

# 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 the heat diffusion of, let's say, a liquid while it spreads through an area. In this study we approach different ways to improve upon the initial solution. The project was devised in three stages. The first one was analysing 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 strong 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 diffu-

sion, 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  $\bar{\phi}$  such that  $\bar{\phi} \rightarrow G(\bar{\phi}) = \begin{pmatrix} 0 \\ 0 \\ \vdots \end{pmatrix}$ . This is accomplished in three different stages:

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

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

## 3 Profiling

The program consists in two major parts, a cycle that computes the  $\phi$  for each cell, using the functions *makeResidual*, which calls the function *makeFlux*, and an FVLib function, *LUFactorize*, which validates the results of the above cycle. Both the calculated mesh and the real mesh, computed by the *LUFactorize*, are presented in the output files, together with the error between them.

After analyzing the application, we conclude that the algorithm has a high workload in the *LUFactorize* function,

## **4 Sequential Optimization**

## **5 Shared Memory Parallel Optimization(OpenMP)**

## **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 graphics board performance using its vector units to diminish the compute time. For this a restructuring of the code is necessary removing most of the memory accesses while maintaining an abstraction of the system. 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.

## **7 Conclusion**