Study and Optimization of a Finite Volume Application

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1 Introduction

High-Performance Computing (HPC) has been a fundamental process to science, in order to make viable certain simulations that require massive amounts of calculation. The use of several optimization techniques has helped decrease the execution time of different algorithms, providing critical results faster, thus helping research move forward at a faster pace.

This document will describe a study about improving the performance of *conv-diff*. This application calculates de heat diffusion of, let's say, a liquid while it spreads though an area. In this study we approach different ways to improve upon the initial solution solution. The project was devised in three stages. The first one was analyzing the original application, building its profile while also developing a better sequential version. On the second stage, a shared-memory parallel version was made (*OpenMP*). Finally on the third stage, a CUDA version is being developed, taking advantage of the massive parallelism modern GPU's have to offer.

This extended abstract presents the application's domain, explaining its uses and objectives. By knowing its domain and profile, a string foundation is created to develop all kinds of different optimizations. From here, an optimized sequential version was developed, as well as an OpenMP shared-memory version. The ongoing and future work and a brief conclusion will be presented in the last sections of this extended abstract.

2 Case Study

The application analyzed for this study is *conv-diff(Convection-Diffusion)*.This application simulates the way heat is transferred in a fluid using the finite-volumes method.To compute the heat diffusion, the surface is represented as a mesh. Being represented by cells and edges, the algorithm will traverse all edges, calculating the contribution of the adjacent cells. This application rests in a Finite Volume Library (FVLib), which handles the structures and some of the logic functions necessary for the problem's solution.

The application's main objective is to compute a vector $\overline{\phi}$ such that $\overline{\phi} \longrightarrow G(\overline{\phi}) = \begin{pmatrix} 0 \\ 0 \\ \vdots \end{pmatrix}$ This is accomplished in three different stages:

1. We begin with a candidate vector ϕ
2. For each edge, we compute the flux F_{ij}, with i and j being the indexes of the adjacent cells
3. For each cell, we compute $\sum |e_{ij}|F_{ij} - |c_i|f_i$

Thus: $\phi = \begin{pmatrix} \phi_1 \\ \vdots \\ \phi_I \end{pmatrix} \longrightarrow G = \begin{pmatrix} G_1 \\ \vdots \\ G_I \end{pmatrix}$

3 Profiling

The program consists in four major parts, reading the initial mesh from a file. Then, using the functions *makeResidual*, which calls the function *makeFlux*, the flux contributions are calculated and the vector phi is built, thus achieving a matrix free implementation. Following this, to calculate the deviation in the results from the previous operations, the function *LUFactorize*. Finally, both the meshes are written to the output files, together with the error between them.

After analyzing the application, we conclude that the algorithm has a very high workload in the *LUFactorize* function, comprising of more than 90% of the execution time.

4 Sequential Optimization

After dissecting the code and understanding the problem at hand, we began to notice several implementation errors, these errors, such as reading the same variable repeatedly from a file and long chains of calculation with a heavy division at the end, were easy to spot, and could clearly been avoided. We changed all those trivial aspects of the application, which required minimal effort. That being said, this simple optimizations paid results. The computation time has been greatly reduced, with the aforementioned *LUFactorize* function taking an even more prominent role in our profile.

```
for (i = 0; i < 10; i++) {
    stuff
}
```

5 Shared Memory Parallel Optimization(OpenMP)

After optimizing the sequential code, we turned our efforts to parallelizing the code. The two loops responsible for the matrix free calculations were ideal candidates. We parallelized both this loops. We had some struggles with data-races in these, but we overcame the problems rather easily. The data-races exist because the mesh is traversed by the edges, however, as we found out, if they are traversed by cell, these data-races no longer exist. Also, the library that was provided includes some iterator style structures. These were also a problem, because, while OpenMP as no problem in parallelizing STL iterators, this doesn't hold for *FVlib*'s iterators. So, we had to convert those to a standard for loop. The code was successfully parallelized, however, results were disappointing, execution time didn't decrease noticeably, hinting at a very memory bound application.

6 On-going and Future Work

After implementing both the sequential version and the OpenMP version, a naïve implementation in CUDA was started. This version aims to take advantage of the GPU's massive parallelism, improving performance using its vector units to diminish computation time. However, for this to be possible, a thorough restructuring of the code is necessary.This is because most of the structures are implemented using pointers, something hinders CPU performance, but also makes it impossible to use CUDA, since we can't have a structure in the device memory pointing to host memory. Thus we are facing the challenge of removing most of the memory accesses while maintaining the abstraction and flexibility currently present in the application. After resolving this issue and other minor ones, we expect to achieve a boost in performance.

In future work, it is expected to develop a optimized CUDA version as well as a OpenMPI. A hybrid version using both CPU and GPU could also be a future implementation to have gains in performance. It is also expected to optimize several areas of code, questioning some decisions like using double-precision versus single-precision. Another area that might require attention is the input parser and the input file's structure.

7 Conclusion

This extended abstract serves as a introduction to the study here presented. The initial results from the implementations of optimized versions, sequential and parallel, shows small improvements in the computed time. Future iterations of the solutions may increase the improvements, shifting the application to a computing bound zone.

Through the development of the solutions some problems were presented, such as the mesh being disperse and the structures implemented with extensive use of pointers. This problems delayed the development of solutions, in particular the CUDA version. The decision of maintaining the abstraction of the system may prove to be a bold direction, but favorable in terms of comprehension.

In the future released paper a deep analysis of the results will be made, showing the performance improvements obtained.