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Coarse-grain Polymer Simulations

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PHY-5320

Introduction to Macromolecules

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Friday

Hands-on workshop for ESPResSo

ESPResSo is not available on windows

- Intro to Unix command-line
- Intro to Python (Espresso 3)
- Intro to TCL (Espresso 2)
- Intro to HOOMD(?)
- Intro to VMD (visual molecular dynamics)
- Example Walkthrough

Server access

http://www.ks.uiuc.edu/Training/Tutorials/Reference/unixprimer.html

Server address: 137.122.32.210

username: user_ID (user_ID)@uottawa.ca

password: user_ID (all in CAPS)

example: `ssh dsean092@137.122.32.210`
`DSEAN092`

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Change your password!

execute the command “passwd”

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verify installation

execute the command “Espresso” (V3)

execute the command “pypresso” (V2)

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Get files

https://github.com/davidsean/Macromolecules.git

```
git clone https://github.com/davidsean/Macromolecules.git
```

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VTF file format

https://github.com/olenz/vtfplugin/wiki/VTF-format

Header: **V**TF **S**tructure **F**ormat (VSF) Define particles

Body: **V**TF **C**oordinate **F**ormat (VCF) particle coordinates for all timesteps

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Header (VSF)

Custom:

```
unitcell 49.99 49.99 49.99
atom 0:599 radius 1 name gel type 3
atom 600:639 radius 1 name ds type 1
atom 640:649 radius 1 name ss type 0
```

```
bond 600::639
bond 690:600
```

Automatic: `writevsf` (Look at User's Guide)

Coordinates (VCF)

Custom:

```
timestep indexed
0 0.0 2.0 2.0
1 50.0 2.0 2.0
2 0.0 2.0 7.0
3 50.0 2.0 7.0
...
```

Automatic: `writevcf` (Look at User's Guide)

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Two files or one?

Separate VSF & VCF for easier analysis

Single VTF is more convenient for loading in VMD

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Limitations

-All particles must be visible (VMD limitation)

-Constant radius, color, etc.. (VMD limitation)

-No dynamic bonds (VMD dynamic bond option)

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Exploit the Limitations!

Only draw the system on the **first** timestep.

Need **custom** VTF write function

Write to disk is slow, this can speed up the sims.

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Custom Colors/Materials

Need **custom** VSF write function

Uniform visuals

Save time

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Constraints

Special “particle types” (mathematical surfaces)

A few geometries to choose from: Cylinder, Plane, Sphere, Maze, Rod, *etc*

No drawing functions are defined!

Have to trust the system, no visual check

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Test this out Now

Look at `DNA.vtf`

Notice the first timestep

Open in VMD

Change all to CPK

(Graphics... Representation... Drawing Method...

Change colors by name, type, color ID

Change a single particle representation to VDW

(create representation... select index 3...

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ESPResSo

User's guide

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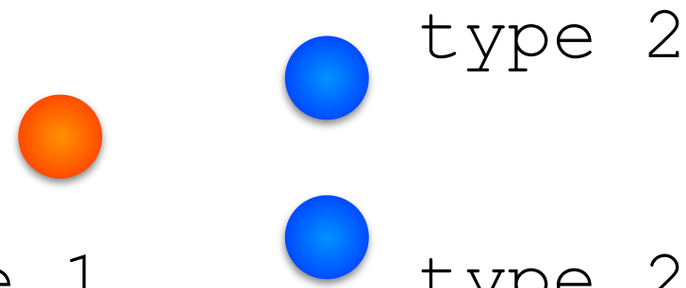
ESPResSo

System parameters, don't modify these

```
thermostat langevin $kBT $gamma
setmd skin 0.4
integrate set nvt
setmd time_step $time_step
```

Non-bonded interactions

$$U_{\mathrm{LJ}}(r) = \begin{cases} 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] + \epsilon & \text{for } r < r_{\mathrm{c}} \\ 0 & \text{for } r \geq r_{\mathrm{c}} \end{cases}$$



inter type_i type_j lennard-jones epsilon sigma r_cut 0.25 0.0

ex.

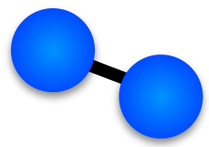
```
inter 1 2 lennard-jones 1.0 1.0 1.2 0.25 0.0
inter 1 1 lennard-jones 1.0 1.0 1.2 0.25 0.0
```

Bonded interactions

$$U_{\mathrm{FENE}}(r) = -\frac{1}{2}\, k_{\mathrm{FENE}}\, {r_0}^2 \ln\left[1 - \frac{r^2}{{r_0}^2}\right]$$

`bond type1`

`bond type 2`



inter bond_ID fene k r_max

ex.

```
inter 1 fene 10 5
inter 2 fene 42 1.5
```

Bonded interactions

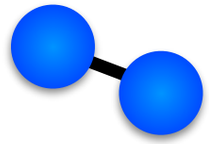
Need to define where the bonds are (individually)

bond type1

particle 2 particle 3

bond type 2

particle 29



particle 44

ONE particle holds the bond:

(don't need to define twice)

part i bond bond_type j

ex.

