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# Application of Mesoscale Dynamics

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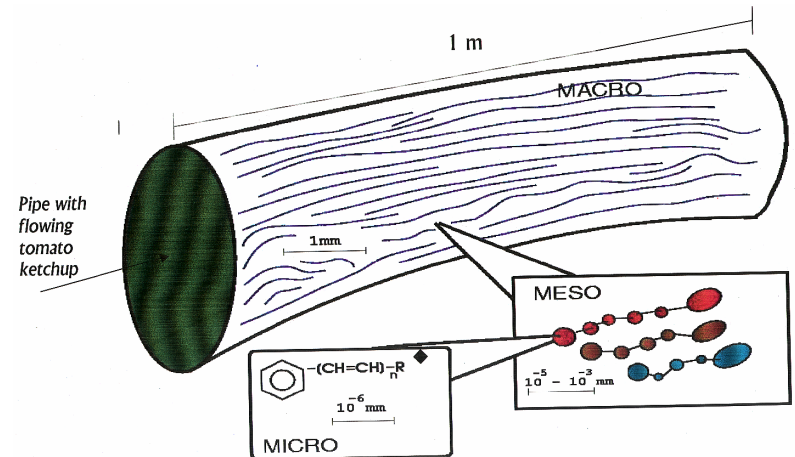
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# What is mesoscale modelling?

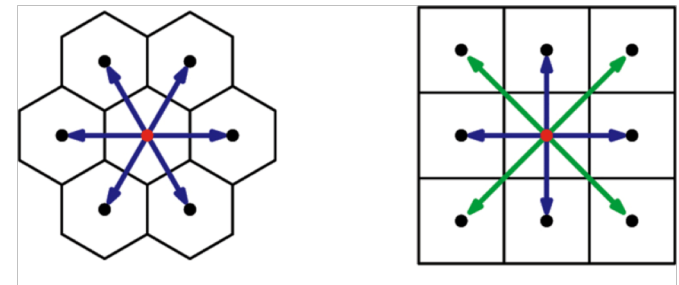
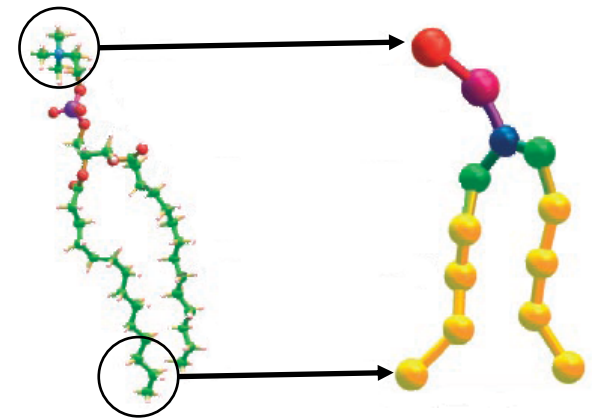
- Mesoscale fits between microscopic (atoms) and macroscopic (continuum fluid)
- Need to consider both thermodynamics and hydrodynamics
  - Atom-like and fluid-like effects
  - Can approach from bottom-up (coarse-graining) or top-down, or even both
- Many complex systems of industrial interest act at mesoscale



Source: Prof. PV Coveney,  
Centre for Computational Science, UCL

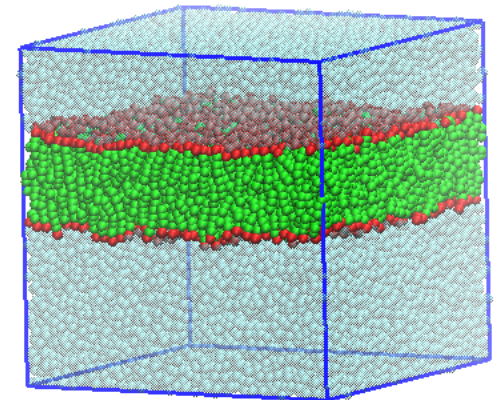
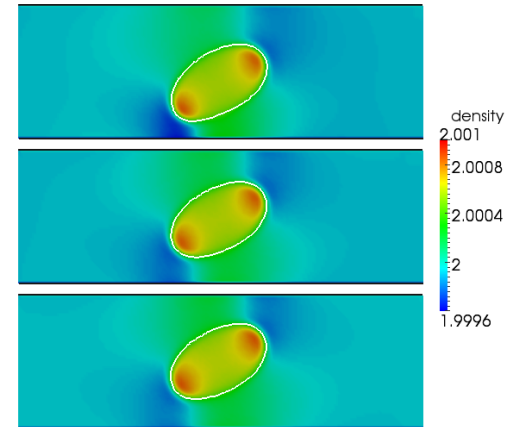
# Mesoscale modelling approaches

- Particles ('beads') can represent a number of atoms or molecules
  - Can fix the degree of coarse-graining, but not compulsory to do so!
- Algorithms determine how these particles move over time
- Two main approaches:
  - Calculate and integrate interaction forces on particles (e.g. DPD)
  - Determine probabilities of finding particles at particular points (e.g. LBE)



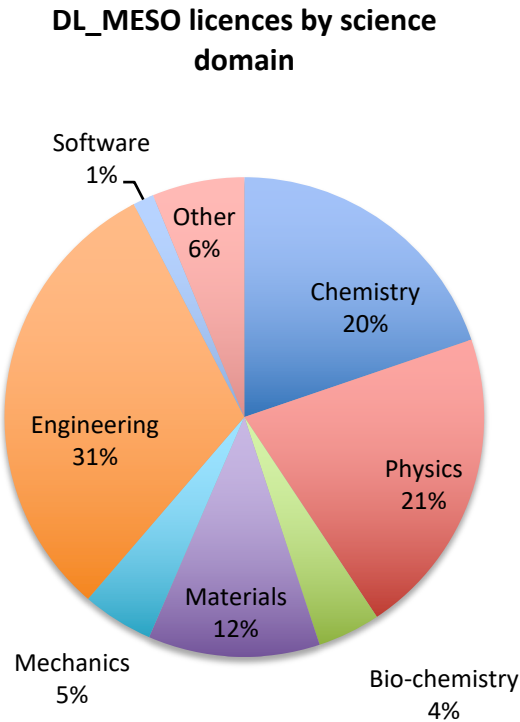
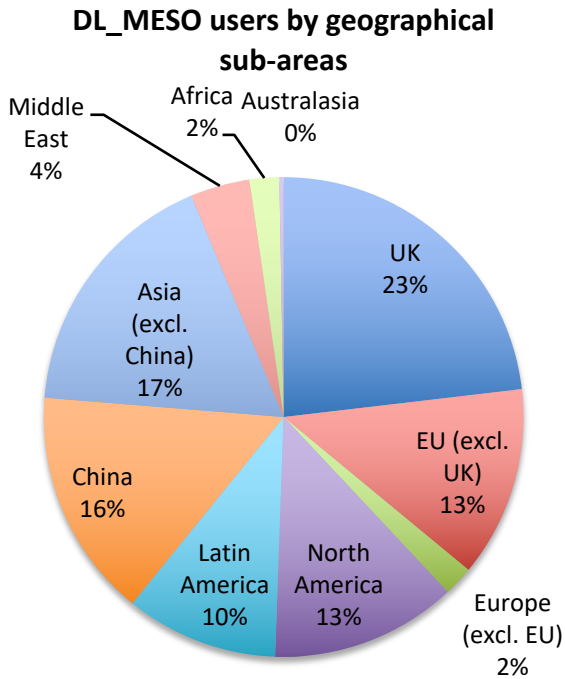
# DL\_MESO

