Global Initiative of Academic Networks (GIAN) Celebrating 10 glorious years 2009-2019

An Introduction To Gpu Computing In Computational Biology
July 15-19, 2019

Discipline of Biosciences and Biomedical Engineering
INDIAN INSTITUTE OF TECHNOLOGY INDORE

Overview
Many of today’s scientific discoveries result from an intrinsic interplay between experimental and theoretical research. For the latter computer support is the dominant resource requirement. Among the most interesting developments in this respect are GPUs (graphics processing units) that combine an enormous computing power with rather modest power consumption needs and negligible infrastructure requirements. However, implementing even the most trivial algorithm on the GPU can be a daunting programming exercise with many of the architectural characteristics of the GPU to be permanently taken into account in order to make the porting process to the GPU a successful experience.

CUDA is the standard API for code development targeting the GPU and a number of impressive examples have already been given in diverse areas from particle physics to computational biology. CUDA allows simple extensions of standard C/C++/Fortran code with GPU-specific instructions via a set of specific functions. In this way thousands of cores available on the GPU can be leveraged to work in parallel and thus carry out significant fractions of the computational workload on the device. The present lecture series is offering a systematic step-by-step introduction into GPU computing from the perspective of the newcomer. Basic design principles will be established, central programming techniques acquired and a number of state-of-the-art programs examined that efficiently employ the GPU and are frequently used in computational biology.

Objectives
- Introducing participants to GPU computing.
- Acquiring basic skills in using CUDA for basic programming tasks frequently arising in STEM.
- Providing exposure to practical problems in software development and applied computational biology through hands-on exercises.
- Surveying different high and low level approaches in scientific GPU computing.

DAY 1
Lecture 1: Basic introduction to GPUs and Principles of CUDA
Lecture 2: Modern Hardware Models, specific Features, explaining usage of Standard Tools for CUDA development
Tutorial 1: Recapitulation of basic programming techniques (C and Fortran), first steps with CUDA etc.

DAY 2
Lecture 3: CUDA Toolkit 1
Lecture 4: CUDA Toolkit 2
Tutorial 2: Real-world applications for CUDA

DAY 3
Lecture 5: Introduction to molecular dynamics (MD) simulations
Lecture 6: MD simulations of biological macromolecules
Tutorial 3: Designing a mini-project, e.g. numerical integration, simulating a biomolecules

DAY 4
Lecture 7: GPUs on computational biology and medicines
Lecture 8: Poisson-Boltzmann (PB) Simulations on the GPUs
Tutorial 4: Hands-on exercises with CHARMM, AMBER, GROMACS

DAY 5
Lecture 9: Exemplification of the Potential of GPUs to explore new domains
Lecture 10: Free energy simulations on GPUs
Tutorial 5: Problem solving session

Who can attend
- Researchers in basic science and engineering from all types of institutions including higher education, government organizations and R&D laboratories
- Students at all levels (BTech/MSc/MTech/PhD)

Accommodation
The accommodation will be provided on chargeable basis:
- In case of guest house accommodation, kindly write to guesthouse@iiti.ac.in

Registration Procedure
The registration can be done
Step 1:
The payment can be made By Demand Draft: Demand Draft should be drawn in favor of “Registrar, IIT Indore”, payable at Indore Or By NEFT Transfer: Registration fee can be paid through NEFT. Transfer of the amount can be done to the A/c number given below:
Name of the Beneficiary: Registrar, Indian Institute of Technology Indore
Name of Bank: Canara Bank
Branch Code: IIT Indore, Simrol Campus Branch
Beneficiary Account No.: 1476100127440
Bank MICR Code: 452015003
Bank IPS Code: CNRB0006223

Step 2:
After completing the payment of registration fee, fill the application form available at http://gian.iiti.ac.in/register.php to complete the registration. If payment is made through Demand Draft, send your Demand Draft to the course coordinator (also e-mail the scanned copy of the Demand Draft to parimal@iiti.ac.in)

Registration deadline: 10th July 2019