Science and Technology Facilities Council

Guide to DPD exercises

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Mesoscale exercises

Put together practical exercises on DPD and LBE

- Available in Jupyter notebooks from the workshop folder on GitLab, designed to run in (non-GPU) STFC Cloud Environment:

  git clone https://gitlab.com/ccp5/workshop.git WORKSHOP

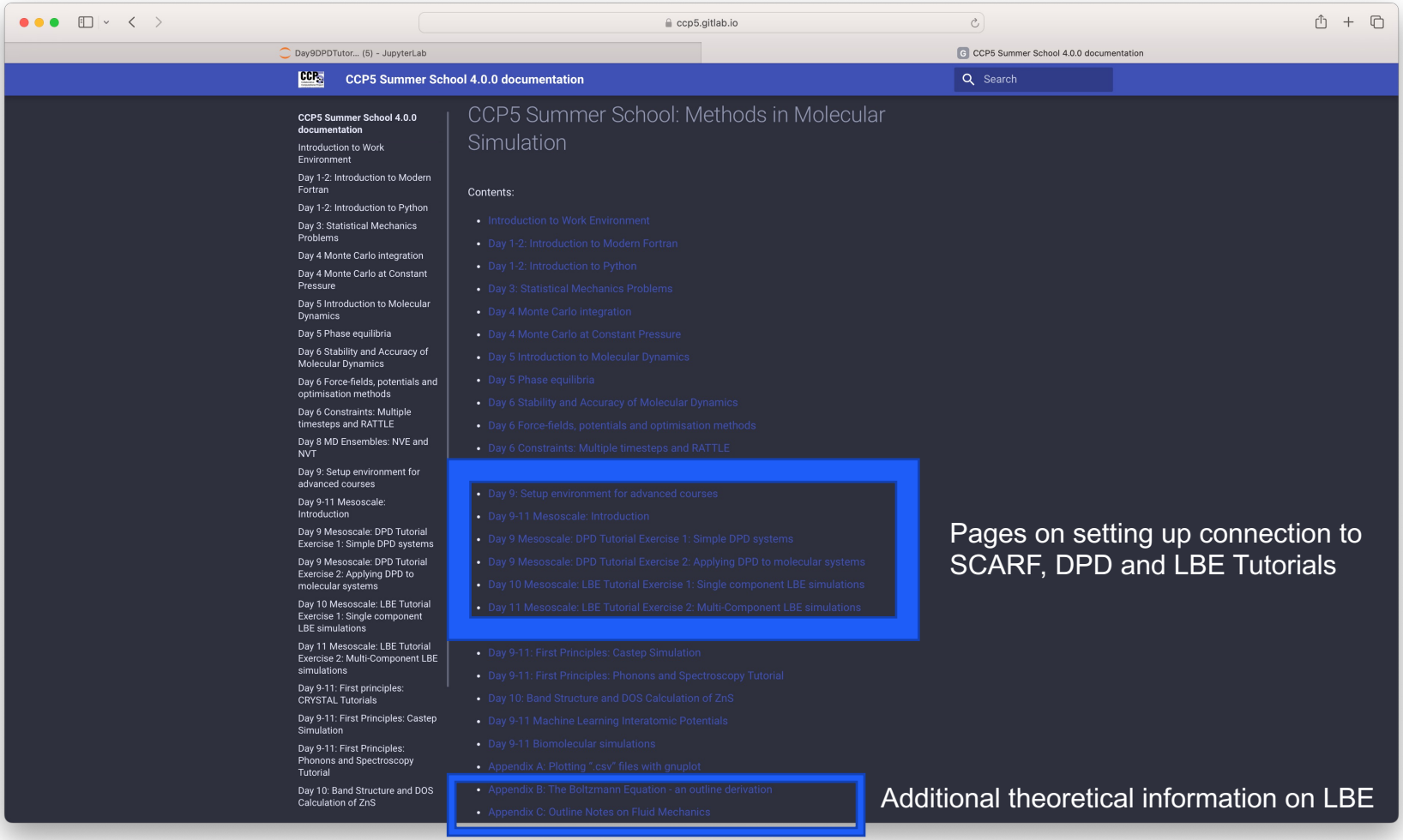
- DPD Exercises available in WORKSHOP/Day_9Meso
- LBE Exercises available in WORKSHOP/Day_10Meso and WORKSHOP/Day_11Meso
- Information also available via main CCP5 Summer School exercises page:

