MODYLAS tutorial

11th CMSI young researcher technical workshop

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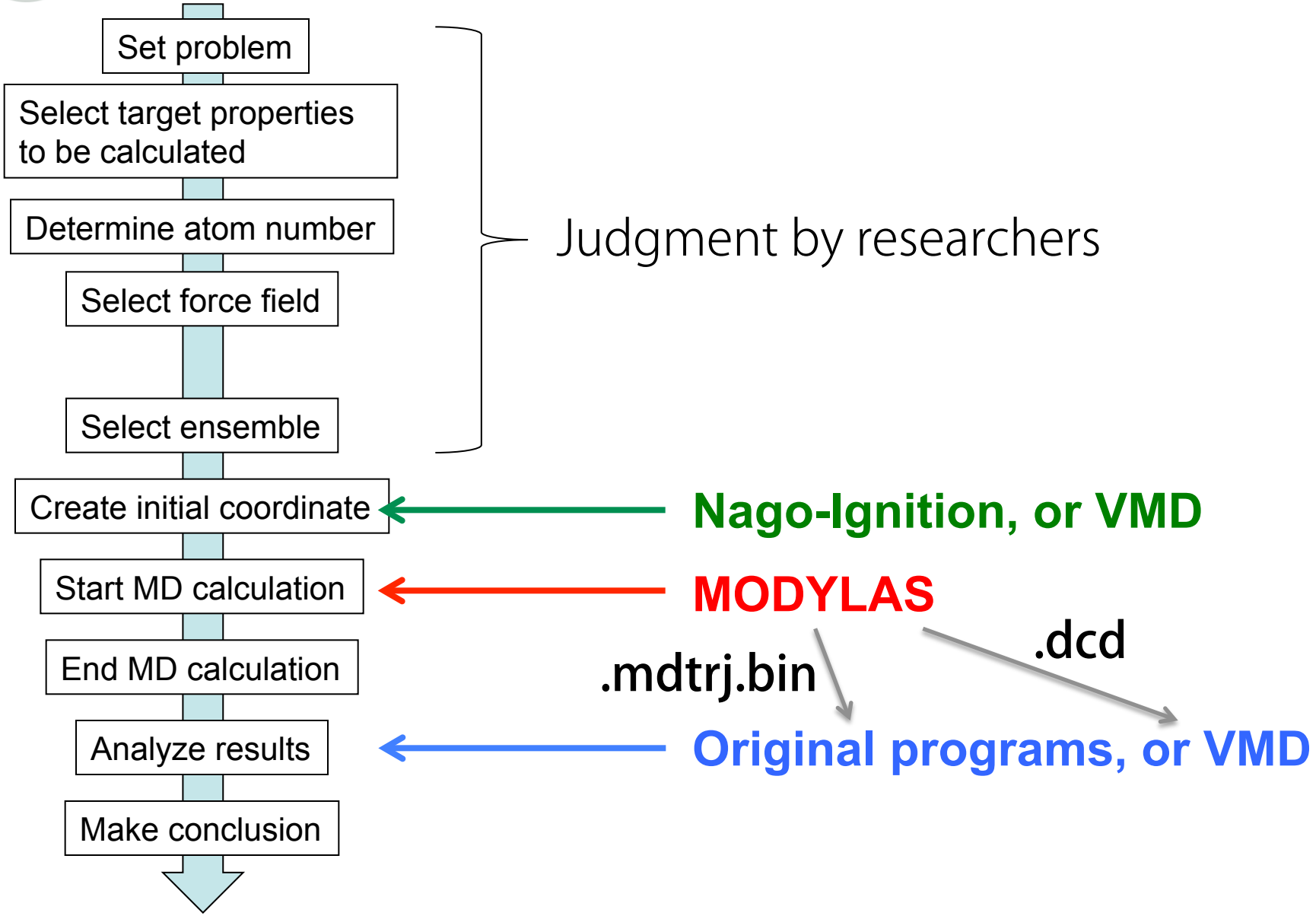
4-6th, Feb, 2015

Procedure of research by MD calculation



Outline of Nano-Ignition

- **Software to prepare a set of input files for MODYLAS**
  (... and RSDFT/TAPP ??)

- **Developed in "NAREGI" project**

sessionname.mddef
sessionname.mdff
sessionname.mdxyz

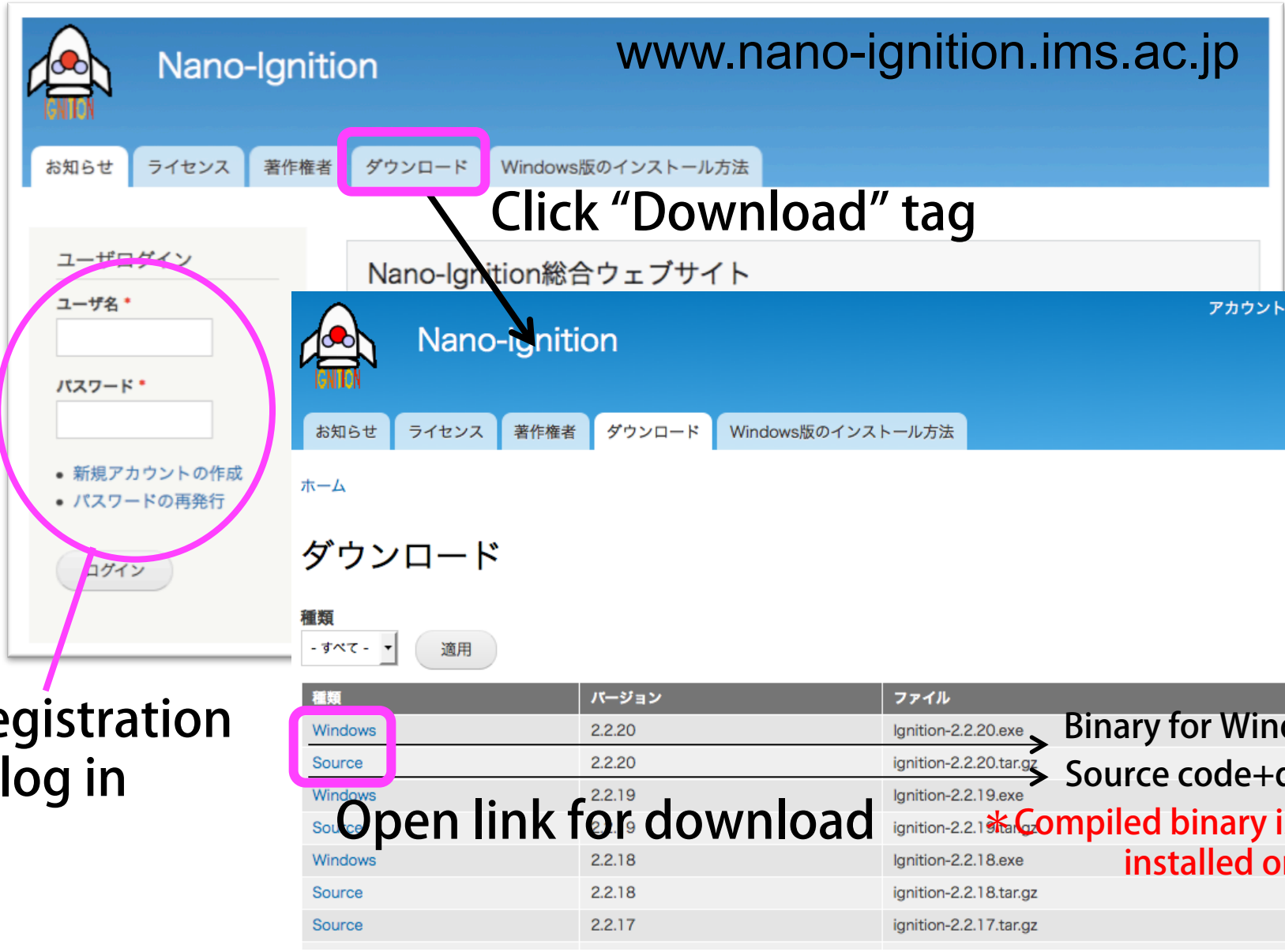
- **Language**
  C (without parallelization)

- **Source code**
  Available at www.nano-ignition.ims.ac.jp
  Newest version is 2.2.20

