An Approach for Designing Hardware Accelerators

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PhD Forum - VLSI-SoC 2010, Madrid, Spain, September 2010

Introduction

Huge increase of complexity in algorithms and applications for scientific computing -larger amounts of data available for analysis (e.g., genomic databases); 
-need for more accurate and precise results (e.g., Computational Chemistry).

Solution: stream-based computing model and GPUs as prototyping platforms to facilitate the design and testing of hardware accelerators for such applications.

Hardware Design Procedure

1st Step: Kernel Design Procedure

- Place & Route results
- Experimental setup used

2nd Step: Design of the Processing Unit (PU)

- Tune the Datapath Control Unit (DCU) according to the algorithm.

3rd Step: Overall System Integration

- Replicate the Processing Unit (PU) according to the available hardware.

Future Work: Induced Dipoles

- One of the major bottlenecks found in Molecular Mechanics applications is the computation of polarizable force fields, namely the computation of the induced dipoles.
- TINKER is a Molecular Mechanics application that includes such computations.
- We have obtained a stream-based implementation of this algorithm and prototyped it on GPUs.

Most relevant publications:


Acknowledgments: We would like to thank to all co-authors of the above publications, to HiPEAC for a 3 month collaboration grant, and to the Portuguese Foundation Fundação para a Ciência e Tecnologia for the SFRH/BD/36041/2007 PhD scholarship.