  ccp5.gitlab.io/summerschool

  - Points to notebooks for each exercise
  - Additional background information on exercises, theory and brief C programming guide (needed for LBE exercises)
  - Download link to these slides on the DPD exercises

- Possible to run notebooks on your own laptops: see CCP5 Summer School exercises page for details (including required Python modules)

Mesoscale exercises



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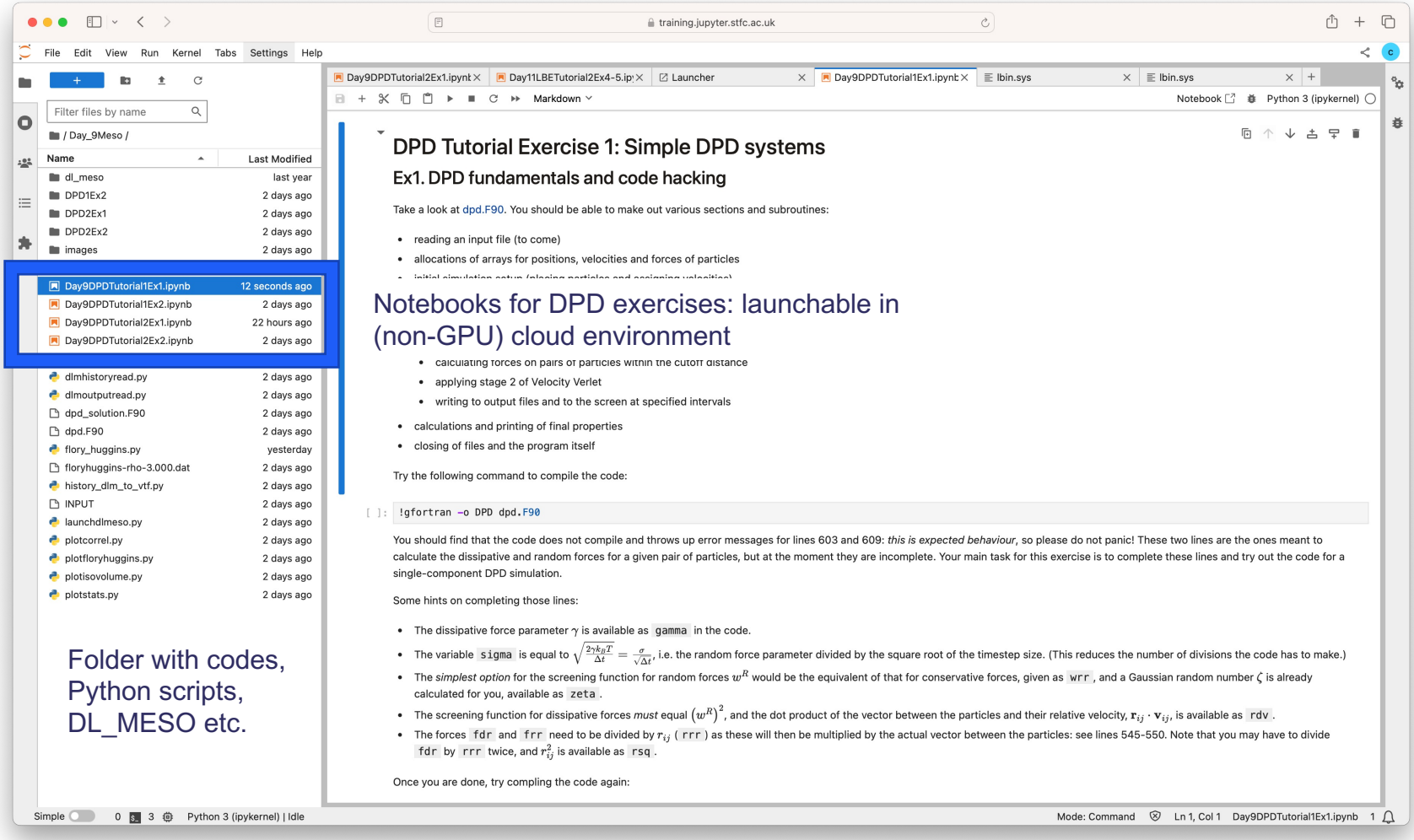
DPD Jupyter notebooks