- **License**

User registration system; Prohibition of redistribution; Obligation of literature citation (more detail, see web page)

Download Nano-Ignition



Nano-Ignition: compilation

Go to the untar-zipped folder

>cd ignition-2.2.20/

Set of compilation environment

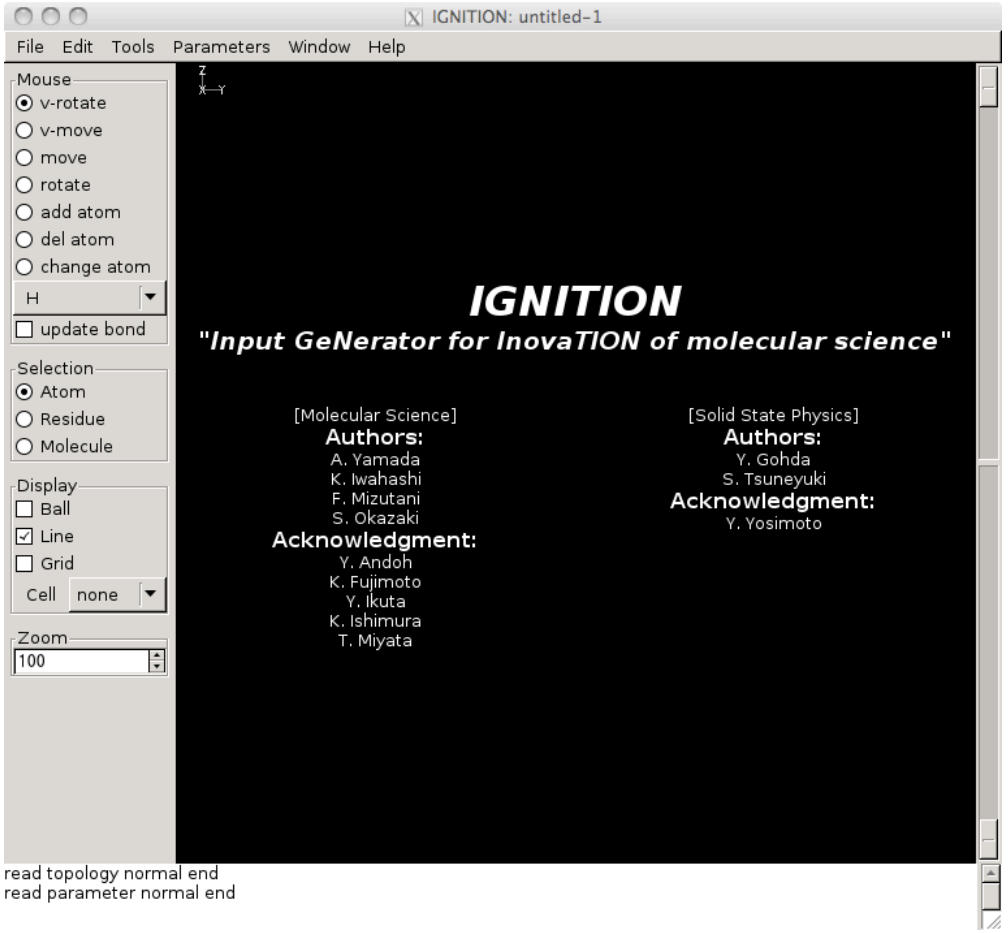
>./configure

Compile

>make

Start up

>./ignition/ignition



Pre-compiled binary is available in this lecture by

>source /opt/MateriApps/ignition/ignitionvars.sh psi

>source /home/materiapps/ignition/ignitionvars.sh phi

>ignition

Nano-Ignition: I/O structure

Molecule coordinate file
.pdb

Ex) water.pdb

CHARMM
Topology file

Ex) top_all22_prot.rtf

CHARMM
Parameter file

Ex) par_all22_prot.prm

Nano-Ignition

Available operations:

- 3D representation of inputted molecules
- Assignment of force field parameters
- Specification of distance constraints
- Specification of unit cell size
- Change of force field parameters
- Addition of hydrogen atoms
- Addition of solvent
- Deletion, insertion, and substitution of molecules
- Copy of molecule,
- Movement of molecules
- Addition of chemical bonds

and so on (see document)

A set of input files for MODYLAS

Calculation condition file
.mddef

Coordinate file
.mdxyz

Force field file
.mdff

Sorry, skip detail in this lecture. See Appendix.

Outline of MODYLAS

MODYLAS: MOlecular DYnamics simulation software for LArge Systems

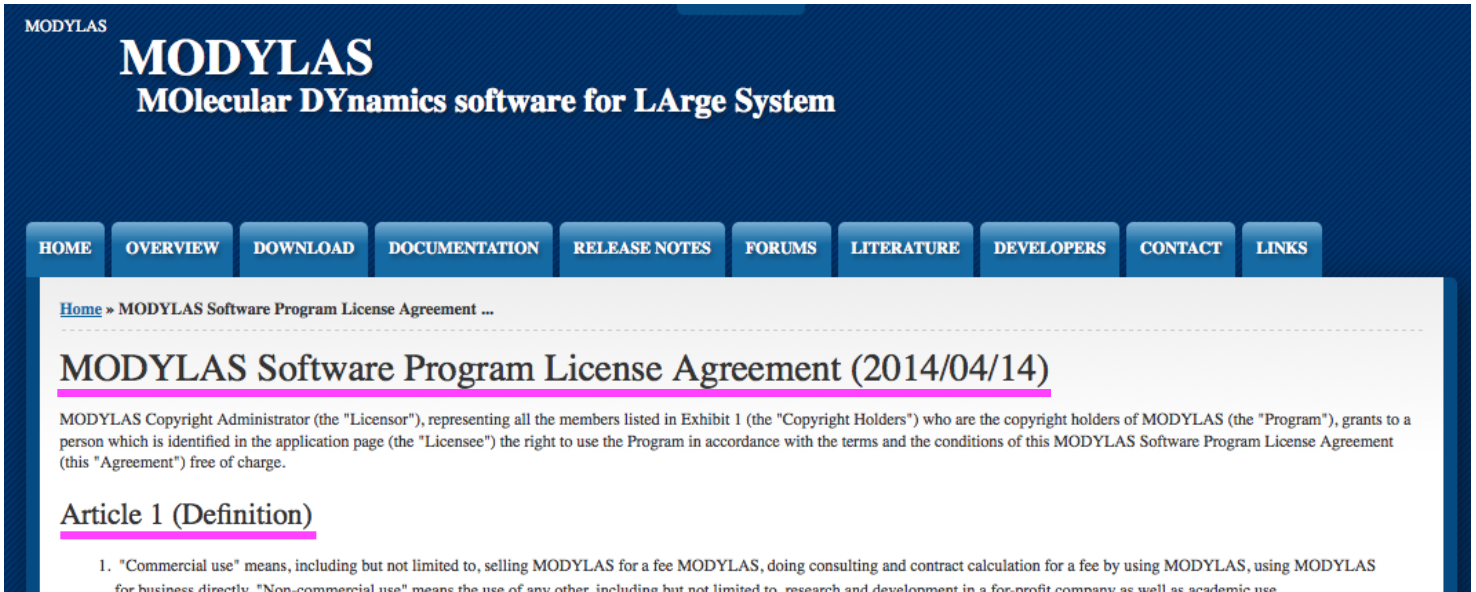
Algorithm	Molecular dynamics calculation
Language	Fortran 77&90
Compiler	frtpx (Fujitsu), ifort (intel), pgf90 (PGI)
Parallelization	MPI/OpenMP/SIMD hybrid
Force field	CHARMM with CMAP [AMBER/OPLS]
Ensemble	NVE, NVT (Nose-Hoover), isotropic NPT (Nose-Anderson), [anisotropic NPT (Nose-Parinello-Rahman)]
Numerical integration	RESPA
Constraint dynamics	SHAKE/ROLL, RATTLE/ROLL
Coulomb interaction	Fast multipole method(FMM), [Particle mesh Ewald method]

Contents in [...] will be supported in future version.

