (Runs #0-#2). Run #3 made slight adjustments to the grid, slightly reducing the size to better fit our previously built pfile. The SW4 "pfile" contains the material properties of the earth model, on a geographic grid of depth profiles. The geographic grid interval is 0.0005 degrees of latitude or longitude, about 42-56 meters in Wellington. Between all the different computational grid spacings, we observed SW4 to make geologically and geophysically reasonable interpolations of the geographic pfile grids, checking model renderings at each stage of resolution increase.

Run #4 was our first attempt at building high-resolution scenarios, increasing maximum source frequency to 1.5 Hz, decreasing grid spacing to 20 m and halving the minimum shear velocity to 175 m/s, which together increased the computational cost by a factor of 16 compared to the 40 m grid. We found that our memory usage requirements exceeded the "defq" partition allowance. To move forward, we received a new resource allocation for large-memory usage: 100,000 core-hour credits on the "bigmem" partition.

Once allocated, we moved forward with Run #4 using 1 node and 48 tasks-per-node. This two second run had a wall-clock time of 33,600 seconds. In Run #5, we ran the full scenario at 40 seconds. We estimated this would have resulted in a 648,000 second wall-clock time (180 hours), which is well over the maximum time allowance for the "bigmem" partition (48 hours) when using 1 node and 48 tasks-per-node, so we increased our job size to 4 nodes. Run #6 changed the image slice parameter (time-steps) from 0.5 seconds to 0.10 seconds to add additional detail within image slices. Runs #6-#9 used identical job directive values. These runs changed the epicenter source location from southwest to east and added 1D scenarios with no basin data. Mesh refinement used in Run #10 increased detail near the model surface where seismic velocities are lower. SW4's mesh refinement feature allows a significant improvement in resolution, while decreasing run-time appreciably.

run	partition	nodes	total tasks	model run-time (s)	wall-clock time (s)	CPU efficiency (%)	max source frequency (Hz)	grid size (m)	grid points	min velocity (m/s)	timesteps
0	defq	1	3	40	8,880	99.69	0.6	100	6,040,151	350	2,315
1	defq	1	16	40	1,897	99.57	0.6	100	6,040,151	350	2,315
2	defq	1	48	40	6,480	99.44	1.2	50	47,919,501	350	4,629
3	defq	1	48	40	9,060	99.58	1.2	50	44,135,630	350	4,629
4	bigmem	1	48	2	33,600	99.61	1.5	20	686,394,474	175	579
5	bigmem	4	192	40	99,000	99.56	1.5	20	686,394,474	175	11,571
6	bigmem	4	192	40	98,940	99.41	1.5	20	686,394,474	175	11,571
7	bigmem	4	192	40	99,060	99.56	1.5	20	686,394,474	175	11,571
8	bigmem	4	192	40	97,620	99.57	1.5	20	686,394,474	175	11,571
9	bigmem	4	192	40	97,614	99.57	1.5	20	686,394,474	175	11,571
10	bigmem	4	192	40	24,720	99.57	1.5	split grid: 20/40	183,879,825/63,255,888	175	6,889

Table 2: Scenario parameters and Slurm job directive values for 11 high-resolution scenarios.

5 PERFORMANCE RESULTS

While using the Rockfish cluster we consistently did not see significant queue times when requesting job batches. Queue time was calculated by comparing job batch submission and end times with wall-clock times. One instance was documented, Run #6, which had 1 hour of queue time due to scheduled system maintenance. Run #0 directly compared processor performance between the MacBook Pro and Rockfish cluster using identical parameters and job directive values. The MacBook Pro had a wall-clock time of 11,400 seconds while Rockfish had a wall-clock time of 8,880 seconds. We expected the Rockfish Intel Cascade Lake processor at 3.0 GHz to take only 47% the wall-clock time of the MacBook Pro Intel i5 at 1.4 GHz, based on clock speed, but it took 78%. For Run #1, output accuracy was verified between the two platforms to seven significant figures using identical parameters and job directive values. Upon analysis of high-resolution scenarios run on "bigmem" partition seen in Figure 3, we can see a linear improvement in timesteps-per-hour up until around 12 wall-clock hours, likely due to the startup cost being amortized over more timesteps. After 12 hours, timesteps-per-hour fluctuates, likely due to scenario parameters and cluster environment at any point, averaging around 420 time-steps per hour.