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DPD practical exercises

Designed to show DPD's capabilities as a mesoscale modelling method

- Two tutorials, each with two exercises (a notebook for each exercise):

    1. Simple DPD systems
        1. DPD fundamentals and code hacking
        2. Parameterising DPD

    2. Applying DPD to molecular systems
        1. DPD mesophases
        2. Lipid bilayers, micelles and vesicles

- Tutorial 1, Exercise 1 uses a simple custom-written code you will need to 'hack' (modify)
- All other exercises use DL_MESO's DPD code (DL_MESO_DPD)
- Python scripts supplied to launch DL_MESO_DPD, convert outputs for visualisation and plot results

Tutorial 1, Exercise 1

Constructing and running a basic DPD code

- Notebook: Day_9Meso/Day9DPDTutorial1Ex1.ipynb
- Starts with a simple DPD code in Fortran90: **`dpd.F90`**
  - Includes a compile-time option to modify how bead pairs are found for force calculations (see later)
- Models a simple fluid – one bead species, no bonds between beads – with a DPD thermostat
- However … the lines calculating dissipative and random forces are incomplete, so the code will not compile
- Your task: complete the lines to calculate dissipative and random forces to get the DPD thermostat to work
  - Two lines in a subroutine (**`calculate_dpd_forces`**) that takes r_{ij}, r_{ij}^2 and $\mathbf{r}_{ij} \cdot \mathbf{v}_{ij}$ as inputs
- Code can be used to explore the properties of a single species

Tutorial 1, Exercise 1

calculate_dpd_forces subroutine (lines 587–611 of dpd.F90)

```
      IF (rrr>1.0e-10_dp) THEN

!     screening function (for conservative force)

         wrr = MAX ((bij - rrr), 0.0_dp)

!     potential calculation

         pot = 0.5_dp * aij * wrr * wrr

!     conservative interaction force

         fcr = aij * wrr / rrr

!     dissipative force (rdv = dot product of vector and relative velocity)

         fdr =

!     random force (zeta = gaussian random number)

         CALL RANDOM_NUMBER (zeta)
         zeta = fac12 * (zeta - 0.5_dp)
         frr =

      END IF
```

Avoids division-by-zero problems

Screening function for conservative forces

Magnitude of conservative force: note division by **rrr** (r_{ij})

Variable **rdv** input into subroutine

Magnitude of dissipative force (missing)

Approximation of Gaussian random number ξ_{ij}

Magnitude of random force (missing)

Tutorial 1, Exercise 1

Hints to complete dissipative and random forces

- Variables available for force parameters:
  - `gamma` γ
  - `sigma` Equal to $\sqrt{\frac{2\gamma k_B T}{\Delta t}} = \frac{\sigma}{\sqrt{\Delta t}}$
- Screening function for random forces w^R: we suggest using the same as for conservative forces (`wrr`), but you can choose something else
- Screening function for dissipative forces:

$$w^D(r_{ij}) = \left[w^R(r_{ij})\right]^2$$

- The forces coming out of the `calculate_dpd_forces` subroutine should be divided by r_{ij}: multiplying these by the actual vector between particles $\mathbf{r}_{ij}$ (e.g. lines 545–550) gives

$$\frac{F_{ij}}{r_{ij}} \times \mathbf{r}_{ij} \equiv F_{ij}\hat{\mathbf{r}}_{ij} = \mathbf{F}_{ij}$$