License

- User registration system
- Prohibition of redistribution of both source and binary codes
- Obligation of literature citation
  [J. Chem. Theory Comp., 9, 3201-3209 (2013)]
- Prohibition of publication of benchmark result without permission
- Obligation of feedback of source code improvement to authors

More detail is described under “Download” tag at www.modylas.org
Japanese license text is included at the beggining of Reference manual (Jpn).



Download MODYLAS

www.modylas.org

MODYLAS

MOlecular DYnamics software for LArge System

HOME | OVERVIEW | DOWNLOAD | DOCUMENTATION | RELEASE NOTE | FORUMS | LITERATURE | DEVELOPERS | CONTACT | LINKS

Home » MODYLAS

MODYLAS

VERSION: 0.9.0beta

COMMENT: work on the K-Computer

If you agree our license, please write your email address to send a URL for download, and then pus

Your personal information filled out below will be used to send MODYLAS news and report activit

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Title

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Dear visitor,

Thank you for your interest.
Please use the following link to download the files:
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This link will be accessible until Wed, 01/22/2014 - 13:31. If you need access after the link expires, don't hesitate to revisit the download page on
http://www.modylas.org/

After registration, e-mail in which download link is included will be sent. Click it for download.

MODYLAS: Folder branching

```
>tar xvfz MODYLAS_1.0.3.tar.gz
```

```
MODYLAS_1.0.3/
    LICENSE.pdf      Software license document
    source/          Source code folder
    binary/          Precompiled binary folder
    sample/          Input samples
    document/        Manual and tutorial documents
```

MODYLAS: Compilation

Go to untar-zipped source folder

```
>cd MODYLAS_1.0.3/source/
```

Set compilation environment

```
>./configure --with-kind-fortran-compiler=FC
```

Compilation

```
>make
```

./src/modylas

will be created.

FC=(K|FX10|INTEL|PGI)

K	: K computer
FX10	: FX10
INTEL	: Intel compiler
PGI	: PGI compiler

Pre-compiled binary is available in this lecture by

```
>source /opt/MateriApps/modylas/modylasvars.sh        psi
>source /home/materiapps/modylas/modylasvars.sh       phi
```

MODYLAS: I/O structure

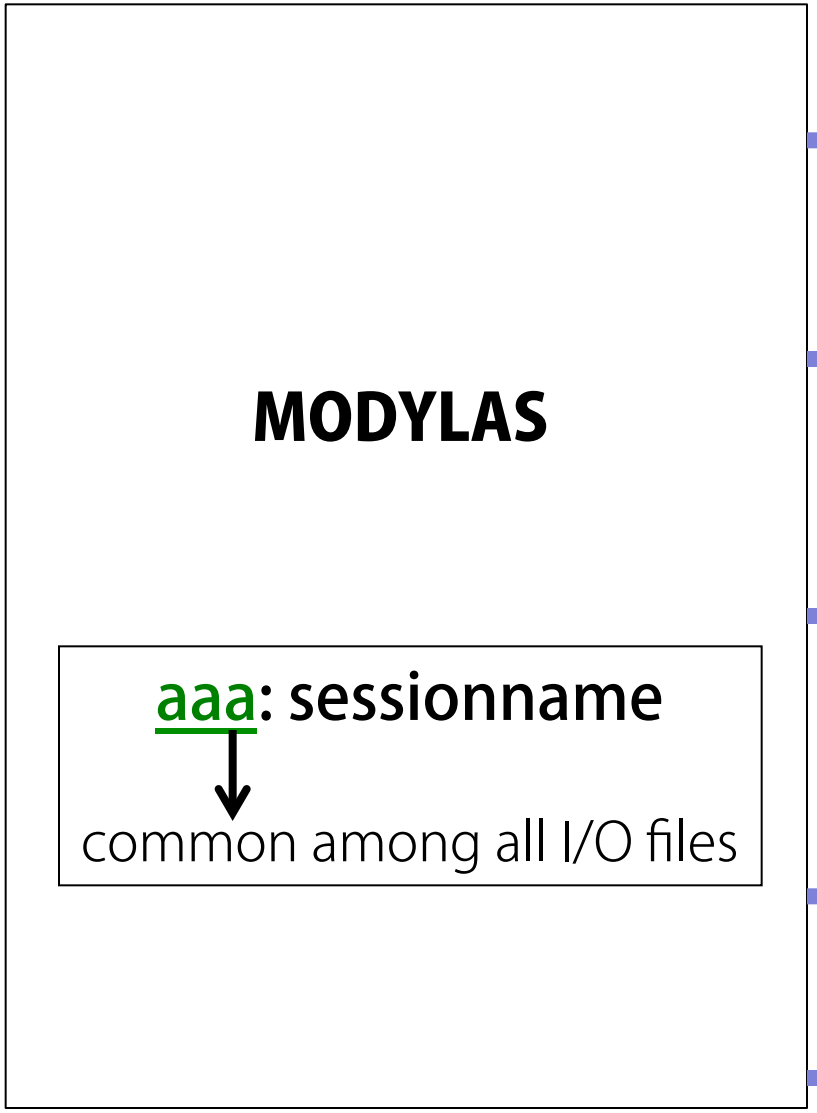
.bin : binary files

A set of input files for MODYLAS

Calculation condition file
aaa.mddef

Coordinate file
aaa.mdxyz

Force field file
aaa.mdff



Execution information
stdout

Monitoring file
aaa.mdmntr

File for restart
aaa.restart.bin, or
aaa.restart.asc

File for analysis
aaa.mdtrj.bin, or
aaa.dcd

Run time information
aaa.mdrun

MODYLAS: Execution

Execution style:

./modylas sessionname

Go to the folder where a set of input files exists

>cd water/

Link executable binary to current directory

>ln –s ../../source/src/modylas ./ *not necessary in this lecture*

Parallel execution (ex. 8 mpi x 1 omp)

>export OMP_NUM_THREADS=1

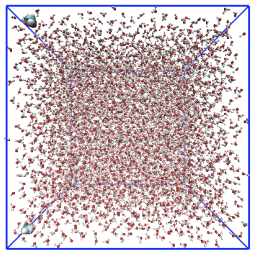
>mpirun –np 8 ./modylas water

Sample shell script 'auto.sh' for psi, phi is prepared

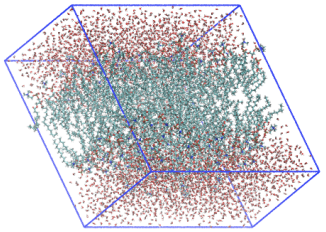
Limitation of execution

MODYLAS_1.0.3 (27th, Jan. 2015) has the following limitation of execution.

✓Cubic unit cell



2.0.0 → Rectangular unit cell → 2.X.0 → Parallelepiped unit cell



✓Periodic boundary condition

✓MPI & OpenMP hybrid parallelization

# of MPI processes*: 2^n (0≤n)
# of OMP threads: no limitation

2.0.0 → 2^n*3^m (0≤n, 0≤m)

✓**# of division of unit cell along axis = 2^k (uniform division only, and 3≤k≤6)**

2.0.0 → **2^k*3^l (nonuniform division)**

✓**Divided unit cell length> 0.5*LJ cut off radius**

L/ncell > 0.5*cutoff

* Addition of –DONEPROC_AXIS to src/Makefile is required.

