Coverletter for ATSPEC

March 10, 2017

Current and Future Work

My name is Rahulkumar Gayatri and I am currently working as a postdoc at the Lawrence Berkeley National Laboratory in the NERSC department. I am in the NESAP program where an application's readiness for the exascale architectures is evaluated. The project involves improving the performance of a compute intensive scientific application on the Cori supercomputer. The aim is to pursue all possible avenues to improve the performance of the application. This includes parallelization, vectorization, improving the memory locality, optimization of cache and register usage. Parallelization will involve both distributed and shared memory approaches using MPI and OpenMP. Exascale programming models such as HPX and kokkos will be explored to determine their usability and performance benefits. I will be working on a seismic wave application that simulates the effects of an earthquake.

2015-2016

Prior to this, I worked on the MOOSE project, a software to simulate the cellular behavior in a human brain. The model simulates the behavior of a cell for a given electric or chemical input. The simulation uses the kinetic and stochastic ODE solvers to model the chemical and electrical interactions inside a cell over multiple time steps. Simulating the entire cell for a single time step is a compute intensive process, hence the cell is divided into multiple smaller compartments. The parallelization was done by distributing the compartments among the available cores.

OpenMP programming model was used to parallelize the MOOSE solvers. I used the OpenMP for-loop and task constructs to parallelize different parts of the simulation. I improved the code by reorganizing the data-structures for better memory and cache access. For certain data structures, I added padding in order to prevent false sharing of data in the cache. The number of OpenMP directives (# pragma OMP parallel) were optimized. Both the solvers achieved a speedup of 5.3X and 6.8X speedup respectively with 8 threads.

2009-2015

For my Doctoral thesis, I worked at the Barcelona Supercomputing Center (BSC), as a PhD student. I worked in the programming models group of the computer science department at BSC. I was involved with the StarSs project, a task based programming model, with implementations for widely used multicore architectures. In the StarSs project, I worked on providing compiler directives and the equivalent runtime support for synchronization of multiple threads. I introduced Software Transactional Memory (STM) based concurrency control mechanism to handle critical memory updates. Later I extended, the concept of speculative memory updates to speculative task generation. StarSs tasks blocked due to synchronization directives were speculatively scheduled before their execution in the program

flow could be confirmed. I implemented a lightweight rollback mechanism in case the speculation fails. This extension improved the performance of parallel codes by 20%.

During my PhD thesis, I also worked on design and implementation of parallel applications using the StarSs framework for it's application repository. I parallelized the Graph500 benchmark, linear iterative solvers such as Gauss-Seidel and Jacobi algorithms and clustering algorithms such as Kmeans and Gmeans. While working on parallelizing applications for the StarSs repository, I used profiling tools such as valgrind and paraver.

Importance of ATSPEC trainings in my future work.

As mentioned above, my current and future work involves programming on large scale computing systems. In that respect, the training provided at ATSPEC such as the *Sturctured parallel programming* and *Performance, SIMD, Vectorization and Performance Tuning* will be highly beneficial for me. Similarly the MPI, OpenMP and the hybrid programming models talks will help me on improving application performance which involves both inter and intra node optimizations. I will also start working on the Titan supercomputer at the Oakridge national laboratory before the start of the training. Hence the GPU specific trainings on day 4 will help me in that regard. Also training and exercises on the numerical algorithms, algebraic solvers and FASTMath will be helpful when working with the scientific computing algorithms.

I have only listed some of the trainings that will directly be effective in my immediete future work. Almost every other training will directly or indirectly help me, like the paraview tool training that is used on Titan supercomputer, or the optimization courses. The presentations such as code documentation are really helpful in writing good code that can later be used by other programmers.

Conclusion

As mentioned above, I have experience in HPC field as a parallel application developer and in the area of development of parallel programming models. Also my current and future work is based on extreme scale computing and the trainings provided at ATSPEC will be immensely helpful in improving the quality of my work. This is the main reason, I believe that I can be one of the candidates that will benefit immensely from this training program.