Tutorial 1, Exercise 1

Compiling code

```
gfortran -o DPD dpd.F90
```

Running code

```
./DPD < INPUT
```

- **INPUT** is a text file with the simulation properties

```
10000          number of time steps
1000           number of equilibration steps
10             sampling interval for properties
900            particle population
300.0          system volume (reduced units)
1.0            temperature (reduced units)
1.0            energy parameters
1.0            particle diameters
4.5            drag coefficient
0.04           time step (LJ units)
.true.         trajectory file option
.true.         write positions (T) or velocities (F)
```

- Commands can be invoked using cells in notebook
- Script available to plot results (e.g. energy, temperature, pressure), VMD can open simulation trajectory for visualisation and some analysis

Tutorial 1, Exercise 1

Speeding up the code

- By default, code uses ‘brute force’ approach to search over all possible particle pairs, check distances and calculate forces if within cutoff
- Code also includes implementation of linked-cell lists, assigning particles to lists for each cell (size of at least the cutoff) and uses the lists to search for particle pairs within each cell and its nearest neighbours

- To invoke linked-cell list version, recompile using additional compiler flag:

```
gfortran –o DPD-FAST –DFAST dpd.F90
```

- Calculation times are measured in both versions of the code so you can compare them
- How does the calculation time vary with the number of beads for each version?

DL_MESO

General purpose mesoscopic modelling software package

- Includes Lattice Boltzmann (LBE) and DPD codes (serial and parallel with MPI and/or OpenMP), Java GUI (optional)

- Created for CCP5 at UKRI STFC Daresbury Laboratory in 2004
  - Now developed for UKCOMES (EPSRC High-End Computing consortium)

- Free for academic use (licence on annual subscription for commercial use)

- Described in Molecular Simulation articles:
  - Seaton *et al.*, *Mol Sim* **39** (10), 796–821 (2013)
  - Seaton, *Mol Sim* **47** (2–3), 228–247 (2021)

- Copy of current version (2.7) included with course materials, available for you to take home with you
  - Small additions included for exercises (makefiles in working directory, additional Python scripts)

Tutorial 1, Exercise 2

Now expanding to two immiscible species

- Conservative force parameter between species higher than those for like-like interactions: particles should separate out

Making use of DPD code in DL_MESO (DL_MESO_DPD)

- Notebook: Day_9Meso/Day9DPDTutorial1Ex2.ipynb
- Unpack and compile serial version and utilities (using makefiles)
- Run DL_MESO_DPD in directory (Day_9Meso/DPD1Ex2) with input files (CONTROL, FIELD)
    - Script available with notebook to launch calculation in background and display progress bar while DL_MESO_DPD runs

Tutorial 1, Exercise 2

Input files for DL_MESO_DPD

```
DL_MESO phase separation example

volume 1000.0
temperature 1.0
cutoff 1.25

timestep 0.01
steps 20000
equilibration steps 0
scale temperature every 10
trajectory 0 100
stats every 100
stack size 100
print every 10
job time 3600.0
close time 200.0

ensemble nvt mdvv

l_scr

finish
```

CONTROL

```
DL_MESO phase separation example

SPECIES 2
A 1.0 0.0 1500
B 1.0 0.0 1500

INTERACTIONS 3
A A dpd   25.0 1.0 1.0
A B dpd  100.0 1.0 1.0
B B dpd   25.0 1.0 1.0

CLOSE
```

Numbers of unbonded beads

Interaction lengths $r_{c,ij}$

Dissipative force parameters γ_{ij}

Conservative force parameters A_{ij}

FIELD

Tutorial 1, Exercise 2

Output files

- `OUTPUT` General output with simulation summaries, error/warning messages and statistical properties (instantaneous and averaged) during simulation
- `export` Simulation restart file (instantaneous particle configuration)
- `REVIVE` Simulation restart file (statistical accumulators and random number states)
- `HISTORY` Simulation trajectory data (in binary)
- `CORREL` Tabulated statistical properties in plottable file