- General purpose mesoscopic simulation software package [1]
  - MPI domain-decomposed codes with optional OpenMP multithreading for:
    - Dissipative Particle Dynamics (DPD)
    - Lattice Boltzmann Equation (LBE)
  - Created in 2004 as CCP5 flagship project:  
[www.ccp5.ac.uk/DL\\_MESO](http://www.ccp5.ac.uk/DL_MESO)
    - Development currently funded under CoSeC for CCP5 and UKCOMES
  - Used widely by academics and industry
  - Last major release (version 2.6) in November 2015: [imminent release of version 2.7](#)

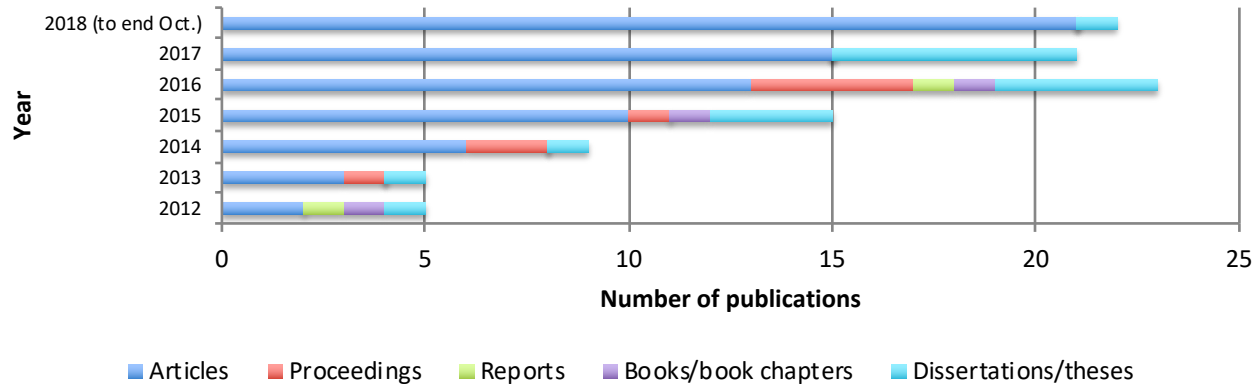


[1] MA Seaton *et al.*, *Mol. Sim.* **39** (10), 796–821 (2013)

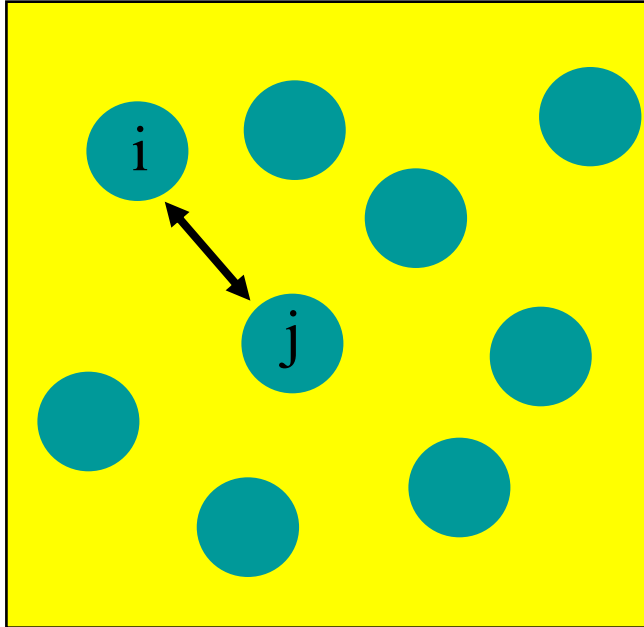
# DL\_MESO users



- 350 registered users of DL\_MESO 2.6
  - Approximately 3:1 using DPD:LBE
  - 100 citations of DL\_MESO to date



# Dissipative Particle Dynamics



- Based on modelling motion of particles ('beads')
  - Represent either collections of physical particles or continuum fluid ('momentum carriers')
  - Usually soft and repulsive
  - Net forces on particles calculated mostly as pairwise contributions: often split into Conservative, Dissipative and Random forces
  - Integrate forces over timestep  $\Delta t$  to determine motion

$$\frac{d^2 \mathbf{r}_i}{dt^2} = \frac{1}{m_i} (\sum_{j \neq i} \mathbf{F}_{ij}^C + \sum_{j \neq i} \mathbf{F}_{ij}^D + \sum_{j \neq i} \mathbf{F}_{ij}^R)$$

# Dissipative Particle Dynamics

- Dissipative force:

$$\mathbf{F}_{ij}^D = -\gamma w^D(r_{ij}) (\hat{\mathbf{r}}_{ij} \cdot \mathbf{v}_{ij}) \hat{\mathbf{r}}_{ij}$$

Distance-based screening function

Relative velocity between particles

- Random force:

$$\mathbf{F}_{ij}^R = \sigma w^R(r_{ij}) \frac{\xi_{ij}}{\sqrt{\Delta t}} \hat{\mathbf{r}}_{ij}$$

Gaussian random number (zero mean, unity variance)

- If following conditions apply [1], dissipative and random forces act together as momentum-conserving thermostat:

$$w^D(r_{ij}) = [w^R(r_{ij})]^2 \text{ and } \sigma^2 = 2k_B T \gamma$$

Related to kinematic fluid viscosity (complex!)

