

About IIT Indore

Indian Institute of Technology Indore located in Madhya Pradesh, known as IIT Indore, is an institute of national importance established by the Government of India in 2009. The discipline of Biosciences and Biomedical Engineering (BSBE) at Indian Institute of Technology Indore was initiated in 2012 that focuses on research in multidisciplinary areas of Biosciences and Biomedical Engineering. Recently IIT Indore debuts with a rank of 351-400 in the Times Higher Education World University Rankings, 2019, 2nd among Indian institutes.

Faculty

Dr. Siegfried Höfner



Dr. Siegfried Höfner holds a senior staff scientist position in the High-Performance Computing Center at Vienna University of Technology, Austria. He is also an adjunct Assistant Professor of Physics at Michigan Technological University, Michigan, USA. He received a M.S. in Biochemistry and a Ph.D. in

Theoretical Chemistry from the University of Vienna, Austria. He was a postdoctoral research fellow at several academic industrial sites including IGBMC Strasbourg, the University of Bologna, Novartis Institutes for BioMedical Research (Vienna), FZ Juelich and MTU before joining the ZID (VSC Team) at the Vienna University of Technology in 2014. His research interests include high performance computing (HPC), computational biophysics, quantum chemistry, continuum electrostatics and large-scale simulations of molecular matter. He is the author of 60 research articles and 5 confidential industrial reports. He has delivered several invited/contributed lectures in various universities and conferences in Europe and North America.

Dr. Parimal Kar



Dr. Parimal Kar is an Assistant Professor in the discipline of Biosciences and Biomedical Engineering at Indian Institute of Technology Indore (IITI). He received a PhD in Computational Biophysics from Michigan Technological University, Michigan, USA. He was a postdoctoral research

fellow at Max Planck Institute of Colloids and Interfaces, Potsdam, Germany and Michigan State University, East Lansing, Michigan, USA. His research interests include multiscale modeling of biomolecular recognitions, structure and dynamics of glycans and proteins using molecular dynamics simulations. He is also interested in developing coarse-grained models of proteins and carbohydrates to simulate these systems to cover biologically relevant spatio-temporal scales.

Fees

The participation fees for taking the course is as follows:

- Participant from outside India: USD 500
- Industry/Research Organizations: Rs 10,000
- Academic Institutions (B.Tech/M.Tech/M.Sc.): Rs 1,500*
- Academic Institutions (PhD/Post-doc): Rs 2,500*
- Academic Institutions (Faculty): Rs 4,000*

The above fee include all instructional materials, computer use for tutorials and assignments, Laboratory equipment usage charges, 24 hr free internet facility. The participants will be provided with accommodation on payment basis.

*Fee concession will be considered for individual having limited financial support

Course Coordinator

Dr. Parimal Kar

Discipline of Biosciences and Biomedical Engineering

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Global Initiative of Academic Networks (GIAN)



An Introduction To Gpu Computing In Computational Biology

July 15-19, 2019

Discipline of Biosciences and Biomedical Engineering (BSBE)

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 easily become 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 developments

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 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

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

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 hostel accommodation, kindly write to hostel@iiti.ac.in
- 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. : 1476101027440

Bank MICR Code : 452015003

Bank IFS Code : CNRB0006223

Step 2:

After completing the payment of registration fee, fill the application form available

<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