Format of MODYLAS input files

Ascii files:

- tag expression　　<xxxx> ..... </xxxx>
  xxxx is given keyword → see also Appendix of Reference manual
- Nested tag structure is available　<xxxx> <yyyy> ... </yyyy> </xxxx>
- Set value to variable by "variable = value"
- A comment is followed by "#"

ex) mddef

```
<output>
# dcd=yes
  <trajectory> start=0 interval=1000 </trajectory>
#  <trjdcd> start=0 interval=1000 </trjdcd>
  <restart> start=0 interval=10000 </restart>
  <monitor> start=0 interval=1 </monitor>
</output>
```

commented out

output mdtrj.bin for every 1000 steps

output mdxyz.bin for every 10000 steps

output .mdmntr for every 1 step

Binary files: unformatted

- mdxyz.bin, and restart.bin has just same data structure

Input file (1) mddef

sessionname.mddef File on which calculation conditions are described

Tag keywords (ver 1.0.0)

name	Meaning	Lower tags and variables
<output>	Output related information	<monitor>, <trajectory>, < restart>, <trjdcd>, ascii, dcd
<integrator>	Numerical integration conditions	<multiple time step>, <shake>, dt, steps
<ensemble>	Ensemble related information	<thermostat>, <barostat>, ensemble, temperature, pressure, velocity_scaling
<intermolecular interaction>	LJ and Coulomb interaction related information	<two body>, <fmm>, <pme>, cutoff, LJcorrection, ncell, type, ULswitch, sterm, nmax
<mpi>	MPI conditions	division, nxdiv, nydiv, nzdiv
<COM>	Thermodynamic integration	constrain_COM, dist_COM, change_distCOM, deltaR, groupAtop, groupAend, groupBtop, groupBend

Input file (2) mdxyz

sessionname.mdxyz File on which atom coordinates and velocities, cell dimension, and thermostat/barostat information are described

Tag keywords (ver. 1.0.0)

Name	Meaning	Lower tags and variables
<atom>	Atom trajectories	<positions>, <velocities>
<thermostat>	Thermostat trajectory	nthermostat, <positions>, <velocities>
<barostat>	Barostat trajectory	mbarostat, <positions>, <velocities>
<periodic cell>	Unit cell dimension and its velocity information	<length>, <angle>, <vboxg>

sessionname.mdxyz.bin binary file of .mdxyz

Input files (3) mdff

sessionname.mdff File on which molecule content of system, FF parameters, constraint conditions, and segment information are described

Tag keywords (ver. 1.0.0)

Name	Meaning	Lower tags and variables
<forcefield>	Kind of force field	type, CMAPVersion
<system>	Molecule content	
<topology and parameters>	Topology and FF parameter information for each molecule species	nspecies, <species>, id, natom, <mass>, <shake pair>, <charge>, <epsilon>, <r>, <bond>, <angle>, <ub>, <dihedral>, <itorsion>, <CMAP>, , nbond, nangle, nub, ndihedral, nitorsion, ncmap, nsegments

sessionname.mdff.bin binary file of .mdff

Output file (1) stdout

```
 nprocs=          8
 nomp  =          1
 MODYLAS version=1.0.3
Input version=1.0.0
 natom=       13284
 mdxyz.bin read end successfully!
 npara=          8
 input,nvoid=          6
 input,nljsp=          0
 input,nclsp=          0
 mdff.bin read end successfully!
 LJ correction term is off
 FMM is selected
 nmax=          4
 lgflg=          0
 ewald sterm is off
 mddef read end successfully!
 MPI auto division
 nxdiv,nydiv,nzdiv=          2          2          2
 No position constrain

 ##### PSHAKE info. #####
 Pshake appllied:          1 /          1

 ************************
 Modylas normally ended!
 ************************
```

# of MPI processes
# of OMP threads

Total number of atoms

LJ and Coulomb interaction condition

3D configuration of MPI processes
(8 processes in total)

Successful completion signal

Output file (2) mdmntr

sessioname.mdmntr File on which mechanical and thermodynamic properties, and cell dimension are plotted as a function of time

Ex) Optimization of initial structure

```
## water_opt.mdmntr -- monitor variables output from MD calculation by modylas
#
# datas below are formated as:
# step     time              Hamiltonian        potential-E        kinetic-E          total energy       temperature        volume
pressure          box-length(x)      box-length(y)      box-length(z)
#                   [sec]          [J/cell]           [J/cell]           [J/cell]           [J/cell]             [K]              [m3]              [Pa]
[m]               [m]                [m]
#
       1  1.000000000000E-15  8.634745670798E-15  8.634745670798E-15  0.000000000000E+00  8.634745670798E-15
0.000000000000E+00  1.406080000000E-25  0.000000000000E+00  5.200000000000E-09  5.200000000000E-09
5.200000000000E-09
       2  2.000000000000E-15  1.449528625793E-15  1.449528625793E-15  0.000000000000E+00  1.449528625793E-15
0.000000000000E+00  1.406080000000E-25  0.000000000000E+00  5.200000000000E-09  5.200000000000E-09
5.200000000000E-09
```

- Format with which data can be directory plotted by gnuplot

> plot 'water_opt.mdmntr u 1:4 w l # of step：potential-E

Output file (3) restart

sessionname.restart.bin File for restart (binary)
sessionname.restart.asc File for restart (ascii)

.asc is created only when .mddef contains <output> ascii=yes </output>

How to restart using binary files：

```
>cp    a00.mddef       a01.mddef
>ln –s a00.restart.bin a01.mdxyz.bin
>ln –s a00.mdff        a01.mdff
>./modylas a01
```

Recommended

How to restart using ascii files：

```
>cp    a00.mddef       a01.mddef
>ln –s a00.restart.asc a01.mdxyz
>ln –s a00.mdff        a01.mdff
>./modylas a01
```

Output file (4) mdtrj.bin

sessionname.mdtrj.bin trajectory file for analysis

Enough amount of trajectories are needed for good statistics

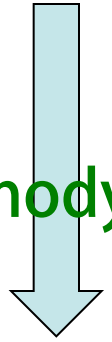
$$\langle A \rangle_{N,V,T} = \frac{\int A(\boldsymbol{r}^N) \exp\left(-\frac{U(\boldsymbol{r}^N)}{k_B T}\right) d\boldsymbol{r}^N}{\int \exp\left(-\frac{U(\boldsymbol{r}^N)}{k_B T}\right) d\boldsymbol{r}^N}$$

.mddef

```
<trajectory>
  start=0 interval=100
</trajectory>
<condition>
  dt=1.0e-15
  steps=10000
</condition>
```

Total 10000 MD steps with Δt=1fs.
"interval=100" means mdtrj.bin is updated by every 100 steps

.mdtrj.bin



Converter:
source/src/modylas-mdtrj2xyz

.xyz

.xyz file can be visualized by VMD

Output file (5) mdrun

sessionname.mdrun Run time information

```
## water_opt.mdrun -- run time information of MD calculation by modylas
#
step:          100
CPU time:       59.000000 [sec]
for MD:         57.767149 [sec]
time/step:       0.577671 [sec/step]
```

Present # of MD steps
Time elapsed by program with I/O
Time elapsed for MD
Time elapsed for one MD step

From this value, guess time to be elapsed by new job.

Visualization of MD calculation results

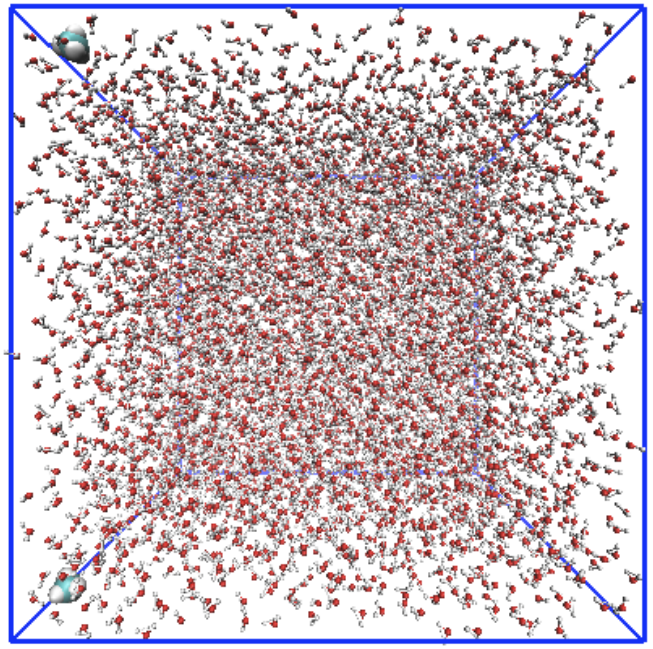
Newly supported from modylas_1.0.3

sessionname.dcd Trajectory file in dcd format (binary)

.dcd file is widely used in biophysical MD calculations. Other MD software (CHARMM, NAMD, etc.), and input generator software (VMD) support reading/outputing .dcd file.

