DynamO Workshop

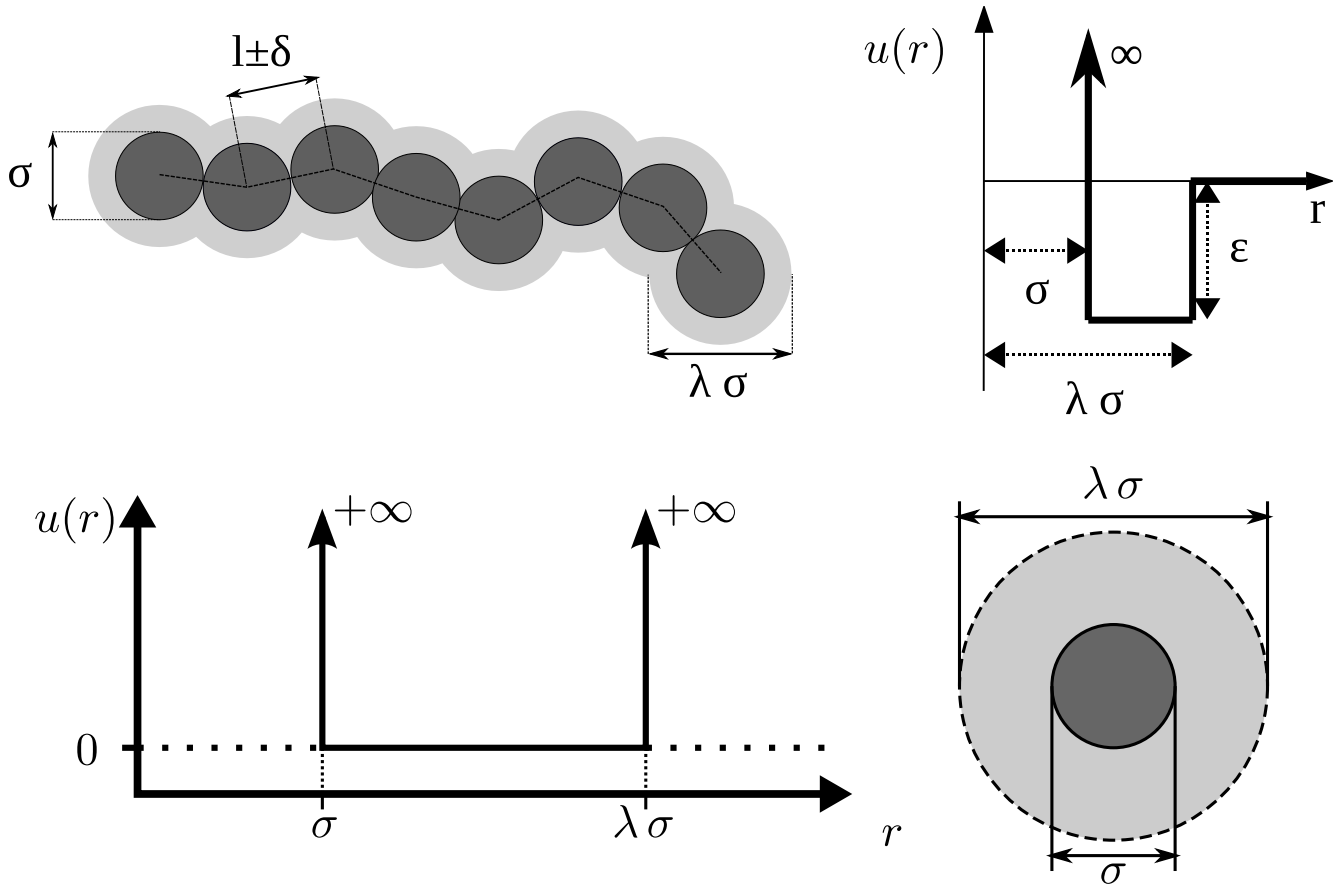
Molecular models

Dr Marcus N. Bannerman & Dr Leo Lue

m.campbellbannerman@abdn.ac.uk leo.lue@strath.ac.uk

Section Outline

Modeling molecules



- Bonds are enforced through an infinitely deep square-well potential.
- Currently within DynamO, there is built-in support for linear chains and rings.

