

■ Hydro MS Example 3: Vary nucleosome placements on template: 1.75 turns

Here are the calculations for the examples given in my paper for a chromatin saturation process. A trimer of positioning sites is envisioned, and the frictional properties of all possible species are calculated. Since when I did these I hadn't yet reactivated the sedimentation coefficient subroutine, I calculate all the sedimentation coefficients all at the end.

First clear the randomizing orientation matrix so that all of the chain pictures will be aligned in the same coordinate system.

```
ClearAll[A0];
A0=IdentityMatrix[3];
```

Define the chain and the nucleosomes for this example. Default parameters include persistence length of 150 bp.

```
turns=1.75;
definebasepair;
definenuke;
definephysicalnuke;
chaininitialize;
wrapbp

n = 20 ; dl = 24.5119

146
```

Now define a couple of things to make the example easier to do. The DNA chain is of length template (bp), and there are nnukes nucleosomes on it. The nucleosomes begin and end the chain. The linker length in bp is calculated, and the "chain" defined. Remember that the chain of segments includes one segment for each free basepair (the linker) and one segment for each nucleosome.

```
ntemplate=624;          (* total length, bp *)

species={{1},{2},{3},{1,2},{1,3},{2,3},{1,2,3}};
nt[spots_]:=ntemplate - Length[spots] wrapbp + Length[spots];
Map[nt,species]

{479, 479, 479, 334, 334, 334, 189}

chain={ {479,{1}},
        {479,{209}},
        {479,{417}},
        {334,{1,64}},
        {334,{1,272}},
        {334,{209,272}},
        {189,{1,64,127}} };

persistence=150 e10;
definebasepair;

collective=True;
test=True;
progress=True;
MonteCarlo=False;

Do[ assembleelements[chain[[isp]]];
    makeAs[chain[[isp]]];
    doKirkwood[chain[[isp]]],
    {isp,Length[species]};

Chain of 479 segments,
with displacements at segments {1}
Stokes offset 3.00764 A at 50 bp
```

```

el0          3.4          A
persistence
length       510.         A
repeat0      10.4         bp/turn
repeat1      10.15        bp/turn
radius       44.916        A
turns        1.75         turns
pitch        -28.571       A/turn
Array of chain lengths (bp)
{0, 478}
Array of friction element positions (bp)
{1, 240}
Array of Stokes radii (A)
{56.8124, 163.022}
...doKirkwood...
i,j,rij:*1 2 645.816 corrected:610.422
Kirkwood results: {f free-draining,f1,s1}
          -7          -7
    4.21008 10    g  3.69942 10    g
    {-----, -----, s1}
          s          s

```

```

Chain of 479 segments,
with displacements at segments {209}
Stokes offset 3.00764 A at 50 bp
el0          3.4          A
persistence
length       510.         A
repeat0      10.4         bp/turn
repeat1      10.15        bp/turn
radius       44.916        A
turns        1.75         turns
pitch        -28.571       A/turn
Array of chain lengths (bp)
{208, 270}
Array of friction element positions (bp)
{104, 209, 344}
Array of Stokes radii (A)
{89.9682, 56.8124, 108.172}
...doKirkwood...
i,j,rij:*1 2 324.43 corrected:320.159
i,j,rij:*1 3 472.918 corrected:446.831
i,j,rij:*2 3 403.033 corrected:394.638
Kirkwood results: {f free-draining,f1,s1}
          -7          -7
    4.88263 10    g  3.44271 10    g
    {-----, -----, s1}
          s          s

```

```

Chain of 479 segments,
with displacements at segments {417}
Stokes offset 3.00764 A at 50 bp
el0          3.4          A
persistence
length       510.         A
repeat0      10.4         bp/turn
repeat1      10.15        bp/turn
radius       44.916        A
turns        1.75         turns
pitch        -28.571       A/turn
Array of chain lengths (bp)
{416, 62}
Array of friction element positions (bp)
{208, 417, 448}
Array of Stokes radii (A)
{147.483, 56.8124, 40.8859}
...doKirkwood...
i,j,rij:*1 2 580.183 corrected:554.514
i,j,rij:*1 3 558.29 corrected:527.493
i,j,rij:*2 3 114.667 corrected:114.52
Kirkwood results: {f free-draining,f1,s1}
          -7          -7
    4.69551 10    g  3.39772 10    g
    {-----, -----, s1}
          s          s

