Fluid and thermal simulations at various scales (2019)
- from first-principles to mesoscopic methods -

Lecturers: Associate Prof. Ikuya Kinefuchi (IK) & Prof. Junichiro Shiomi (JS), Department of Mechanical Engineering, The University of Tokyo.

Time: **6/10 (Mon), 6/11 (Tue), 6/13 (Thu), 6/14 (Fri): 10:00-14:00 (with a lunch break)**
6/12 (Wed): 14:15-18:00 (with a break)

Lecture rooms: 6/10 Mon-6/12 Wed **: Faxén, Fluid physics lab, Teknikringen 8**
6/13 Thu-6/14 Fri **: Munin, Teknikringen 8**
(Munin is close to the other entrance with the von Karman vortex street, same floor as the lab)

Objective:
Simulations at various scales from atomistic to mesoscales have become important in fluid and thermal science and engineering, particularly to understand phenomena involving multi-scales as in any interfacial flows. The lecture aims to provide basic knowledge and practical experience in standard and non-standard calculations at various scales, ranging from first-principles calculations of electrons and interatomic forces to dissipative particle dynamics simulations of mesoscale heat and mass transport.

Day 1 (JS):

I. Basics of quantum calculations
   1. Matter waves
   2. Schrödinger equation (single electron)
   3. Molecules (interatomic bonding)
   4. Many-electrons system by Density functional theory (DFT)
   5. Exercise: Experience “first-principles” DFT calculation

Day 2 (JS)

II. Molecular dynamics ①
   1. Basics of molecular dynamics method
   2. Thermodynamic quantities from equilibrium MD simulations
   3. Transport coefficients
   4. Exercise: Calculate transport coefficient using equilibrium molecular dynamics

Day 3 (KI)

III. Molecular dynamics ②

1. Transport properties from non-equilibrium MD (NEMD) simulations
2. Lees-Edwards boundary condition
3. The DOLLS and SLLOD method
4. Exercise: Calculate transport coefficient using non-equilibrium molecular dynamics

Day 4 (KI)

IV. Dissipative particle dynamics ①

1. Basics of dissipative particle dynamics
2. Conventional model for simple liquid
3. Fluctuation-dissipation theorem
4. Time integration algorithms
5. Exercise: Calculate transport properties of simple liquid using dissipative particle dynamics

Day 5 (KI)

V. Dissipative particle dynamics ②

1. Iterative Boltzmann inversion method
2. Coarse-graining modeling
3. Multiscale / hybrid simulations
4. Exercise: Modify a potential model using the iterative Boltzmann inversion method

Credits: 5.

Grade: Attendance (20%), Homework (40%) and Final Exam (40%)?

Preparation for the exercise (Fluid and Thermal Simulations at Various Scales)

In the exercise of this course, we will conduct first principles calculations, molecular dynamics (MD) simulations, and dissipative particle dynamics (DPD) simulations using the software listed below. **Please install them on your laptop before the exercise.**

(1) A Unix-like environment with the X Window System

[Linux]　Follow the instructions for Windows from step 2.

[Windows]

1. Download Cygwin installer from the project website (https://www.cygwin.com/).
2. Run the installer. During the installation process, select the following packages in addition to those selected by default.

   bc, python3, git, gcc-core, gcc-g++, gcc-fortran, make, xorg-server, gnuplot, vim, emacs
3. After the installation finishes, open a command-line window by clicking "Cygwin64 Terminal" icon.
4. Open `.bashrc` file using your favorite text editor and add the following lines after the comment line "`# User dependent .bashrc file`."

```
export LANG=C
export DISPLAY=:0.0
alias runx='run xwin -multiwindow -noclipboard'
```

5. Type `exit` to close the command-line window.
6. Launch a Cygwin terminal again and type `runx` to start an X11 server. Then, you can find a new icon  on the notification area of the taskbar.

[Mac]

You need to install Xcode (software development tools) and XQuartz (X Window System that runs on OS X). Additionally, you probably want to install Homebrew, with which you can easily install GNU compiler collection and other software.

Xcode https://itunes.apple.com/us/app/xcode/id497799835

XQuartz https://www.xquartz.org/

Homebrew https://brew.sh/

(2) Quantum Espresso (First principles calculation)

[Windows]

1. Download “qe.zip” from the following the AdvanceSoftware Corp website.
2. Put the folder “qe” in an appropriate folder (e.g. under “home” of your Cygwin directory).

https://github.com/advancesoftcorp/espresso/releases/tag/binary_windows

[Mac/Unix]

Download the source code from https://github.com/QEF/q-e/archive/qe-6.4.1.tar.gz

Run the following commands in order:

(a) `tar xzvf q-e-qe-6.4.1.tar.gz`

(b) `cd q-e-qe-6.4.1`

(c) `./configure`

(d) `make pw`

If everything goes well, you will find executable command “pw.x” under “bin” folder.

Pay attention that the step (c) may depend on personal MAC/Unix environment setting. Adjust the environment if you meet any error information.

(2) LAMMPS Molecular Dynamics Simulator

1. Download the source code by typing the following command.

```
git clone -b stable https://github.com/lammps/lammps.git ~/lammps
```

2. Build an executable by typing the following commands.

```
cd ~/lammps/src
make serial
```

If the build process finishes successfully, the last few lines look like:

```
size ../lmp_serial
   text    data     bss     dec     hex filename
3769377   16584     768 3786729  39c7e9 ../lmp_serial
make[1]: Leaving directory '/home/kine/lammps/src/Obj_serial'
```

If the building process fails, edit ~/lammps/src/MAKE/Makefile.serial in accordance with your environment.

(3) VMD - Visual Molecular Dynamics

Download the latest stable version 1.9.3 from the project website.

https://www.ks.uiuc.edu/Research/vmd/

You have to make a registration before downloading the installer.