- Plotting trajectory data requires utility to convert into formats for visualisation software
  - Utilities available with DL_MESO to do this and carry out analyses
  - Also have a Python script with notebook to create a VTF file for visualisation with VMD

- Statistical properties can be plotted using e.g. Excel, gnuplot or Python script (`dlmresultviewer.py`)
  - Python script for plotting also available in notebook

Tutorial 1, Exercise 2

Effect of conservative force parameter on separation

- Flory-Huggins relationship

$$\chi^{AB} \propto \left(A_{ij}^{AB} - A_{ij}^{AA}\right)$$

  - Assumes beads for both components have same sizes and like-like interactions
  - Proportionality constant changes with particle density ρ

- Can measure χ^{AB} from simulations of separating particles, using volume fraction of one species in phase-separated regions (e.g. ϕ_A):

$$\chi^{AB} = \frac{\ln\left[\frac{1-\phi_A}{\phi_A}\right]}{1-2\phi_A}$$

  - Simulations set up by putting beads of each species in one half of an elongated box: can set this up by supplying DL_MESO_DPD with a **CONFIG** file specifying initial positions of beads
  - Vary A_{ij}^{AB}, calculate resulting χ^{AB} values and plot to get relationship

Tutorial 1, Exercise 2

Python script to automate calculations

- **`flory_huggins.py`**: Runs series of DL_MESO_DPD calculations to find volume fraction profiles and estimates χ^{AB} for various A_{ij}^{AB} values (creates **`CONTROL`**, **`FIELD`** and **`CONFIG`** files automatically)
  - Runs in notebook, displays progress bars for calculations/analyses
  - Suggest recompiling DL_MESO_DPD to use OpenMP multithreading to speed up calculations

- Script supplied with notebook to read file produced by **`flory_huggins.py`** and plot results
  - Concentration profiles: ϕ_A vs. x
  - Plot of χ^{AB} vs. $\Delta A_{ij} = A_{ij}^{AB} - A_{ij}^{AA}$

- Questions:
  - Does value of A_{ij}^{AA} affect above relationship and the graph?
  - (Optional) What happens if the total bead density ρ is changed?

Tutorial 2, Exercise 1

Applying DPD to molecular systems: adding bonds to form amphiphilic dimers

- Notebook: Day_9Meso/Day9DPDTutorial2Ex1.ipynb
- Including harmonic bonds between two beads that interact differently with a solvent – one hydrophilic, one hydrophobic – to form two-bead molecules
- Solutions of these molecules form mesophases (stable structures at equilibrium)
  - Functions of temperature and concentration of solute (dimers)
- Simulation and analysis workflow:
  - Run DL_MESO_DPD with different **`FIELD`** files (but same **`CONTROL`** file each time), each representing a different dimer concentration
    - Can run more than one calculation at a time
  - Look at trajectories and create isosurface volume plots of one species in molecule (hydrophobic beads) to visualise phases
  - Calculate order parameters to help detect different mesophases (semi-)automatically (i.e. without needing to visualise them)

Tutorial 2, Exercise 1

```
DL_MESO amphiphile mesophase example

volume 10.0 10.0 20.0
temperature 1.0
cutoff 1.0
global bonds

timestep 0.02
steps 50000
equilibration steps 10000
scale temperature every 1000
trajectory 10000 1000
stats every 1000
stack size 100
print every 1000
job time 3600.0
close time 10.0

ensemble nvt mdvv

l_scr

finish
```