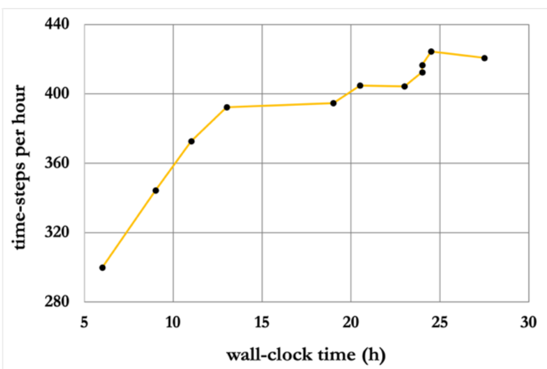
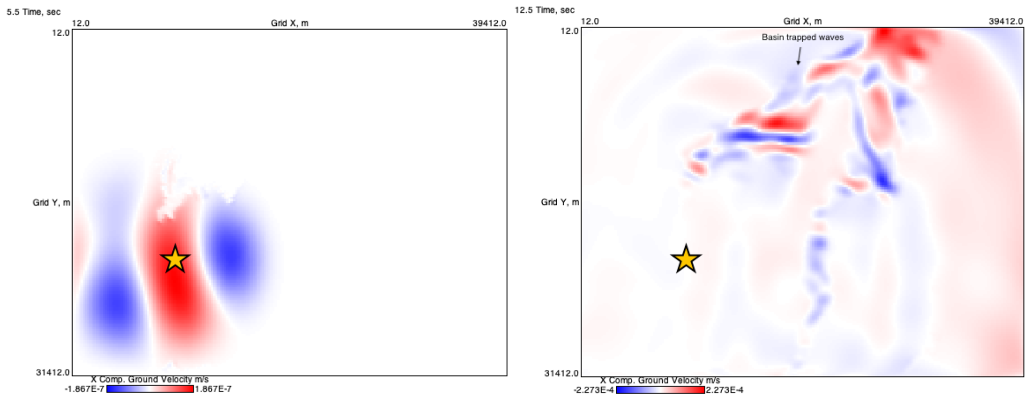


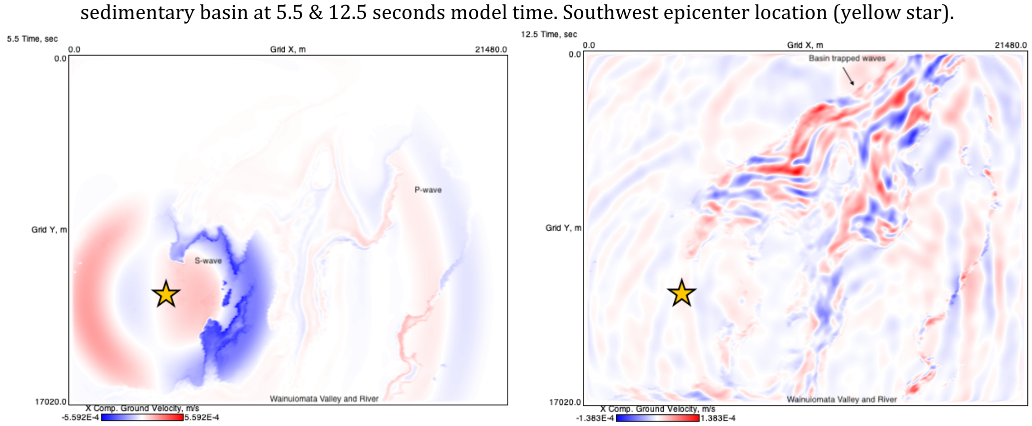
Figure 2: Time-steps per hour, wall-clock time (h).