# Dissipative Particle Dynamics

- Conservative forces can take many forms, but most frequently used form is by Groot and Warren [1]:

$$\mathbf{F}_{ij}^C = \begin{cases} A_{ij} \left(1 - \frac{r_{ij}}{r_c}\right) \hat{\mathbf{r}}_{ij}, & r_{ij} < r_c \\ 0, & r_{ij} \geq r_c \end{cases}$$

Conservative force parameter

Interaction length (cutoff radius)

- Gives quadratic potential and quadratic equation of state:

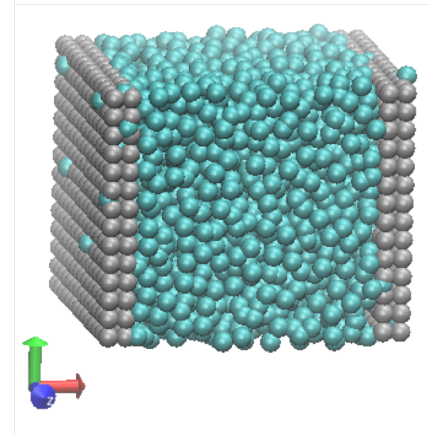
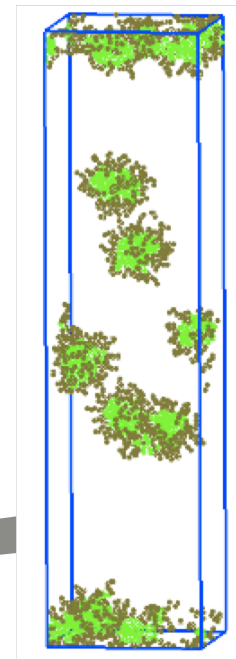
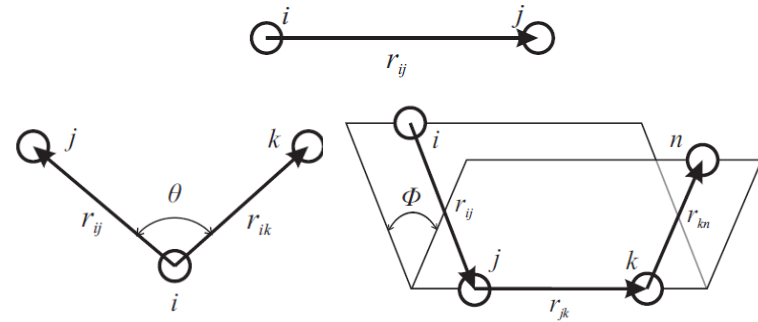
$$p \approx \rho k_B T + 0.101 A_{ij} \rho^2 r_c^4 \quad (\rho > 2)$$

- Soft potential allows larger timestep than classical MD: can often reach equilibrium state quickly



# Dissipative Particle Dynamics

- In addition to Groot-Warren conservative forces, can also include:
  - Bonded interactions (stretching, angles, dihedrals)
  - Electrostatic interactions (usually based on Ewald sums or P<sup>3</sup>M with charge smearing)
  - Many-body (density-dependent) interactions
  - Surface interactions (planar surfaces or based on frozen beads)



# DL\_MESO\_DPD

- DL\_MESO's DPD code [1]
  - Models (soft) particles with a pairwise thermostat (DPD or others)
  - Pairwise potentials: Groot-Warren, many-body DPD, LJ, WCA
  - Can include bonded and charge-based interactions
  - Non-periodic boundary conditions available: hard planar surfaces with wall interactions, frozen beads, Lees-Edwards shearing boundaries
- Uses text files as inputs (similar to DL\_POLY):
  - CONTROL, FIELD, (optional) CONFIG
- DL\_MESO includes utilities to process and analyse results
  - e.g. visualization (in VMD), RDFs, isosurface plots, phase detection

# DL\_MESO\_DPD: Input files

```
DL_MESO amphiphile mesophase example
```

```
volume 10.0 10.0 20.0
temperature 1.0
cutoff 1.0
global bonds

timestep 0.01
steps 200000
equilibration steps 20000
scale temperature every 1000
trajectory 20000 1000 0
stats every 1000
stack size 100
print every 1000
job time 7200.0
close time 10.0
```

```
ensemble nvt mdvv
```

```
finish
```

```
DL_MESO amphiphile mesophase example
```

```
SPECIES 3
```

```
A 1.0 0.0 0 0
B 1.0 0.0 0 0
C 1.0 0.0 8400 0
```

```
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 C dpd 0.0 1.0 5.625
B B dpd 25.0 1.0 5.625
B C dpd 50.0 1.0 5.625
C C dpd 25.0 1.0 5.625
```

```
CLOSE
```

CONTROL file (simulation information)

FIELD file (interaction information)

rch  
ation

# DPD units

- Can use any system of consistent units, most often:
  - Mass  $[M]$ : mass of a DPD bead
  - Length  $[L]$ : interaction cutoff distance (related to volume of bead)
  - Energy  $[E]$ : product of Boltzmann constant ( $k_B$ ) and datum temperature
  - All above often set to 1 in simulations for numerical accuracy

- DPD time unit derived from fundamental units:

$$[T] = [L] \sqrt{\frac{[M]}{[E]}}$$

- Temperature related to kinetic energy:

$$k_B T = \frac{2E_k}{3N_f}$$

# How to parameterise DPD

- Conservative force parameters
  - For interactions between beads of same type (like-like), we can make use of equation of state and relate to isothermal compressibility:

$$\begin{aligned}\kappa^{-1} &= \frac{V_{bead}}{k_B T \kappa_T} \\ &= \frac{1}{k_B T} \left( \frac{\partial p}{\partial \rho} \right)_T \\ &= 1 + \frac{2\alpha A_{ij} \rho}{k_B T}\end{aligned}$$

$\kappa$  is dimensionless form of compressibility: value depends on real volume of a DPD bead

- e.g. for water (one molecule per bead),  $\kappa^{-1} \approx 16$  and:

$$A_{ij} \approx \frac{75k_B T}{\rho}$$

Density in DPD simulations often set to 3: gives commonly-used conservative force parameter of 25

# How to parameterise DPD

- Conservative force parameters
  - Unlike species interactions can affect e.g. hydrophobicity
  - Can connect conservative force parameter to Flory-Huggins solution theory [1] (assuming  $A_{ij}^{AA} = A_{ij}^{BB}$ ):

Represents energy of mixing

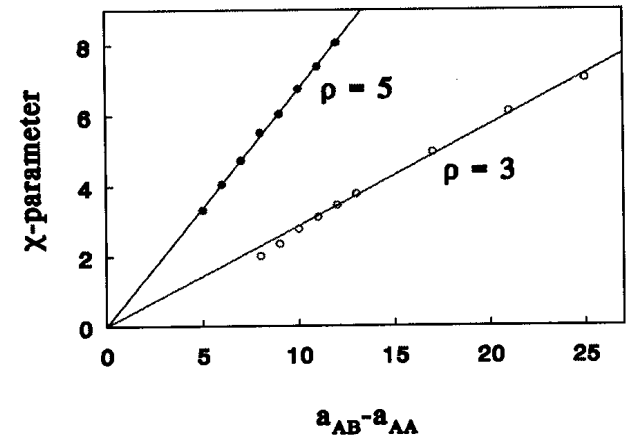
$$\chi_{AB} \propto (A_{ij}^{AB} - A_{ij}^{AA})$$