part 2 bond 1 3

part 29 bond 2 44

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Real Polymer

With excluded volume

LJ between everyone, FENE bond only with neighbours

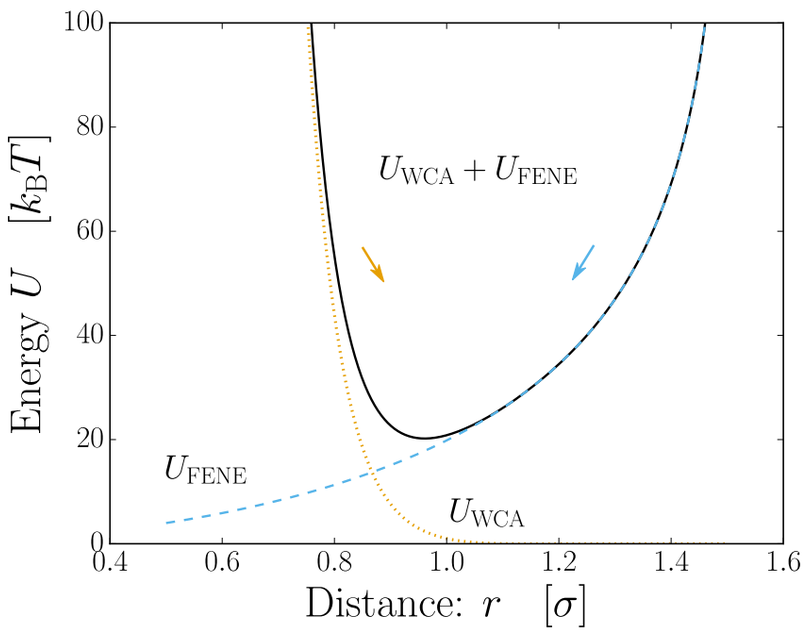
```
inter 1 1 lennard-jones 1.0 1.0 1.2 0.25 0.0

inter 1 fene 10 5
```

Ideal Polymer

No excluded volume

~~LJ between everyone~~, FENE bond only with neighbours

(FENE bond + LJ) only with neighbours



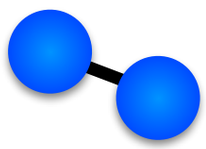
Tabulated this, and call it “Bond”

Do not define other interactions

Ideal Polymer

No excluded volume

```
bond type 2
particle 29
```

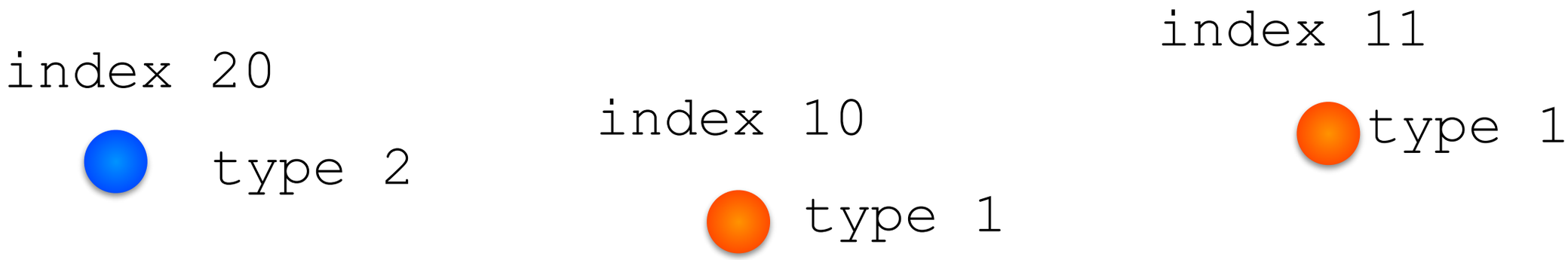


```
particle 44
```

inter bond_ID tabulated bond file_name

```
inter 2 tabulated bond "tabulated_KG.txt"

part 29 bond 2 44
```

Place a particle



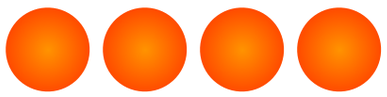
part index pos x y z type type

```
part 20 pos 1.2 2.3 0.2 type 2
part 10 pos 0.9 4.3 0.2 type 1
part 11 pos 1.2 6.3 0.2 type 1
```

2-ways to init a Polymer

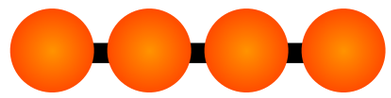
(manual or automatic)

1) Init as a line



```
for {set p 0} {$p<$n_mono} {incr p} {
 part $p pos [expr $p] 2.3 1.2 type 1
}
```

+ manually define FENE bonds between neighbours



```
for {set p 1} {$p<$n_mono} {incr p} {
 part $p bond $bondID_fene [expr $p-1]
}
```

2) Or use ESPResSo's built-in method

```
  polymer 1 $n_mono 1.0 start 0 pos 0.2 2.3 1.2 mode
PSAW bond $bond_ID
```

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Poke it!

fix a particle in space

```
part 2 fix 1 1 1
```

or just in the x-dimension

```
part 2 fix 1 0 0
```

add a constant external force

```
part 2 ext_force 0.1 0.0 0.0
```

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Try this now

open polymer.tcl

Simulate an IDEAL polymer

Simulate a REAL polymer

Try a straight-line init

Try a “random”-ish init

Try two polymers?

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Try this now

open polymer.tcl

Simulate an IDEAL polymer

Simulate a REAL polymer

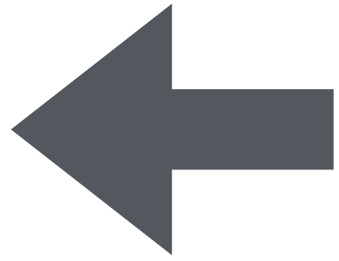
A straight-line init

A “random”-ish init

Try two polymers?

Place a force on an end

Fix certain monomer in space



Try a few combinations of these ideas