6 CONCLUSIONS

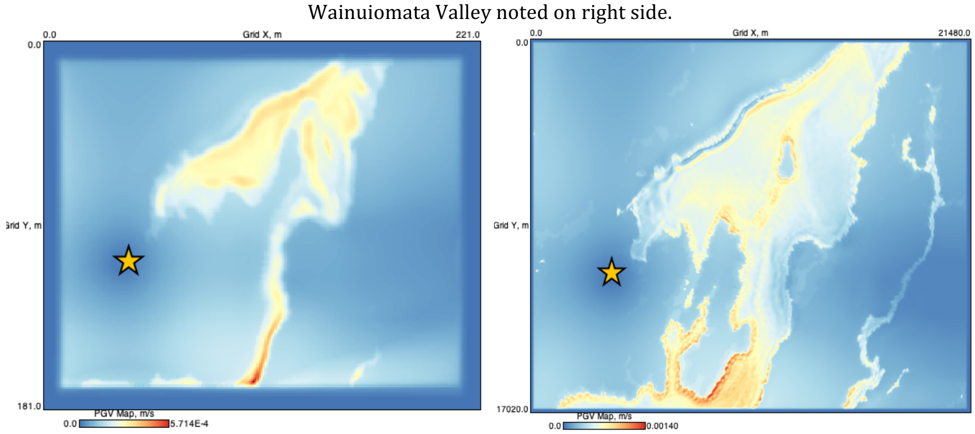
All high-resolution scenarios run with the ARCH Rockfish supercomputing cluster were successful, running to completion without any errors. Scenarios completed after using notably less allocation than preliminary usage estimates. Job efficiency was above 99% for all configurations tested. As a result, runs used a much smaller proportion of our allocation than initially expected. After project completion, a large portion of core-hours are still available for future research endeavors. In the future, we hope to streamline cluster processes to complete all previous non-ergodic scenarios at high-resolution under our remaining “bigmem” partition allocation. The high-resolution simulations enabled by Rockfish yield improved scientific results.



Figures 3 & 4: Low-resolution M3.3 event ground velocity snapshots showing wave resonance within Wellington's sedimentary basin at 5.5 & 12.5 seconds model time. Southwest epicenter location (yellow star).



Figures 5 & 6: High-resolution M3.3 event ground velocity snapshots showing wave resonance within Wellington's sedimentary basin at 5.5 & 12.5 seconds model time. Southwest epicenter location (yellow star), Wainuiomata Valley noted on right side.



Figures 7 & 8: Low-resolution PGV Map (left). High-resolution PGV Map (right).

Figures 3 & 4 show low-resolution snapshots run using the MacBook Pro. Figures 5 & 6 show high-resolution snapshots of the same scenarios built using Rockfish. Both scenarios show earthquake wave propagation and resonance across Wellington's sedimentary basin from a magnitude 3.3 earthquake. We saw an increase in detail within the southern, eastern and center regions. On the eastern (right) side, Figures 5 & 6 show resonance within Wainuiomata Valley, a large suburb of Lower Hutt. This region is not discernable in the low-resolution models. In Figures 7 & 8, we compare low-resolution and high-resolution scenarios built using a southwest-epicenter source. The high-resolution PGV shaking map built using Rockfish (Figure 8) shows a substantial increase in detail, especially within the southern, eastern and center regions. Wave resonance within the basin is most visible for both models in the upper right as regions of brighter color.

Our final model incorporated SW4's mesh refinement feature, which decreased run-time from 27 hours to just under seven hours while preserving efficiency. This improvement in performance allows for the incorporation of topographic data, which will provide an increase in both quality and data precision for the models. In future scenarios, we aim to add this feature. Based on our results, we strongly recommend incorporating mesh refinement, to enable high-resolution results with reduced wall-clock time. When comparing the MacBook Pro directly with the Rockfish system, we saw a significant decrease in wall-clock time for all scenarios and submitting multiple jobs at once significantly increased productivity. In addition, visual improvements were considerable.

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