```

```

Chain of 334 segments,
with displacements at segments {1, 64}
Stokes offset 3.00764 A at 50 bp
el0      3.4      A
persistence
length    510.      A
repeat0    10.4      bp/turn
repeat1    10.15     bp/turn
radius     44.916    A
turns      1.75      turns
pitch      -28.571    A/turn
Array of chain lengths (bp)
{0, 62, 270}
Array of friction element positions (bp)
{1, 32, 64, 199}
Array of Stokes radii (A)
{56.8124, 40.8859, 56.8124, 108.172}
...doKirkwood...
i,j,rij:*1 2 114.667 corrected:114.52
i,j,rij:*1 3 216.181 corrected:215.094
i,j,rij:*1 4 389.412 corrected:373.65
i,j,rij:*2 3 117.624 corrected:117.463
i,j,rij:*2 4 380.308 corrected:368.775
i,j,rij:*3 4 403.033 corrected:394.638
Kirkwood results: {f free-draining,f1,s1}
      -7      -7
      5.03067 10 g 2.86755 10 g
      {-----, -----, s1}
              s              s

```

```

Chain of 334 segments,
with displacements at segments {1, 272}
Stokes offset 3.00764 A at 50 bp
el0      3.4      A
persistence
length    510.      A
repeat0    10.4      bp/turn
repeat1    10.15     bp/turn
radius     44.916    A
turns      1.75      turns
pitch      -28.571    A/turn
Array of chain lengths (bp)
{0, 270, 62}
Array of friction element positions (bp)
{1, 136, 272, 303}
Array of Stokes radii (A)
{56.8124, 108.172, 56.8124, 40.8859}
...doKirkwood...
i,j,rij:*1 2 403.033 corrected:394.638
i,j,rij:*1 3 715.09 corrected:667.661
i,j,rij:*1 4 692.236 corrected:638.584
i,j,rij:*2 3 405.636 corrected:397.074
i,j,rij:*2 4 382.279 corrected:370.687
i,j,rij:*3 4 114.667 corrected:114.52
Kirkwood results: {f free-draining,f1,s1}
      -7      -7
      5.03067 10 g 3.25362 10 g
      {-----, -----, s1}
              s              s

```

```

Chain of 334 segments,
with displacements at segments {209, 272}
Stokes offset 3.00764 A at 50 bp
el0      3.4      A
persistence
length    510.      A
repeat0    10.4      bp/turn
repeat1    10.15     bp/turn
radius     44.916    A
turns      1.75      turns
pitch      -28.571    A/turn
Array of chain lengths (bp)
{208, 62, 62}
Array of friction element positions (bp)
{104, 209, 240, 272, 303}

```

```

Array of Stokes radii (A)
{89.9682, 56.8124, 40.8859, 56.8124, 40.8859}
...doKirkwood...
i,j,rij:*1 2 324.43 corrected:320.159
i,j,rij:*1 3 301.232 corrected:294.874
i,j,rij:*1 4 317.637 corrected:307.905
i,j,rij:*1 5 358.974 corrected:344.322
i,j,rij:*2 3 114.667 corrected:114.52
i,j,rij:*2 4 216.181 corrected:215.094
i,j,rij:*2 5 177.429 corrected:175.527
i,j,rij:*3 4 117.624 corrected:117.463
i,j,rij:*3 5 111.337 corrected:110.777
i,j,rij:*4 5 114.667 corrected:114.52
Kirkwood results: {f free-draining,f1,s1}
      -7          -7
      5.46506 10  g  2.58136 10  g
      {-----, -----, s1}
          s          s

Chain of 189 segments,
with displacements at segments {1, 64, 127}
Stokes offset 3.00764 A at 50 bp
el0      3.4      A
persistence
length    510.      A
repeat0    10.4      bp/turn
repeat1    10.15     bp/turn
radius     44.916    A
turns      1.75      turns
pitch      -28.571    A/turn
Array of chain lengths (bp)
{0, 62, 62, 62}
Array of friction element positions (bp)
{1, 32, 64, 95, 127, 158}
Array of Stokes radii (A)
{56.8124, 40.8859, 56.8124, 40.8859, 56.8124, 40.8859}
...doKirkwood...
i,j,rij:*1 2 114.667 corrected:114.52
i,j,rij:*1 3 216.181 corrected:215.094
i,j,rij:*1 4 177.429 corrected:175.527
i,j,rij:*1 5 207.821 corrected:203.999
i,j,rij:*1 6 245.647 corrected:238.957
i,j,rij:*2 3 117.624 corrected:117.463
i,j,rij:*2 4 111.337 corrected:110.777
i,j,rij:*2 5 178.214 corrected:176.266
i,j,rij:*2 6 184.858 corrected:181.459
i,j,rij:*3 4 114.667 corrected:114.52
i,j,rij:*3 5 216.181 corrected:215.094
i,j,rij:*3 6 177.429 corrected:175.527
i,j,rij:*4 5 117.624 corrected:117.463
i,j,rij:*4 6 111.337 corrected:110.777
i,j,rij:*5 6 114.667 corrected:114.52
Kirkwood results: {f free-draining,f1,s1}
      -7          -7
      5.6131 10  g  2.15597 10  g
      {-----, -----, s1}
          s          s

