

Application Guidelines for Computational Science Alliance Summer School 2017

1. Overview

Computational Science Alliance is aiming to train experts for numerical simulations in various fields of computational science. In this summer school 2017, we hold a three-day summer school. The summer school consists of three lectures with exercises: (1) development of a small first principles electronic structure calculation program and its application to a simulation of hydrogen molecules under classical electric fields, (2) parallelization of a finite-difference time-domain method (FDTD method) for the Maxwell's equations and simulation of time evolution of electromagnetic fields using a supercomputer (Readbush-U), and (3) numerical simulation of quantum many-body problems by using Krylov subspace method and matrix product state (tensor network states) methods. During the summer school, participants will make applications, perform parallel simulations by using a supercomputer, and learn about how to select proper application to solve problems efficiently.

2. Schedule and Venue

Start: August 23rd, 2017, Close: August 25th, 2017.

Large seminar room 2, Information Technology Center on the Hongo Campus.

<http://www.itc.u-tokyo.ac.jp/files/ehongo.pdf>

*Detailed schedule is at the bottom of this document

3. Target participants of the summer school

Under graduate, master course, doctor course students, and young researchers (such as postdoc and research assistants) who belong to the University of Tokyo.

Maximum number of participants: about 20.

4. Requirement for participation

- (1) A participant must belong to the University of Tokyo.
- (2) A participant must have an ECCS (Educational Campus-wide

Computing System) account at least at the beginning of the summer school.

- (3) A participant is expected to be familiar with file operations, editing, and commands in the UNIX system.
- (4) A participant is expected to have basic knowledge for programming and programming languages (c, fortran, ...).

In order to use supercomputer, you must be staying in Japan for more than six months. If you are a student from abroad, please include the information whether you are staying in Japan more than six months or not. (Even if you have not been in Japan more than six months, you can participate in topics which do not use the supercomputer.)

5. Fee

Registration fee: free

We plan to collect about 2000 yen for an informal discussion with meal.

6. Application

Please send email to summerschool@compsci-alliance.jp by describing the following information.

- Name
- Affiliation 1: Faculty (e.g. Faculty of Science)
- Affiliation 2: Department (e.g. Department of Physics)
- (For students) year
- Email address
- Phone number
- Topics you are interested in (you may attend every topic). This is a survey for preparations. Regardless of your selection here, you can participate to all topics on the summer school if you want.

For students who have not been registered with the computational science alliance, please register yourself with the computational science alliance

through <http://www.compsci-alliance.jp> .

We will send email when we accept your registration. If you do not receive any responses until August 9th, please ask the secretariat (secretariat@compsci-alliance.jp) .

If you cancel your participation, please ask the secretariat as soon as possible.

7. Registration deadline

August 8th, 2017

8. Contact

Computational science alliance secretariat:
secretariat@compsci-alliance.jp

Tentative program

8/23 (Wed.)

10:00 – 11:30 “How to use supercomputer”

11:30 – 12:45 Lunch

12:45 – 14:15 Lecture & Exercise (1)

14:30 – 16:00 Lecture & Exercise (2)

16:15 – 17:45 Lecture & Exercise (3)

18:00 Dinner (informal discussion)

8/24 (Thu.)

10:00 – 11:30 Lecture & Exercise (1)

11:30 – 12:45 Lunch

12:45 – 14:15 Lecture & Exercise (2)

14:30 – 16:00 Lecture & Exercise (3)

16:15 – 17:45 Discussion

8/25 (Fri)

10:00 – 11:30 Lecture & Exercise (1)

11:30 – 12:45 Lunch

12:45 – 14:15 Lecture & Exercise (2)

14:30 – 16:00 Lecture & Exercise (3)

16:15 – 17:45 Discussion & Presentation

Lecture & Exercise (1):

Lecturer: Dr. Jun-Ichi Iwata (Department of Applied Physics)

Contents: Making (time dependent) density functional theory (DFT) with local density approximation (LDA), and performing a first-principle simulation of hydrogen molecules under classical electric fields.

Lecture & Exercise (2):

Lecturer: Dr. Masaharu Matsumoto (Department of Computer Science)

Contents: Parallelizing a finite-difference time-domain method (FDTD method) for the Maxwell's equations and learning a simulation of time evolution of electromagnetic fields on a supercomputer.

Lecture & Exercise (3):

Lecturer: : Dr. Tsuyoshi Okubo (Department of Physics) and Dr. Youhei Yamaji (Department of Applied Physics)

Contents: Performing simulations of quantum many-body problems by using Krylov subspace method and matrix product method (tensor network method).

- All of the lectures contain exercises. In addition, we will have discussion and presentation for the results obtained by the simulations.