- Density-dependent relationships can be determined from simulations, e.g. for  $\rho = 3$ :

$$\chi_{AB} \approx 0.286(A_{ij}^{AB} - A_{ij}^{AA})$$

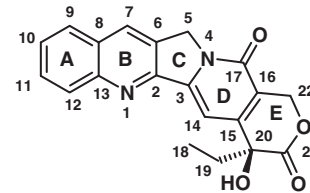
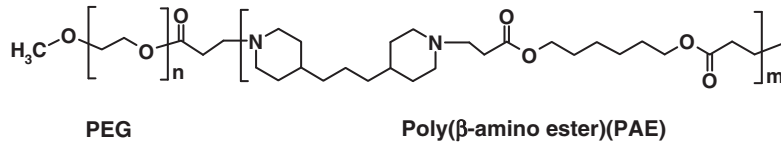
$$A_{ij}^{AB} \approx A_{ij}^{AA} + 3.50\chi_{AB}$$

If  $\chi$ -parameters are available, can use them to find DPD conservative force parameters



# Example: drug loading/release<sup>[1]</sup>

- Copolymer PAE-PEG with water and camptothecin (CPT)



Camptothecin (CPT)

- Conservative force parameterisation

- Can estimate Flory-Huggins  $\chi$ -parameters by calculating energies of mixing:

$$\chi_{AB} = \frac{\Delta E^{mix} V_{ref}}{RT \phi_A \phi_B V}$$

$$\Delta E^{mix} = E_{AB} - (E_A + E_B)$$

- Mixing energies calculated from classical MD simulations (NPT ensembles) of pure and mixed components with COMPASS force field

[1] Luo and Jiang, *J Control Release* **162**, 185–193 (2012)

# Example: drug loading/release

- Two sets of conservative force parameters  $A_{ij}$

	H <sub>2</sub> O	CPT	PEG	PAE
H <sub>2</sub> O	25.00	48.22	26.05	125.23
CPT		25.00	22.28	22.49
PEG			25.00	46.81
PAE				25.00

Drug loading: pH  $\approx$  7.4

Can bond PAE and PEG beads together to form copolymers (e.g. 28 PAE beads and 10 PEG beads represent PAE<sub>12580</sub>-PEG<sub>4850</sub>)

	H <sub>2</sub> O	CPT	PEG	PAE
H <sub>2</sub> O	25.00	48.22	26.05	19.10
CPT		25.00	22.28	82.04
PEG			25.00	23.63
PAE				25.00

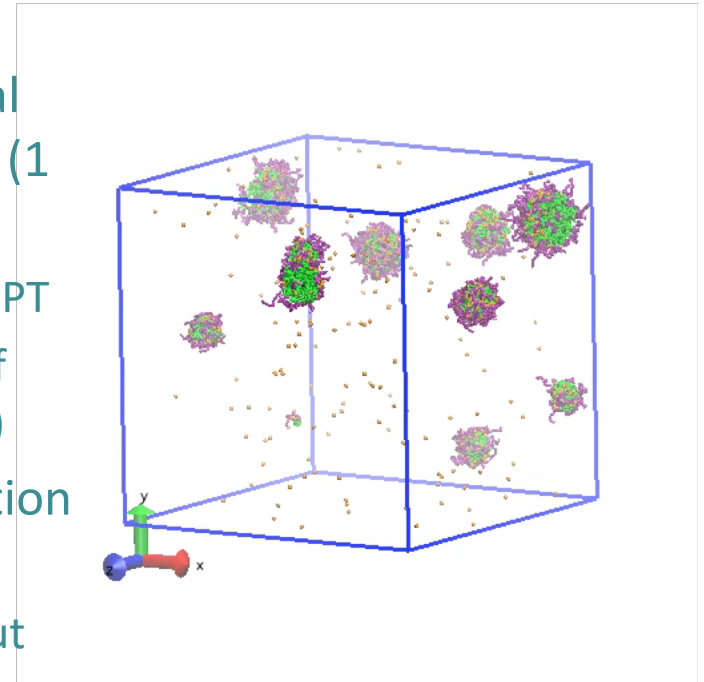
Drug release: pH  $\approx$  6.4

PAE replaced with hydrated form: note changes to hydrophobicity between PAE and water/CPT/PEG



# Example: drug loading/release

- DPD simulations with DL\_MESO
  - Ran drug loading simulation from initial randomly distributed state over 900ns (1 million timesteps)
    - PAE-PEG form vesicles encapsulating CPT
    - Took approx. four hours on 96 cores of Hartree Centre machine (BlueWonder)
  - Last timeframe of drug loading simulation used as initial state for drug release
    - Vesicles swell, break open and push out CPT due to drop in pH
  - Drug release simulation ran for 90ns
  - Loading efficiency closely matches experimental observation



Simulation courtesy: Nidhi Raj

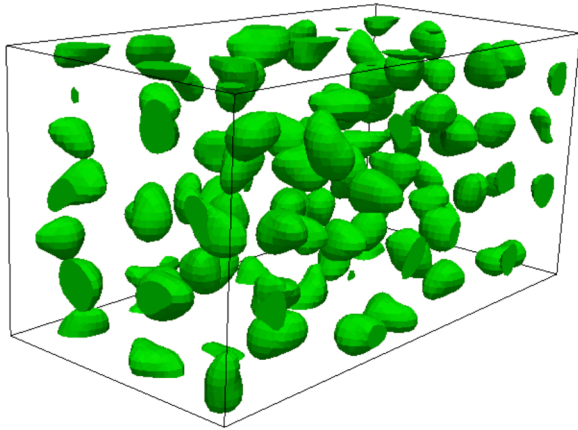
# Phase determination in DPD

- Simplest (slowest) method: visualise and take a look!
- Automatic phase detection, e.g.
  - Calculate order parameters for system, e.g. second moment of isosurface normal distribution [1]:
$$\mathbf{M} = \int \mathbf{nn} p(\mathbf{n}) d\mathbf{n}$$
  - Normalised eigenvalues of symmetric tensor  $(\mu_1, \mu_2, \mu_3)$  give indication of shapes for particle structures, e.g. spheres, tubes, flat sheets

[1] Prinsen *et al.*, *Phys Rev Lett*, **89** (14), 148302 (2002)