CONTROL

```
DL_MESO amphiphile mesophase example (30% composition)

SPECIES 3
A 1.0 0.0 0
B 1.0 0.0 0
S 1.0 0.0 8400

MOLECULES 1
AB
nummols 1800
beads 2
A 0.0107636 -0.0112540 -0.249515
B -0.0107636 0.0112540 0.249515
bonds 1
harm  1 2 100.0 0.50
finish

INTERACTIONS 6
A A dpd  25.0 1.0 5.625
A B dpd  30.0 1.0 5.625
A S dpd   0.0 1.0 5.625
B B dpd  25.0 1.0 5.625
B S dpd  50.0 1.0 5.625
S S dpd  25.0 1.0 5.625

CLOSE
```

NOTE: beads involved in molecules not included in totals here

name of molecule type

number of molecules in system

configuration for molecule insertion

bond stretching interaction

FIELD

(30 vol% concentration)

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Tutorial 2, Exercise 1

Order parameters for automatic mesophase detection

- Assign function (often a Gaussian) for selected particles based on their positions onto a density grid
- Density grid can be used to find isosurfaces and determine normals
- Can calculate second moment of isosurface normal distribution

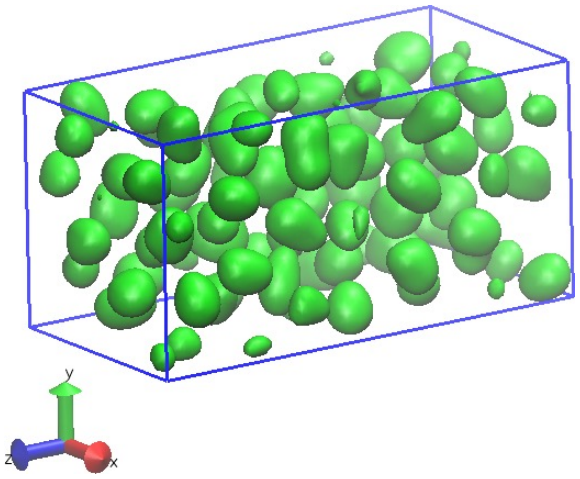
$$\mathbf{M} = \int \mathbf{nn} p(\mathbf{n})\, d\mathbf{n}$$

- Eigenvalues of second moment (μ_1, μ_2, μ_3) in numerical order normalised to sum to 1 can be used to determine mesophase shape

- All of the above can be determined by **`isosurfaces.exe`** utility
  - Directly reads **`HISTORY`** file, uses one bead species selected by user for density plots written to VTK files (readable by ParaView)
  - Eigenvalues are printed on screen and in text file for each trajectory frame
  - Python scripts in notebook can launch utility and plot eigenvalues

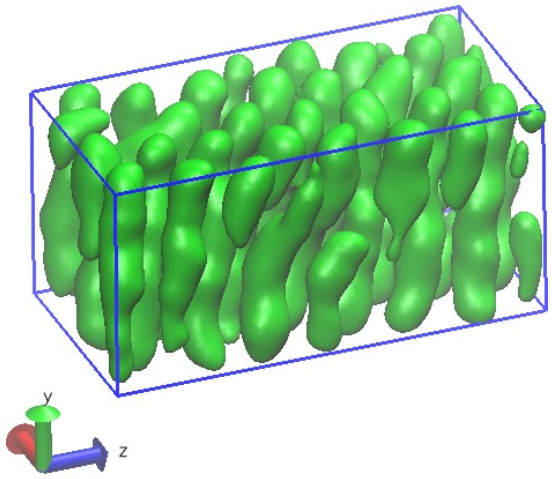
Tutorial 2, Exercise 1

Probable mesophases



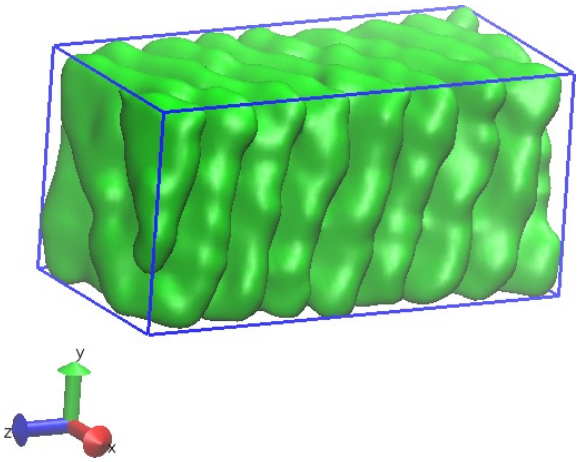
Isotropic (L_1)