Configuration file

dynamod command:

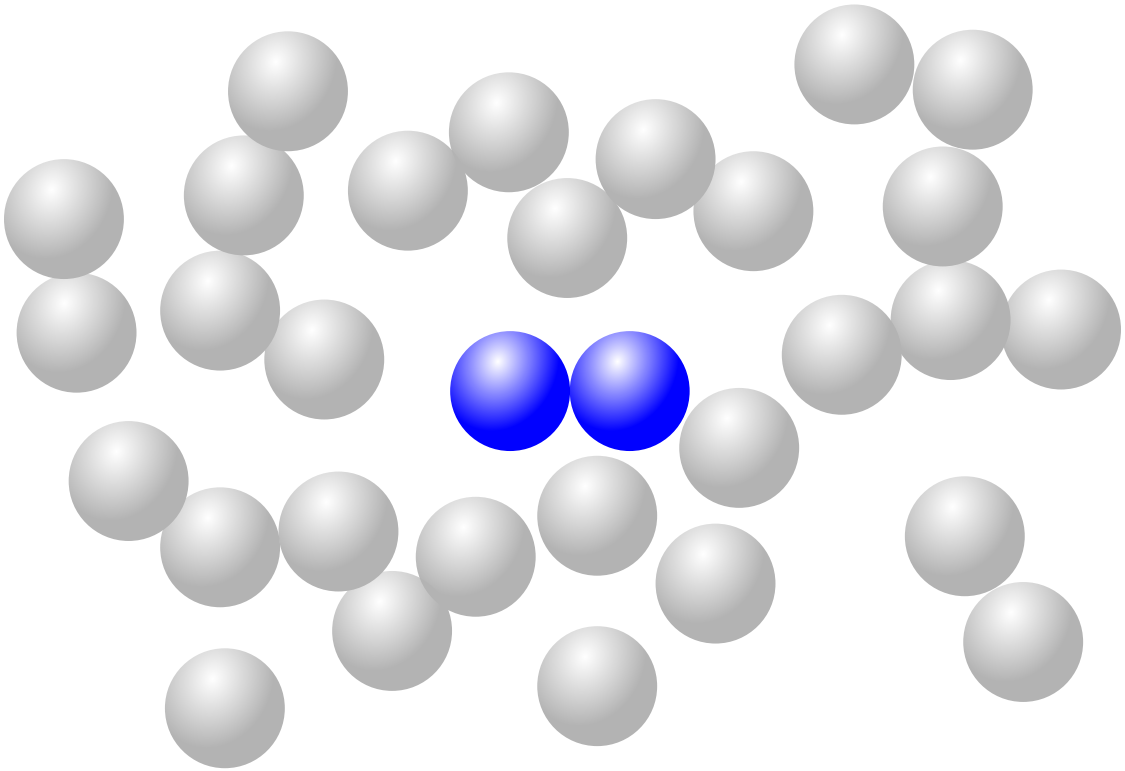
```
dynamod --packing-mode 2 --i1 50
```

configuration file:

```
...
<Interactions>
<Interaction Type="SquareBond" Diameter="0.90000000000000013"
  Lambda="1.2222222222222223"
  Name="Bonds" Elasticity="1">
    <IDPairRange Type="Chains"
      Start="0" End="15" Interval="16"/>
</Interaction>
...
</Interactions>
...
```