# Phase determination in DPD

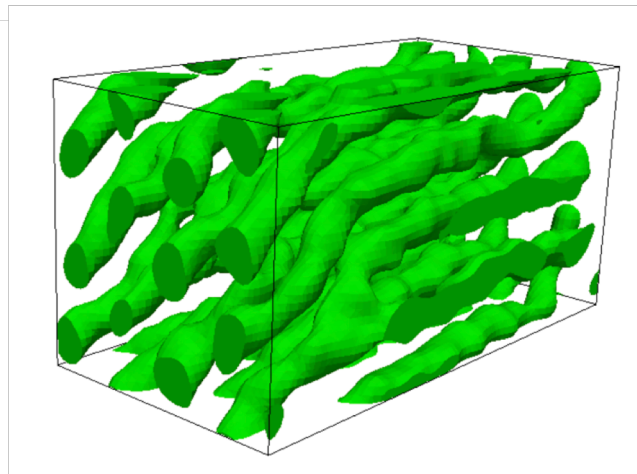
- Example: solutions of dimer amphiphilic surfactant [1]
  - Two-bead molecules: one hydrophilic, one hydrophobic
  - Hydrophobic phases used for isosurface plots



30 vol%

isotropic phase

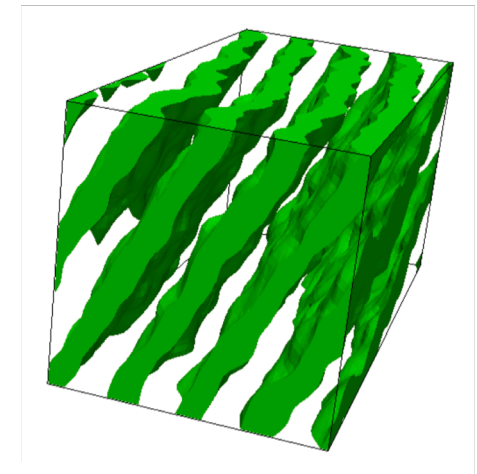
$$\mu_1 \approx \mu_2 \approx \mu_3 \approx \frac{1}{3}$$



55 vol%

hexagonal phase

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



75 vol%

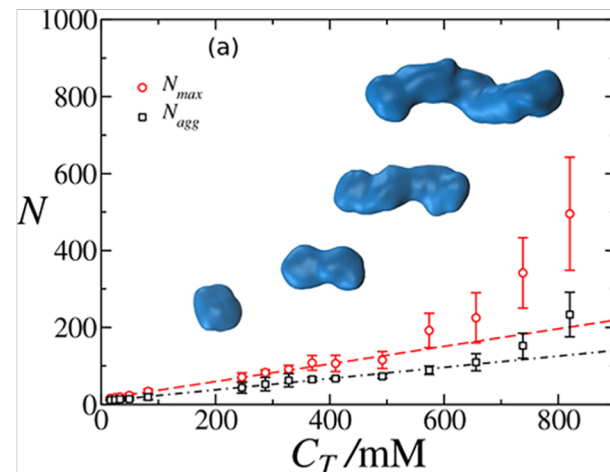
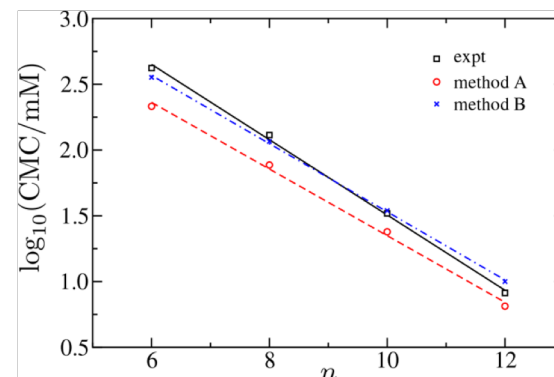
lamellar phase

$$\mu_1 < 0.05, \mu_2 < 0.15$$

[1] Prinsen *et al.*, *Phys Rev Lett*, **89** (14), 148302 (2002)

# Example: micelle properties

- DPD simulations of alkyl sulphate surfactants (6–12 carbon atoms) [1]
  - Protocols to find CMCs from particle simulations [2]
  - DPD parameterisation using water-octanol partition coefficients [3]
  - Bond and angle potentials
  - Gaussian smeared charges for sodium ( $\text{Na}^+$ ) and sulphate ( $\text{CH}_2\text{OSO}_3^-$ ) beads
- Obtained close quantitative fit for CMCs to experiment, observed sphere-to-rod transition for SDS



[1] Anderson *et al.*, *J Chem Theory Comput*, **14** (5), 2633–2643 (2018)

[2] Johnston *et al.*, *J Phys Chem B*, **120** (26), 6337–6351 (2016)

[3] Anderson *et al.*, *J Chem Phys*, **147** (9), 094503 (2017)

# Rheological properties of DPD

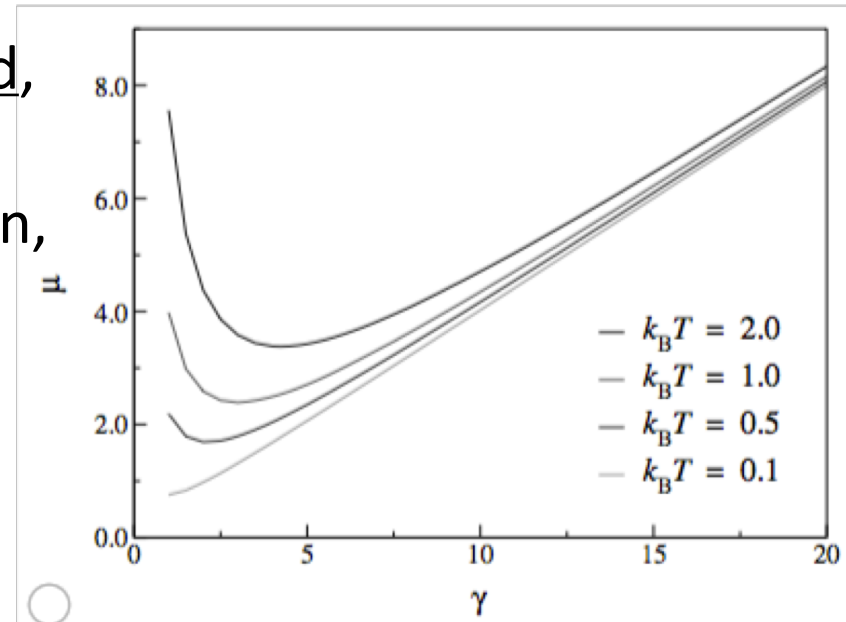
- If no conservative forces applied, kinematic viscosity depends on random force weighting function,
  - e.g. if

$$w^R(r_{ij}) = \begin{cases} 1 - \frac{r_{ij}}{r_c}, & r_{ij} < r_c \\ 0, & r_{ij} \geq r_c \end{cases}$$