Q. How to output dcd file from modylas?
A. Add following two lines in .mddef

```
<output>
 dcd=yes          ＊default : no
 <trjdcd> start=0 interval=100 </trjdcd>
</output>
```



Visualization of trajectory using VMD:

Required files

- .dcd file
- .pdb file
- .psf file for analysis (optional)

>vmd system.pdb result.dcd

Tutorial : Equilibration of bulk water

(1) Log in to psi or phi

(2) Set environment for modylas execution

```
>source /opt/MateriApps/modylas/modylasvars-1.0.3-1.sh      psi
>source /home/materiapps/modylas/modylasvars.sh             phi
```

(3) Copy sample inputs to current directory

```
>cp -r /opt/wakate/modylas/water/ ./                       psi
>cp -r /opt/wakate/modylas/water/ ./                       phi
```

Tutorial : Equilibration of bulk water

(4) Execute sample shell

>cd water/
>sh auto.sh

auto.sh for psi

8procs x 1thread

```
#!/bin/sh
#PBS -l nodes=1:ppn=8
#PBS -q small
#PBS -N wat_opt-nvt-npt
#PBS -j oe
source /opt/MateriApps/modylas/modylasvars-1.0.3-1.sh

export OMP_NUM_THREADS=1
export PARALLEL=1
cd $PBS_O_WORKDIR

mpiexec -np $PBS_NP modylas water_opt

cp    water.mddef_for_nvt      water_nvt.mddef
ln -s water_opt.mdff           water_nvt.mdff
ln -s water_opt.restart.bin    water_nvt.mdxyz.bin
mpiexec -np $PBS_NP modylas water_nvt

cp    water.mddef_for_npt      water_npt.mddef
ln -s water_opt.mdff           water_npt.mdff
ln -s water_nvt.restart.bin    water_npt.mdxyz.bin
mpiexec -np $PBS_NP modylas water_npt
```

optimization

NVT ensemble
5,000 steps

NPT ensemble
10,000 steps

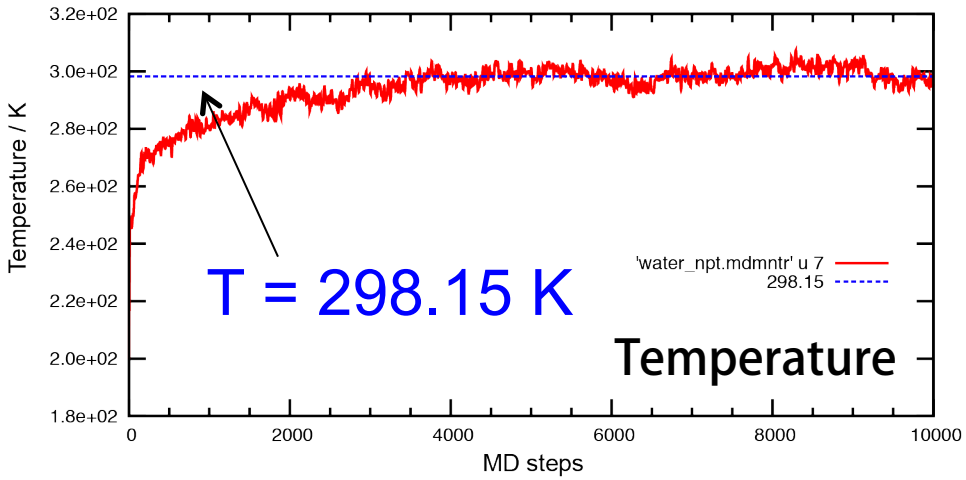
auto.sh for phi
is a little different,
but content is same