Section Outline

Thermodynamic perturbation theory



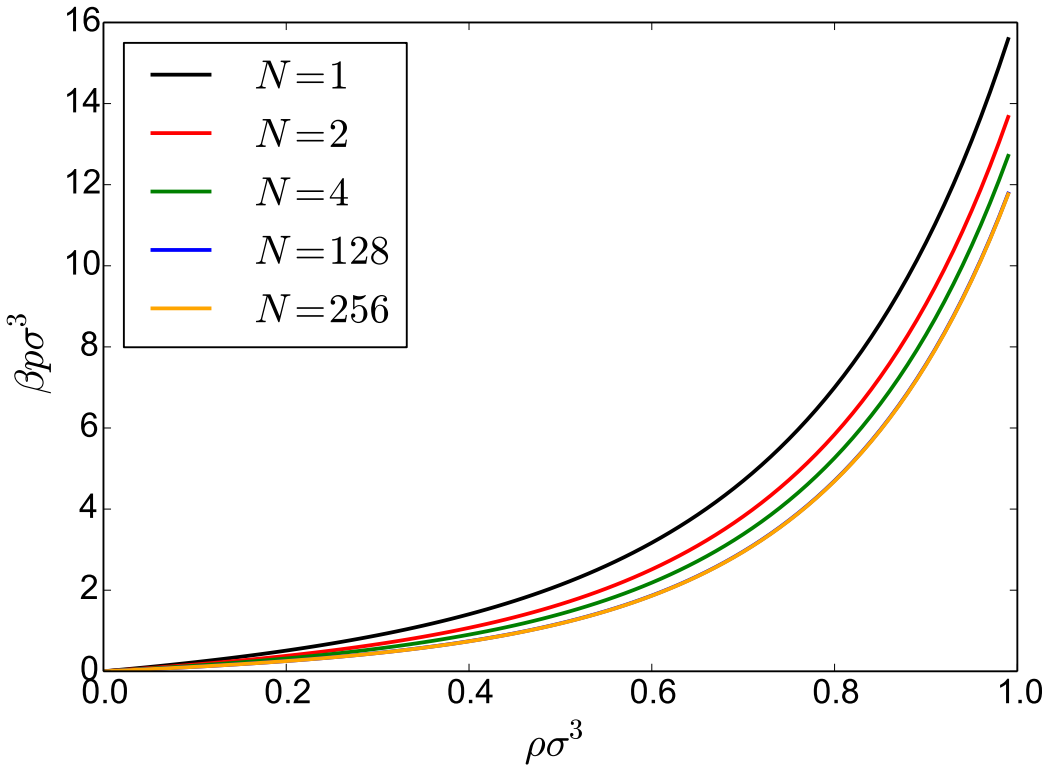
Free energy of a system of molecules:

$$F^{\mathrm{res}}(c_p, \beta, V, N) = F^{\mathrm{res}}_{\mathrm{ref}}(Nc_p, \beta, V) + F^{\mathrm{bond}}$$

$$F^{\mathrm{bond}}(c_p, \beta, V, N) \approx -N_p N_{\mathrm{bonds}} k_B T \ln y_{\mathrm{ref}}(l; Nc_p, \beta)$$

where N_{bond} is the number of bonds per molecule.

Thermodynamic perturbation theory



$$Z = \beta p / c_p = N + N Z_{\mathrm{ref}} - (N-1)\left[1 + \rho \frac{\partial \ln y_{\mathrm{ref}}}{\partial \rho}\right]$$

Section Outline

Modeling molecules

Thermodynamic perturbation theory

Building a multi-molecule configuration

Building multi-molecule configuration file

Create a single chain configuration:

```
dynamod --pack-mode 2 --i1 16 --f1 1 --thermostat 100
```

Arrange the configuration in a low density lattice:

```
dynamod --pack-mode 3 --density 0.001 \
--i1 0 --xcell 3 --ycell 3 --zcell 3  \
--s1 config.out.xml.bz2
```

Fix bonding constraints

Change bonding entry from

```
...
<Interaction Type="SquareBond" Diameter="0.8999999999999991"
  Lambda="1.222222222222223" Name="Bonds" Elasticity="1">
  <IDPairRange Type="Chains"
    Start="0" End="15" Interval="16"/>
</Interaction>
...
```

to

```
...
<Interaction Type="SquareBond" Diameter="0.8999999999999991"
  Lambda="1.222222222222223" Name="Bonds" Elasticity="1">
  <IDPairRange Type="Chains"
    Start="0" End="1727" Interval="16"/>
</Interaction>
...
```

Eliminate CaptureMap tag

```
...
<Interaction Type="SquareWell" Diameter="1" Elasticity="1"
  Lambda="1.5" WellDepth="1" Name="Bulk">
    <IDPairRange Type="All"/>
    <CaptureMap>
      <Pair ID1="1" ID2="3" val="1"/>
      <Pair ID1="2" ID2="4" val="1"/>
      <Pair ID1="9" ID2="11" val="1"/>
      ...
    </CaptureMap>
</Interaction>
...
```

Compress the configuration

Compress the configuration to the desired density

```
dynarun --engine 3 --growth-rate 1 --target-density 0.1 \
  config.out.xml.bz2
```

Zero momentum and rescale velocities

```
dynamod --zero-momentum --rescale-T 100 -o config.out.xml.bz2 \
config.out.xml.bz2
```

Run simulation

```
dynarun --engine 1 -c 1000000 config.out.xml.bz2
```