$\mu_1 \approx \mu_2 \approx \mu_3 \approx \frac{1}{3}$



Hexagonal (H_1)

$\mu_1 < 0.1, \mu_1 \ll \mu_2, \mu_3$



Lamellar (L_α)

$\mu_1 < 0.1, \mu_2 < 0.15,$

$\mu_1, \mu_2 \ll \mu_3$

Eigenvalues shown here are for guidance based on experience in carrying out simulations: they are not definitive!

Running DL_MESO_DPD on SCARF

DL_MESO_DPD available on SCARF for Tutorial 2, Exercise 2

- Parallel version of DL_MESO_DPD has been compiled on SCARF, available for practical exercises inside a shared folder
- Logging on to SCARF:

```
ssh scarf
```

- Submitting batch job to queue using Slurm:

```
sbatch dpdjob
```

- Job script runs **`traject_vtf.exe`** utility immediately after DL_MESO_DPD finishes to produce VTF file from **`HISTORY`** file
  - VTF file can be transferred to your own machine for visualisation in VMD
  - Folders available in environment to copy results from each calculation

Running DL_MESO_DPD on SCARF

Job submission script

- Runs DL_MESO_DPD on 32 cores for up to an hour and creates VTF trajectory file for visualisation
- Runs DPD code in directory where job is submitted
- Creates standard output and error files with filenames based on job number
- Uses reservation code for CCP5 Summer School and exclusive running of job on allocated cores
- Uses precompiled executables for DL_MESO_DPD and **`traject_vtf.exe`** utility in shared folder

```
!/usr/bin/env bash
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=32
#SBATCH -t 01:00:00
#SBATCH -o %j.out
#SBATCH -e %j.err
#SBATCH --exclusive
#SBATCH --reservation=ccp5_pre
#SBATCH -C scarf21
cd $PWD
CWD=/work4/training/ccp5/meso
mpirun -srun $CWD/dpd.exe
$CWD/traject_vtf.exe
```