Tutorial : Equilibration of bulk water

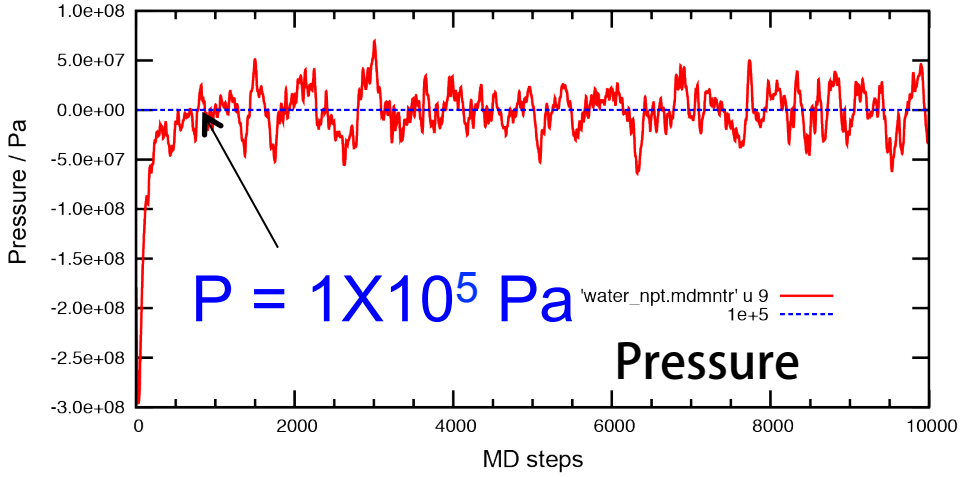
(5) View result

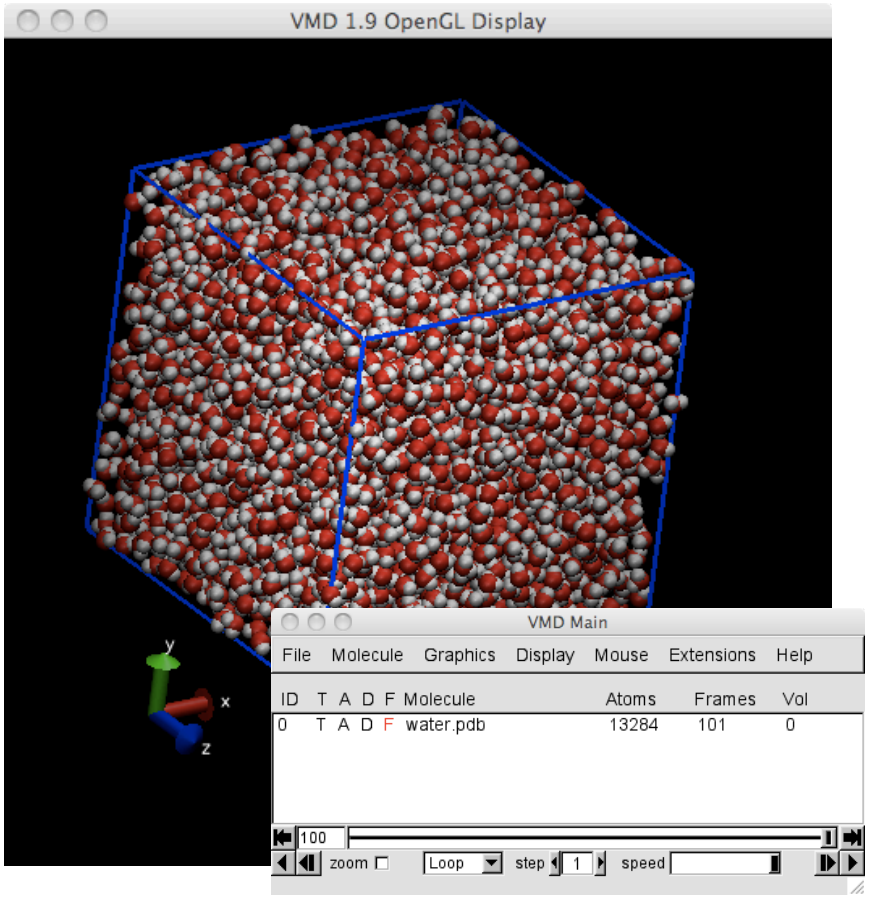
NPT ensemble
10,000 steps

gnuplot> p 'water_npt.mdmntr' u 7



gnuplot> p 'water_npt.mdmntr' u 9





>vmd water.pdb water_npt.dcd

Tk console> pbc box –center origin

Appendix

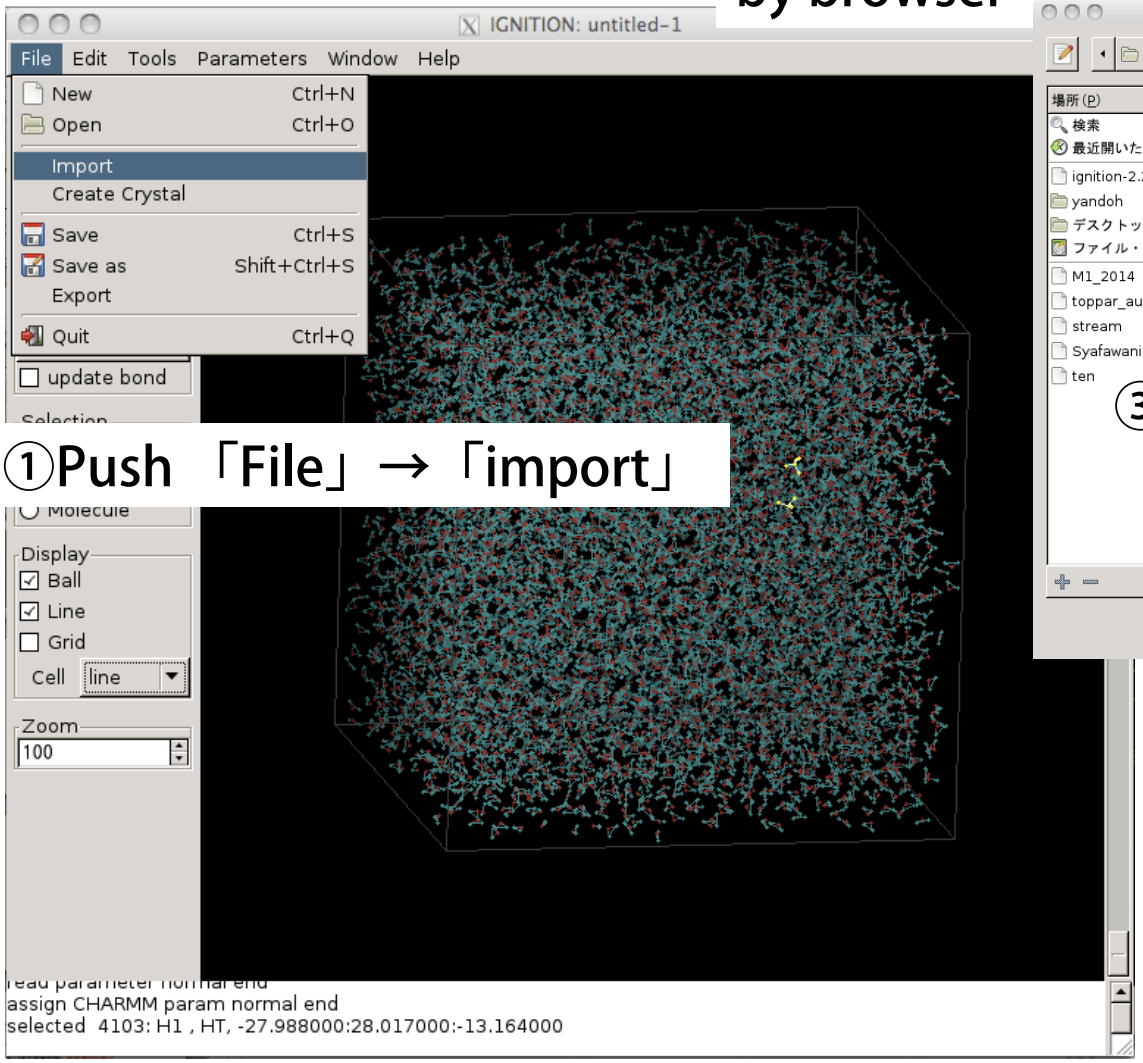
Nano-Ignition: folder branching

```
>tar xvfz ignition-2.2.20.tar.gz
ignition-2.2.20/
    configure   ./configure script
    ignition/     source code folder (*.c, *.h)
    document/          document
    template/   template of output files
    addhydrogen/      optional code folder to add hydrogen atoms
    solvent/      optional code folder to add solvent
    copyMolecule/      optional code folder to copy molecule
            ⋮
```

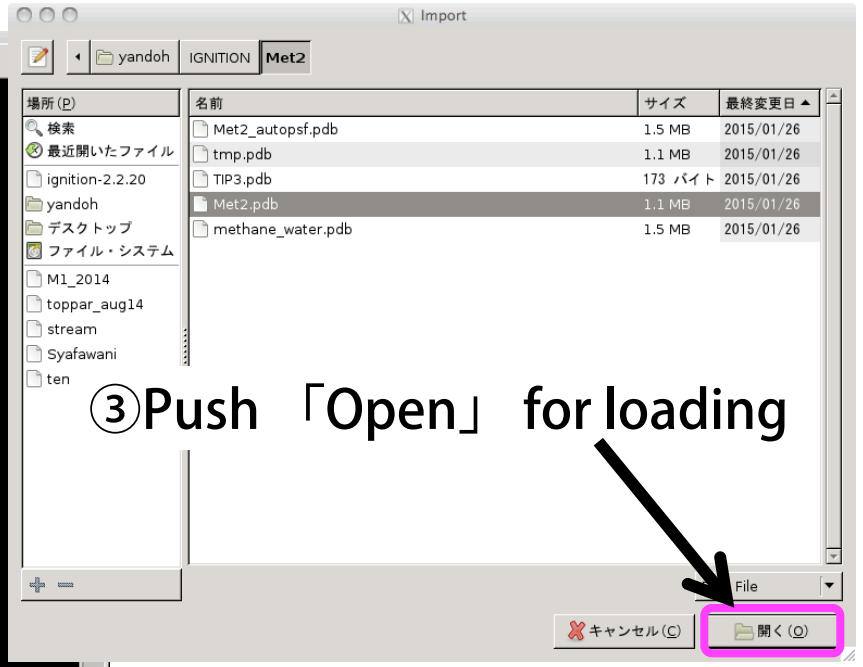
How to use Nano-Ignition (1)