- viscosity and diffusivity are [1,2]:

$$\mu \approx \frac{45k_B T}{4\pi\gamma r_c^3} + \frac{2\pi\gamma\rho^2 r_c^5}{1575}$$

$$D \approx \frac{45k_B T}{2\pi\gamma\rho r_c^3}$$

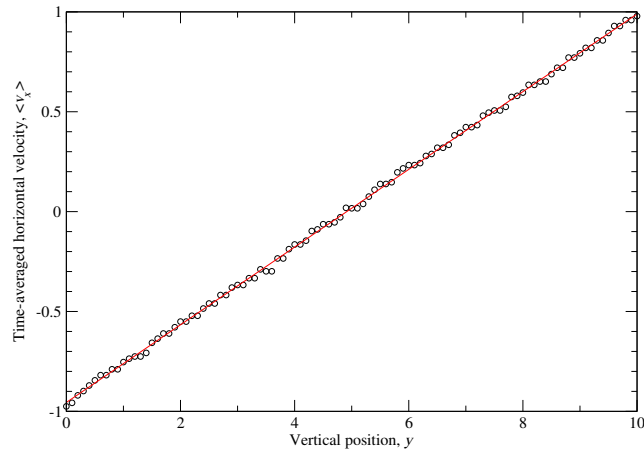


Schmidt number  $\frac{\nu}{D} = \frac{\mu}{\rho D}$  of order 1: a bit low for liquids? (May need alternative pairwise thermostat, e.g. Lowe-Andersen)

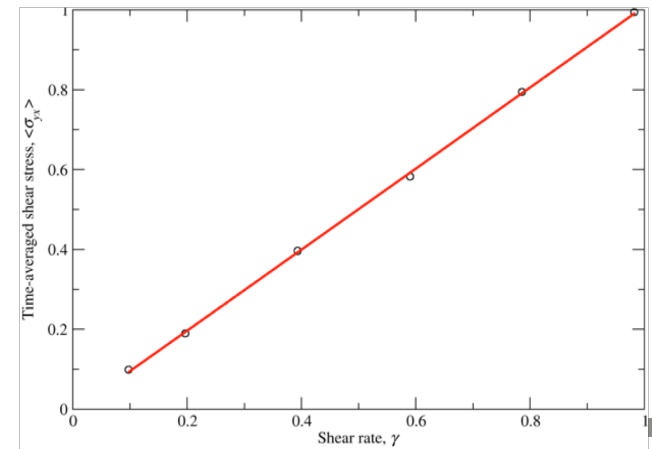
[1] Marsh *et al.*, *Phys Rev E*, **56** (2), 1676–1691 (1997)  
 [2] Visser *et al.*, *J Comput Phys* **214** (2), 491–504 (2006)

# Rheological properties of DPD

- Lees-Edwards boundaries
  - Used to obtain linearly shearing flows: can set different constant velocity gradients (shear rates)
  - Measure shear stresses in simulation box
  - Relationship between shear stress and shear rate gives dynamic viscosity (divide by density to give kinematic viscosity)



Linear velocity profile of simple fluid



Stress vs. shear rate plot for simple fluid: constant dynamic viscosity  $\mu$  of  $\sim 1.0145$

# Summary: Advantages of DPD

- Momentum-conserving thermostat: correct fluid hydrodynamics guaranteed
- Soft potentials allow larger time steps than classical MD: equilibrium reached more quickly
  - Generally short-range cutoffs: easier to parallelise
- Comparatively few particles needed to represent large chemical species
  - Can also preserve general structures with localised interactions
- Parameterisations available to represent basic chemical effects (e.g. hydrophobicity)

# Lattice Boltzmann Equation

- Based on statistical mechanics: probabilities of finding particles
  - Define distribution function  $f$ : sums of various moments give fluid density, momentum etc.
  - Evolution of distribution function given by Boltzmann equation: split into propagation and collisions

$$\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla f = C_{12}$$

Two-body uncorrelated collisions

- Plenty of mathematics links the (mesoscopic) Boltzmann equation to the (continuum) Navier-Stokes equations for fluid flows
  - No direct connection necessary between rarefied gas particles modelled by Boltzmann equation and a real fluid, but can consider particles like collections of molecules



# Lattice Boltzmann Equation

- Apply Boltzmann equation to regular grid
  - Distribution function  $f_i$  definable for each lattice link  $i$ 
    - Discretising both time  $\Delta t$  and space  $\Delta x$
  - Particle movement restricted to lattice links  $\mathbf{e}_i$  joining grid points (usually nearest neighbours)
  - Can represent evolution as separate collision and propagation stages:
    - Collision:  $f_i(\mathbf{x}, t^+) = f_i(\mathbf{x}, t) + C_i$
    - Propagation:  $f_i(\mathbf{x} + \mathbf{e}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t^+)$
  - Macroscopic fluid properties:

$$\rho(\mathbf{x}, t) = \sum_i f_i(\mathbf{x}, t), \rho(\mathbf{x}, t)\mathbf{u}(\mathbf{x}, t) = \sum_i f_i(\mathbf{x}, t)\mathbf{e}_i$$

Local nature of grid-based collisions (and near-local propagation) make LBE easily parallelisable with domain decomposition: tends to scale very well with number of processor cores

# Lattice Boltzmann Equation

- Collisions can be defined based on deviation from local equilibrium (function of fluid density and velocity):

$$f_i^{eq}(\rho, \mathbf{u}) = \rho w_i \left[ 1 + 3(\mathbf{e}_i \cdot \mathbf{u}) + \frac{9}{2}(\mathbf{e}_i \cdot \mathbf{u})^2 - \frac{3}{2}u^2 \right]$$

- Simplest form uses a single relaxation time (Bhatnagar-Gross-Krook: BGK scheme)

$$C_i = - \frac{f_i(\mathbf{x}, t) - f_i^{eq}(\rho(\mathbf{x}, t), \mathbf{u}(\mathbf{x}, t))}{\tau}$$

Numerical representation of particles colliding together at grid points: still makes physical/chemical sense

- Relaxation time  $\tau$  related to kinematic viscosity of fluid:

$$\nu = \frac{1}{3} \left( \tau - \frac{1}{2} \right) \frac{\Delta x^2}{\Delta t}$$

# DL\_MESO\_LBE

- DL\_MESO's LBE code
  - Models particles moving on two- or three-dimensional grids
  - Various collision operators, mesoscopic interactions and boundary conditions (including stationary solid objects)
  - Can couple solute diffusion and heat transfer to fluid flows
- Uses text files as inputs:
  - `lbin.sys`, `lbin.spa`, (optional) `lbin.init`
- DL\_MESO includes utilities to initialise LBE simulations and gather results for visualisation and analysis (in Paraview)