```

Calculate sedimentation coefficients

First check "sediment" routine for a mononucleosome core particle

```

sediment[{1,{1}},1.09 10^-7 g/s]

{np, nchain, mass1, vbar1}
{{1, {1}}, 146, 204860, 0.655926}

1.06806 10^-12 s

```

```

flvalues={3.69942,3.44271,3.39772,2.86755,
           3.25362,2.58136,2.15597} 10^-7 g/s;
Do[Print["\n",sediment[chain[[isp]],flvalues[[isp]]],
   {isp,Length[chain]}];

{np, nchain, mass1, vbar1}
{{479, {1}}, 624, 520340, 0.591704}
-13
9.49818 10 s

{np, nchain, mass1, vbar1}
{{479, {209}}, 624, 520340, 0.591704}
-12
1.02064 10 s

{np, nchain, mass1, vbar1}
{{479, {417}}, 624, 520340, 0.591704}
-12
1.03416 10 s

{np, nchain, mass1, vbar1}
{{334, {1, 64}}, 624, 628840, 0.619016}
-12
1.38108 10 s

{np, nchain, mass1, vbar1}
{{334, {1, 272}}, 624, 628840, 0.619016}
-12
1.2172 10 s

{np, nchain, mass1, vbar1}
{{334, {209, 272}}, 624, 628840, 0.619016}
-12
1.53419 10 s

{np, nchain, mass1, vbar1}
{{189, {1, 64, 127}}, 624, 737340, 0.63829}
-12
2.04401 10 s

```

■ Hydro MS Example 3: Generate sedimentation distributions for trimer

```

ss={8.1,9.5,10.2,10.3,13.8,12.2,15.3,20.4};

fcoop[x_]:=Module[{a,b},
  a=(1-x);
  b=x;
  {a,0,0,0,0,0,0,b}];
frand[x_]:=Module[{a,b},
  a=(1-x);
  b=x;
  {a^3,a^2 b,a^2 b,a^2 b,a b^2,a b^2,a b^2,b^3}];

Print[MatrixForm[{ss,fcoop[0.5]}]]

8.1    9.5    10.2    10.3    13.8    12.2    15.3    20.4
0.5    0      0      0      0      0      0      0.5

Print[MatrixForm[{ss,frand[0.5]}]]

8.1    9.5    10.2    10.3    13.8    12.2    15.3    20.4
0.125  0.125  0.125  0.125  0.125  0.125  0.125  0.125

```

Demonstrate that the sum of species fractions is always unity for both models

```

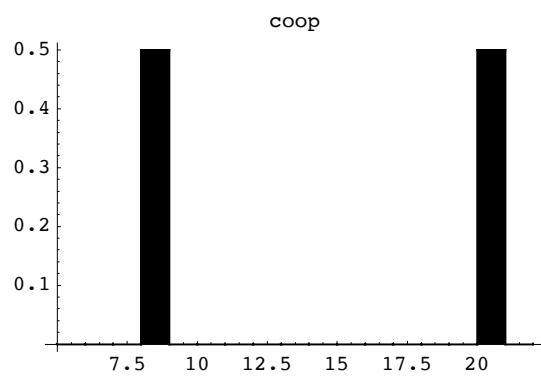
Print[Simplify[Apply[Plus,fcoop[x]]]];
Print[Simplify[Apply[Plus,frand[x]]]];

1
1

```

```
wdistribution[ss,fcoop[0.5],1,0,5,22,0,"coop"];
```

```
{17, 1, 8}  
binned...  
top summed...  
Average is 14.25
```



```
wdistribution[ss,frand[0.5],1,0,5,22,1,"rand"];
```

```
{17, 1, 8}  
binned...  
top summed...  
Average is 12.475
```