Load .pdb file

②Push 「import」, then select .pdb file by browser



①Push 「File」→「import」

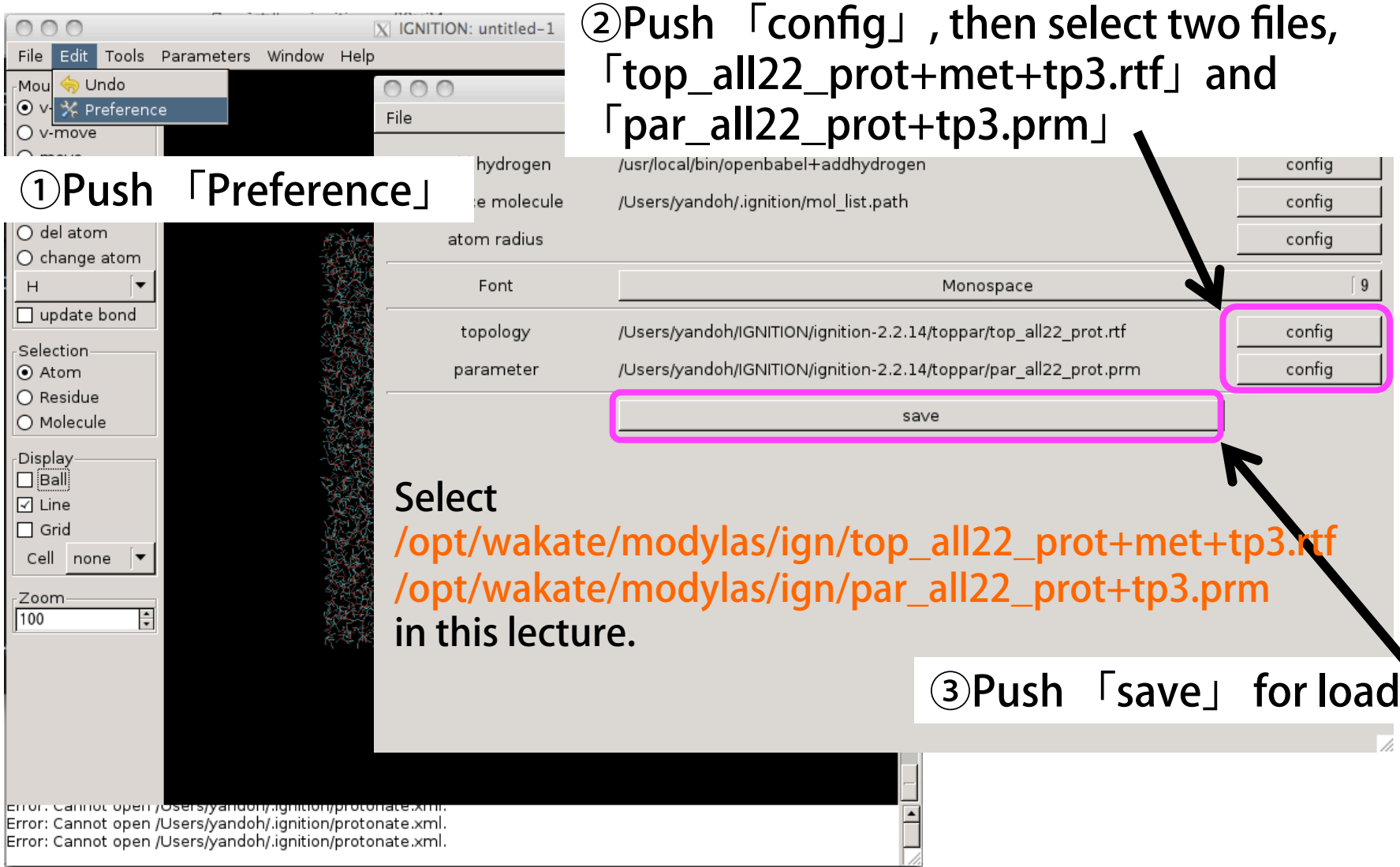


③Push 「Open」 for loading

Select
/opt/wakate/modylas/water/water.pdb
in this lecture.
(water 4428 molecules)

How to use Nano-Ignition (2)

Load topology and parameter files



①Push 「Preference」

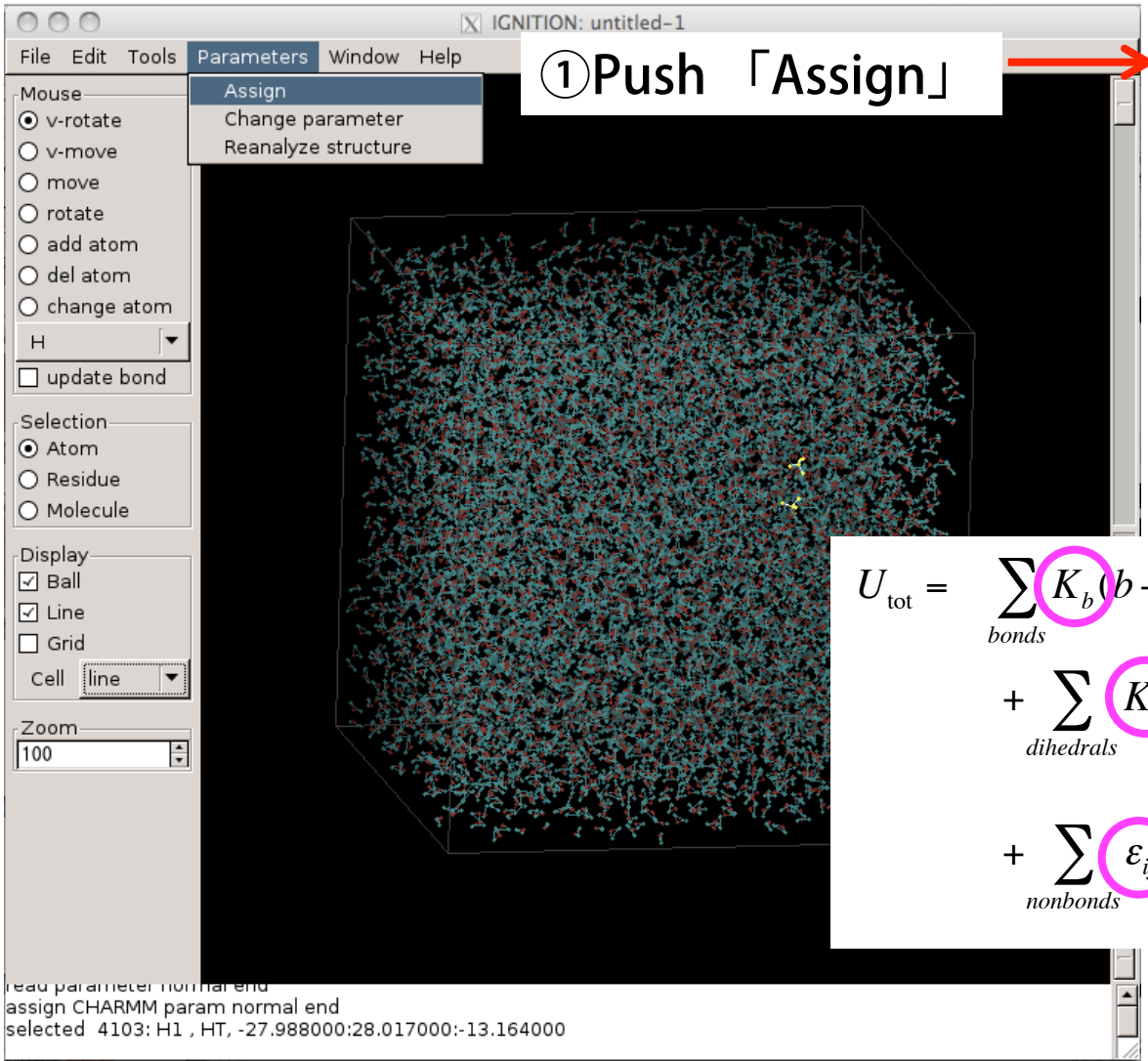
②Push 「config」, then select two files,
「top_all22_prot+met+tp3.rtf」and
「par_all22_prot+tp3.prm」

Select
/opt/wakate/modylas/ign/top_all22_prot+met+tp3.rtf
/opt/wakate/modylas/ign/par_all22_prot+tp3.prm
in this lecture.

③Push 「save」 for loading

How to use Nano-Ignition (3)