# DL\_MESO\_LBE: Input files

```
space_dimension      2
discrete_speed       9
number_of_fluid      2
number_of_solute     0
temperature_scalar   0
phase_field          0
grid_number_x      150
grid_number_y      50
grid_number_z      1
domain_boundary_width 1
incompressible_fluids 0
collision_type        BGKGuo
interaction_type      Lishchuk
output_format         VTK
total_step            400000
equilibration_step   5000
save_span             500
noise_intensity       0.0
sound_speed           540.0
kinetic_viscosity     0.001
relaxation_fluid_0    1.0
relaxation_fluid_1    1.0
bulk_relaxation_fluid_0 1.0
bulk_relaxation_fluid_1 1.0
interaction_0         0.0
interaction_1         0.0034
interaction_2         0.0034
interaction_3         0.0
segregation           1.4
```

lbin.sys (left):  
simulation properties;  
note keywords in bold  
are mandatory, but  
order is not!

lbin.spa (right):  
boundary conditions  
at specified grid points  
(represented by  
numerical codes);  
constructing this file is  
easiest using  
DL\_MESO GUI

```
131 49 0 149
132 49 0 149
133 49 0 149
134 49 0 149
135 49 0 149
136 49 0 149
137 49 0 149
138 49 0 149
139 49 0 149
140 49 0 149
141 49 0 149
142 49 0 149
143 49 0 149
144 49 0 149
145 49 0 149
146 49 0 149
147 49 0 149
0 49 0 149
149 49 0 149
1 0 0 13
148 0 0 13
2 0 0 13
3 0 0 13
4 0 0 13
5 0 0 13
6 0 0 13
7 0 0 13
8 0 0 13
```

# LBE units

- Based on lattice grid used for simulations
- Lattice spacing  $\Delta x$  and time step  $\Delta t$  can be related to 'real world' properties, i.e.

- Speed of sound: 
$$c_s = \frac{1}{\sqrt{3}} \frac{\Delta x}{\Delta t}$$

- Kinematic viscosity: 
$$\nu = \frac{1}{3} \left( \tau - \frac{1}{2} \right) \frac{\Delta x^2}{\Delta t}$$

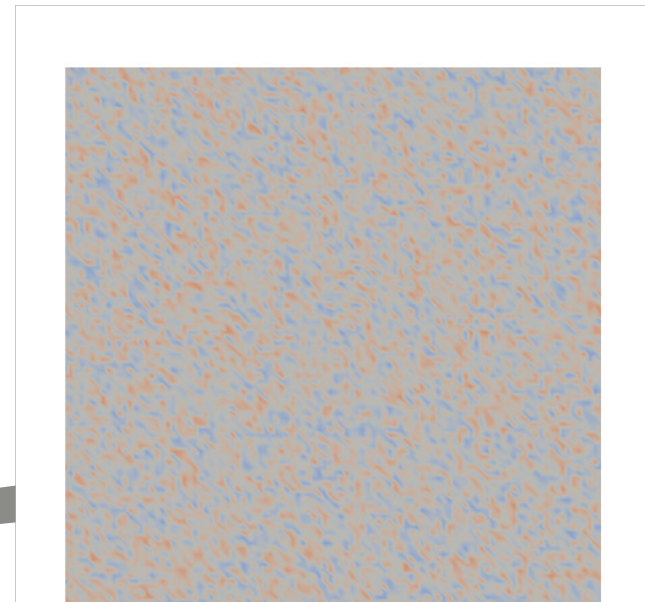
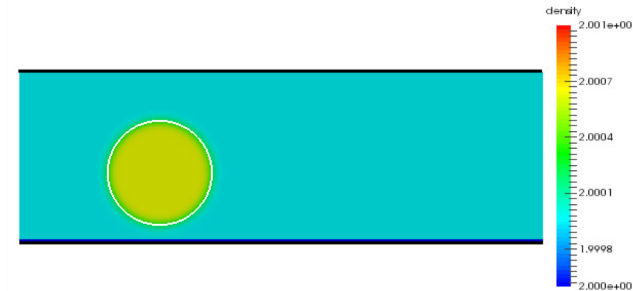
- Pressure and density related to equation of state, which by default (without mesoscopic interactions) is:

$$p = \rho c_s^2$$

- Density is a comparatively free parameter: usually set to around 1 to maximise available calculation precision

# Multiple fluids/phases

- Collision operator can include application of forces
  - Constant (body) forces
  - Interfacial forces between phases or multiple fluids
- Interfaces between fluids emerge: no need to explicitly track them
- Several methods available based on required phenomena:
  - Macroscopic interfacial tension [1]
  - Pseudopotentials (functions of density) [2]
  - Free-energy functionals [3]



[1] Halliday *et al.*, *Phys Rev E*, **73**, 056708 (2006)

[2] Shan and Chen, *Phys Rev E*, **47**, 1815–1819 (1993)

[3] Swift *et al.*, *Phys Rev Lett*, **75** (5), 830–833 (1995)

# Multiple fluids/phases

- Example: Shan/Chen pseudopotential approach

- Interaction force based on spatial gradients of pseudopotentials:

$$\mathbf{F}^a = -c_s^2 \psi_a \sum_b g_{ab} \nabla \psi_b = -\psi_a \sum_b g_{ab} \sum_i w_i \psi_b(\mathbf{x} + \mathbf{e}_i \Delta t) \mathbf{e}_i$$

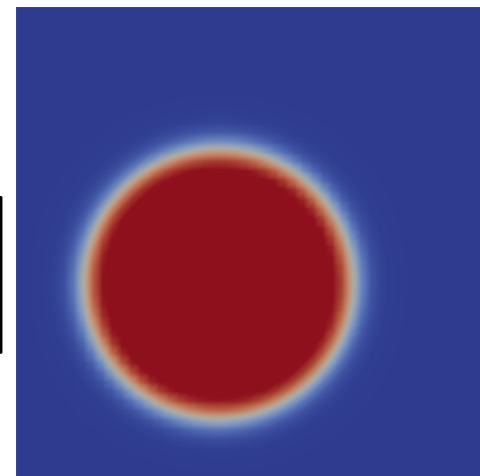
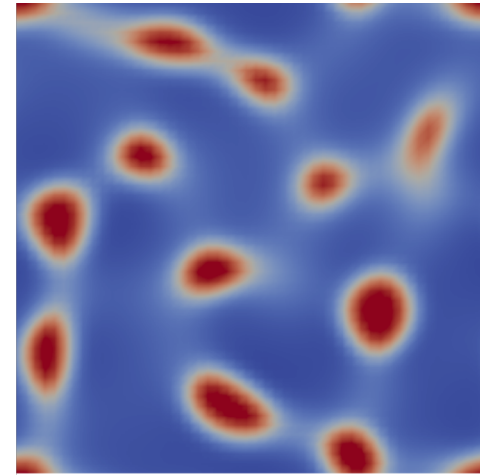
- Can apply for single fluid, separates spontaneously into liquid and vapour phases below critical point
- Gives particular one-fluid equation of state:

$$p = \rho c_s^2 + \frac{1}{2} g c_s^2 \psi^2$$

- Can rearrange equation above to give required pseudopotential for desired equation of state [1]:

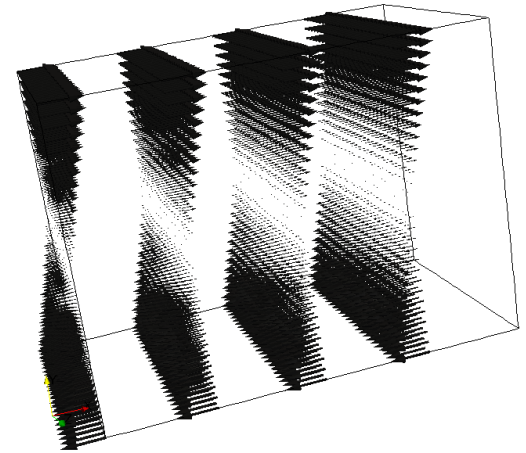
$$\psi = \sqrt{\frac{2(p(\rho, T) - \rho c_s^2)}{g c_s^2}}$$

Set  $g = \pm 1$  to ensure square root taken on positive value



# Boundary conditions

- LBE boundary conditions can be simple and intuitive
  - Bounce-back: no-slip boundary
  - Simple and computationally cheap to apply for both planar boundaries and more complicated geometries
- Schemes available to apply constant density/velocity accurately:
  - Zou/He (non-equilibrium BB) [1]
  - Inamuro [2]
  - Regularised boundaries [3]



[1] Zou and He, *Phys Fluids*, **9** (6), 1591–1598 (1997)

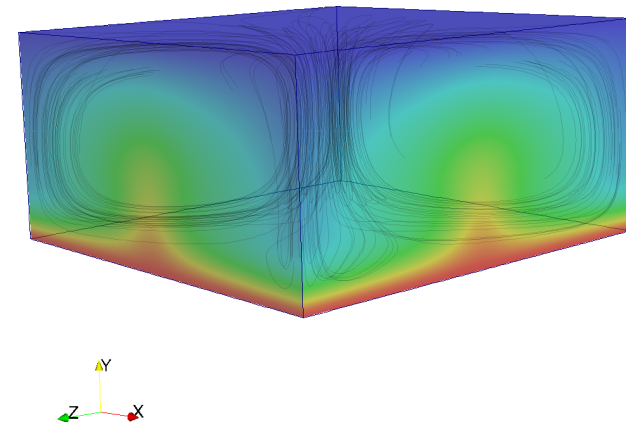
[2] Inamuro *et al.*, *Phys Fluids*, **7** (12), 2928–2930 (1995)

[3] Latt *et al.*, *Phys Rev E*, **77** (5), 056703 (2008)



# Diffusion and heat

- Simplification of local equilibrium distribution function gives diffusive (viscosity-dominated) flows [1]
  - Can be used to model solute diffusion and/or temperature fields coupled to bulk fluid(s)
  - Relaxation times represent diffusivities in similar way to kinematic viscosity
- Heat transfer boosted by convection
  - Either set equation of state or use additional force that depends on fluid temperature (e.g. Boussinesq approximation)



[1] Inamuro *et al.*, *J Comput Phys*, **179** (1), 201–215 (2002)

# Non-Newtonian rheologies

- Non-Newtonian fluids have non-constant viscosities, usually a function of shear rate  $\dot{\gamma}$ , e.g.

- Power law fluid:  $\mu = k\dot{\gamma}^{n-1}$

- Can set LBE relaxation time based on local viscosity:

$$\tau(\mathbf{x}, t) = \frac{3\mu(\mathbf{x}, t)\Delta t}{\rho\Delta x^2} + \frac{1}{2}$$

- How to calculate shear rate?

Stress tensor:

$$\dot{\gamma} = \sqrt{\sum_{\alpha,\beta} \left( \frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} \right)^2}$$

Momentum-flux tensor:

$$\dot{\gamma} = \sqrt{\frac{\sum_{\alpha,\beta} \sum_i e_{i,\alpha}^2 e_{i,\beta}^2 (f_i - f_i^{eq})^2}{\rho c_s^2 \tau \sqrt{2}}}$$

Based solely on local values for given grid point, but implicit in relaxation time

# How to parameterise LBE

- Use relationships for speed of sound and kinematic viscosity:

$$c_s = \frac{1}{\sqrt{3}} \frac{\Delta x}{\Delta t}$$
$$\nu = \frac{\mu}{\rho} = \frac{1}{3} \left( \tau - \frac{1}{2} \right) \frac{\Delta x^2}{\Delta t}$$

Can set relaxation time  $\tau$  to ensure numerical stability, i.e. not too close to 0.5

- Local equilibrium distribution function generally an approximation for low Mach numbers:

$$\text{Ma} = \frac{u}{c_s} \leq 0.15$$

- Dimensionless numbers useful to represent flows, e.g. Reynolds number:

$$\text{Re} = \frac{uL}{\nu}$$

Flow characteristics independent of absolute values for fluid velocity, viscosity and system length scale: systems with equal Reynolds numbers will behave in the same way.

# Phase determination in LBE

- Output from DL\_MESO\_LBE includes fluid densities at each grid point:

- Can define phase index, e.g.

$$\phi_{ab} = \frac{\rho_a - \rho_b}{\rho_a + \rho_b}$$

- Value of  $\phi_{ab}$  will be positive if rich in fluid/phase  $a$  (+1 if pure  $a$ ), negative if rich in fluid/phase  $b$  (-1 if pure  $b$ )
- Boundary between fluid/phases usually diffuse in multiple-fluid/phase LBE simulations, but can use phase index to define boundary region

# Summary: Advantages of LBE

- Statistical mechanics basis gives correct fluid behaviour: rheology automatically part of model
- Grid-based calculations run efficiently on massively parallel computers
- Intuitive models for interactions between particles (collections of molecules)
  - Collisions, mesoscopic interactions
- Multi-fluid/phase flows, complex geometries, coupled mass/heat transfer and non-Newtonian rheologies comparatively straightforward to apply

# Practical exercises

- Six available for this workshop (three DPD, three LBE)
  - Range of simulations using DL\_MESO's codes
  - Vary in terms of difficulty and computing requirements: can all use laptops/desktop, but multiple cores/threads will help
  - Representative of main functionalities in DL\_MESO and what DPD and LBE can do
  - The exercises and presentation available from DL\_MESO website:

[www.ccp5.ac.uk/DL\\_MESO](http://www.ccp5.ac.uk/DL_MESO)