`dpdjob`

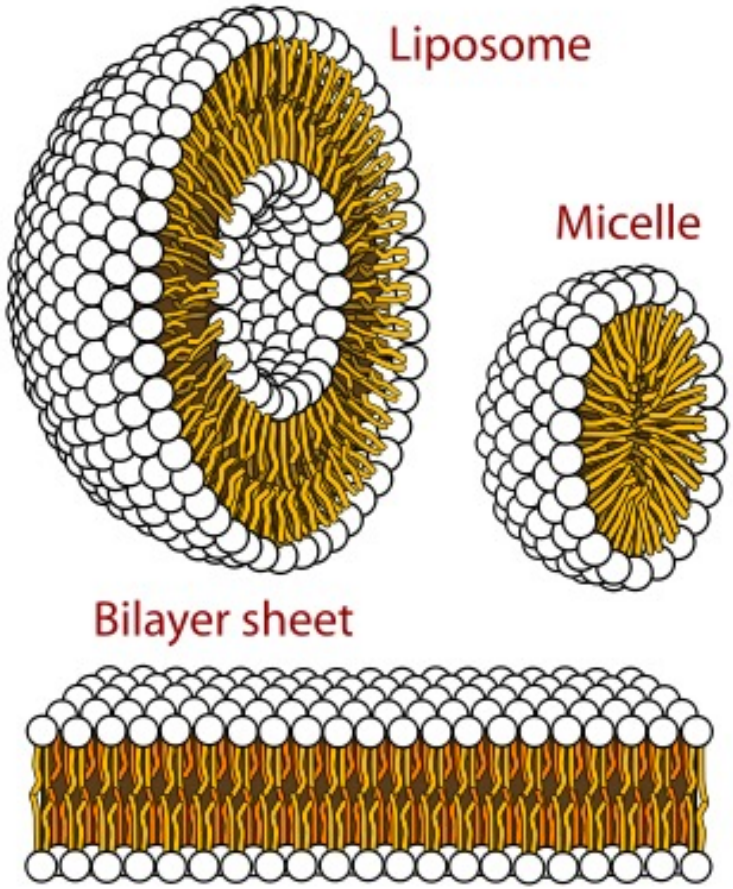
Tutorial 2, Exercise 2

Lipid molecules in solution

- Notebook: Day_9Meso/Day9DPDTutorial2Ex2.ipynb
- Each molecule consists of one hydrophilic bead and six hydrophobic beads bonded together
- We can optionally include additional potentials to fix angles between pairs of bonds:

$$U_{ijk} = A\left[1 + \cos\left(m\theta_{ijk} - \theta_0\right)\right]$$

- Depending on molecule concentration and bond straightness, molecules can form into bilayers, micelles or vesicles (liposomes)



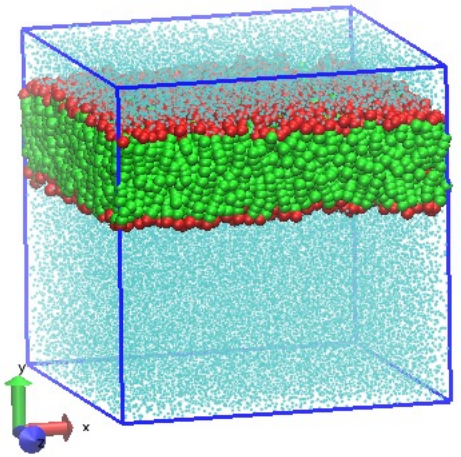
Tutorial 2, Exercise 2

Lipid molecules in solution

- Starting with DL_MESO_DPD simulation that **should** generate a bilayer sheet
  - `FIELD` file sets number of lipid molecules and interactions (including bond angles)

- Start by modifying FIELD file to switch off bond angle potentials, e.g. setting $A = 0$
  - This will still enable angles to be measured and recorded in `CORREL` file

- Try a lower molecule concentration (with and without bond angles)
  - What structures will result?



Tutorial 2, Exercise 2

```
[...]
SPECIES 3
H         1.0 0.0 0
C         1.0 0.0 0
W         1.0 0.0 35152

MOLECULES 1
HC6
nummols 2000
beads 7
H         -0.0172847 0.383451 0.2849
C         -0.016165 0.381111 -0.215093
C         0.280007 0.0703806 0.0412832
C         0.440339 -0.359403 -0.157664
C         0.00469362 -0.136529 -0.260333
C         -0.455453 -0.119133 -0.0654933
C         -0.236136 -0.219878 0.3724
bonds 6
harm  1 2 128.0 0.50
harm  2 3 128.0 0.50
harm  3 4 128.0 0.50
harm  4 5 128.0 0.50
harm  5 6 128.0 0.50
harm  6 7 128.0 0.50
angles 5
cos   1 2 3 20.0 0.0 1.0
cos   2 3 4 20.0 0.0 1.0
cos   3 4 5 20.0 0.0 1.0
cos   4 5 6 20.0 0.0 1.0
cos   5 6 7 20.0 0.0 1.0
finish
[...]
```

adjust for molecule concentration
(keep total number of beads constant)

adjust these values for bond angle potentials (A, θ_0, m)

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Before you finish …

Registering for DL_MESO

- If you want to use DL_MESO for your own research (either DPD or LBE), please register via the website

www.ccp5.ac.uk/DL_MESO

DL_Software Digital Guide

- If you want more information about DL_MESO, the mesoscale modelling methods it includes and/or other DL_Software packages, we have an online guide available at

https://dl-sdg.github.io/