Assign force field parameters

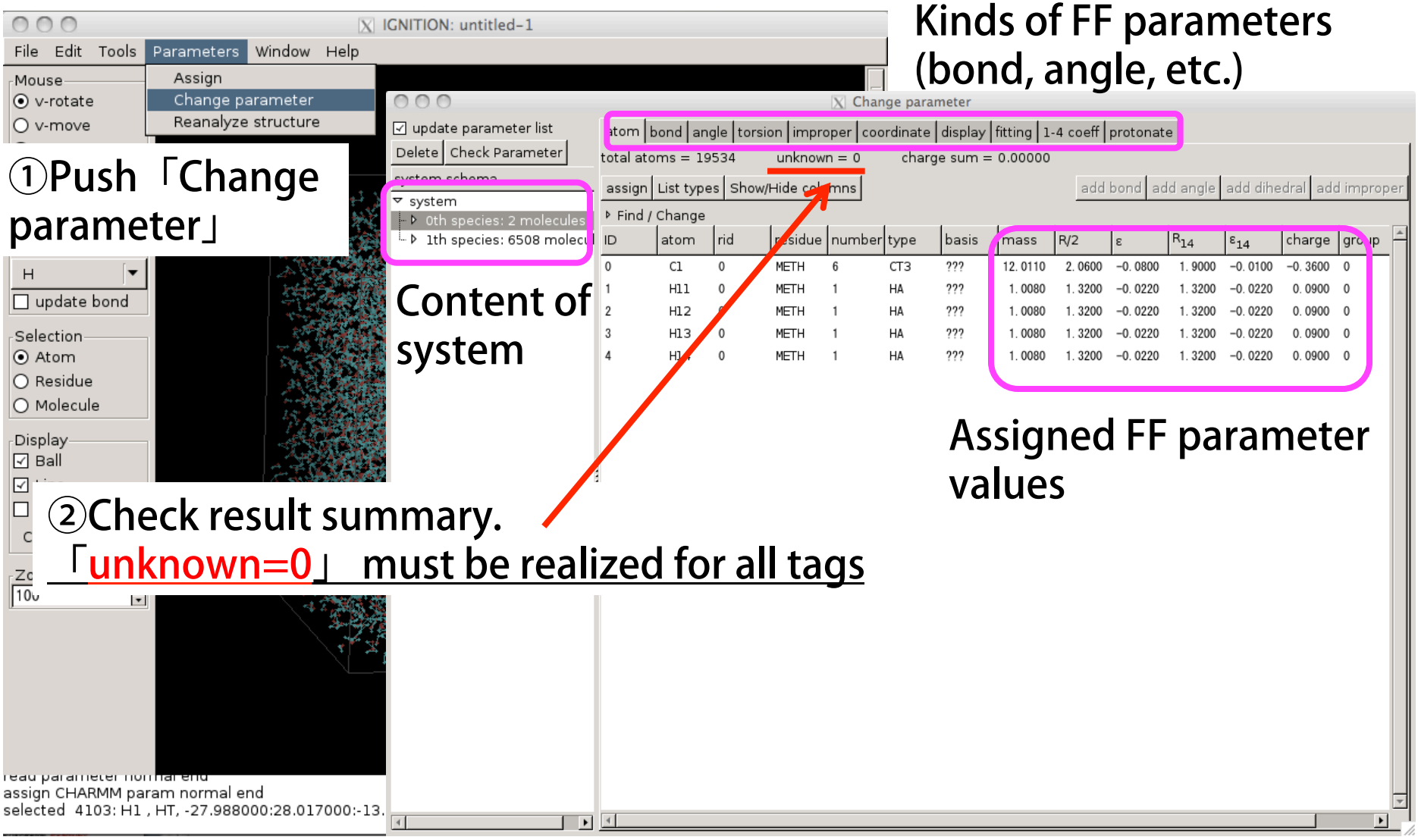


FF parameters are loaded from topology and parameter files

$$U_{\mathrm{tot}} = \sum_{bonds} K_b (b - b_0)^2 + \sum_{angles} K_\theta (\theta - \theta_0)^2 + \sum_{ub} K_{ub} (s - s_0)^2$$
$$+ \sum_{dihedrals} K_\phi [1 + \cos(n\phi - \delta)] + \sum_{impropers} K_\psi (\psi - \psi_0)^2$$
$$+ \sum_{nonbonds} \varepsilon_{ij} \left[\left(\frac{R_{ij}}{r_{ij}} \right)^{12} - 2 \left(\frac{R_{ij}}{r_{ij}} \right)^{6} \right] + \frac{q_i q_j}{r_{ij}}$$

How to use Nano-Ignition (4)

Check whether FF parameters are assigned or not



Kinds of FF parameters (bond, angle, etc.)

①Push「Change parameter」

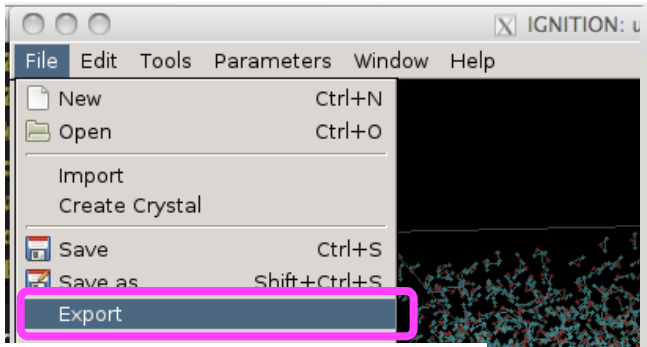
Content of system

②Check result summary.
「unknown=0」 must be realized for all tags

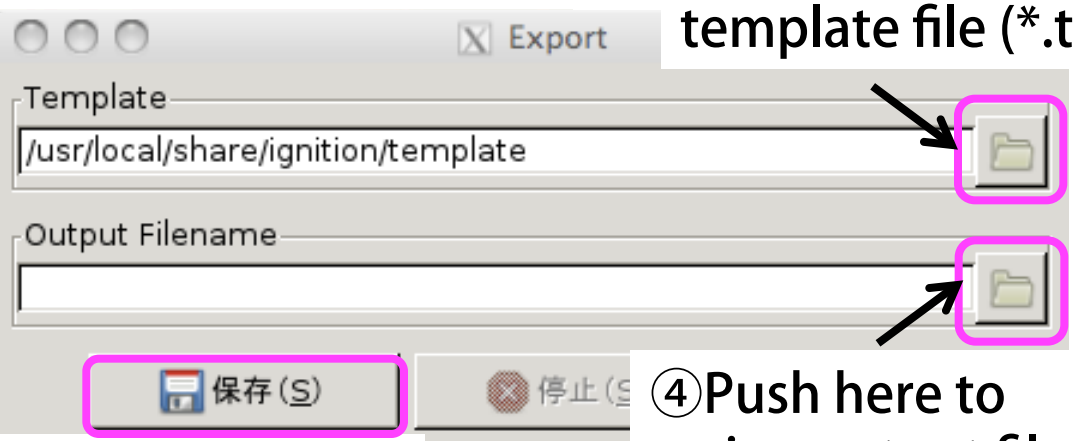
Assigned FF parameter values

How to use Nano-Ignition (5)

Export a set of inputs for MODYLAS



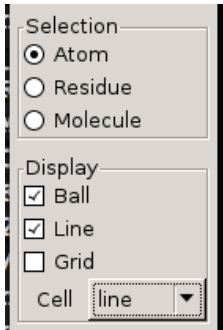
①Push 「Export」



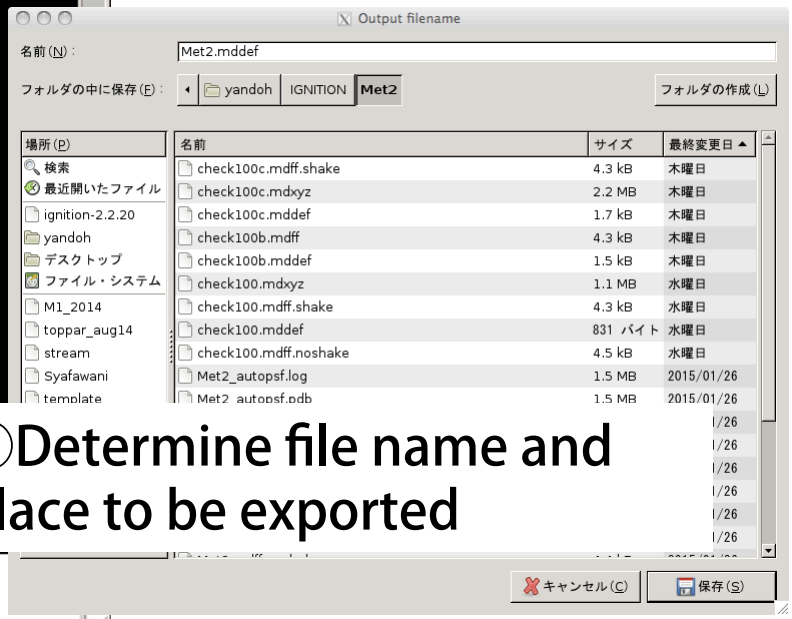
②Push here to select template file (*.tpt)

④Push here to assign output file

⑥Push 「save」



③Select each template file in /opt/wakate/modylas/ign/ folder:
mdff-1.0.0.tpt (for .mdff)
mdxyz-1.0.0.tpt (for .mdxyz)
mddef-1.0.0.tpt (for .mddef)



⑤Determine file name and place to be exported

Nano-Ignition: I/O structure

Molecule coordinate file
.pdb

Ex) water.pdb

CHARMM
Topology file

Ex) top_all22_prot.rtf

CHARMM
Parameter file

Ex) par_all22_prot.prm

Nano-Ignition

Available operations:

- 3D representation of inputted molecules
- Assignment of force field parameters
- Specification of distance constraints
- Specification of unit cell size
- Change of force field parameters
- Addition of hydrogen atoms
- Addition of solvent
- Deletion, insertion, and substitution of molecules
- Copy of molecule,
- Movement of molecules
- Addition of chemical bonds

and so on (see document)

A set of input files for MODYLAS

Calculation condition file
.mddef

Coordinate file
.mdxyz

Force field file
.mdff

End ignition after output these files

Questions and request to Nano-Ignition/MODYLAS

Nano-Ignition:

Kensuke Iwasahi, Technical associate, Institute for Molecular Science (IMS)
E-mail: iwahashi@ims.ac.jp

MODYLAS:

Submit questions and request to Forum on Web page
http://www.modylas.org/forum

Direct e-mail to Y.A. is unfavorable.