

CHR 2 November 1994

These are the examples that form part of my hydrodynamics paper.

■ Paper: Use Kirkwood and vary the number of turns

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

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

Then define a couple of things to make the example easier to do... Here 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.

```
linker[length_,t_]:=length-t wrapbp;
ns[length_,t_]:=2+linker[length,t];
chain[length_,t_]:= {ns[length,t],{1,ns[length,t]}};

template=354;
nnukes=2;

turns=1.75;
chain[template,nnukes]

{64, {1, 64}}
```

I reset the persistence length and now will calculate the Kirkwood estimates of the frictional coefficients. This procedure (Kirkwood) does not require Monte Carlo trials, remember, so I don't need to bother anymore with A0.

```
template=354;
nnukes=2;
collective=True;
test=True;
progress=True;
MonteCarlo=False;

definebasepair;
Do[ turns=turns0;
  definenuke;
  definephysicalnuke;
  assembleelements[chain[template,nnukes]];
  makeAs[chain[template,nnukes]];
  doKirkwood[chain[template,nnukes]],
{turns0,1.5,2.0,0.1}];

n = 20 ; dl = 21.0801
Chain of 106 segments,
with displacements at segments {1, 106}
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           1.5             turns

pitch           -28.571         A/turn
Array of chain lengths (bp)
{0, 104, 0}
Array of friction element positions (bp)
{1, 53, 106}
Array of Stokes radii (A)
{55.7171, 56.2669, 55.7171}

...doKirkwood...
i,j,rij:*1 2 174.723
i,j,rij:*1 3 328.72
i,j,rij:*2 3 177.669
  Kirkwood results: {f free-draining,f1,s1}
                    -7              -7
      3.21167 10   g  2.0895 10   g
  {-----, -----, s1}
      s              s

n = 20 ; dl = 22.4569
Chain of 90 segments,
with displacements at segments {1, 90}
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         1.6             turns

pitch         -28.571         A/turn
Array of chain lengths (bp)
{0, 88, 0}
Array of friction element positions (bp)
{1, 45, 90}
Array of Stokes radii (A)
{56.1394, 50.5685, 56.1394}

...doKirkwood...
i,j,rij:*1 2 151.701
i,j,rij:*1 3 291.824
i,j,rij:*2 3 154.673
  Kirkwood results: {f free-draining,f1,s1}
                    -7              -7
      3.11871 10   g  1.96407 10   g
  {-----, -----, s1}
      s              s

n = 20 ; dl = 23.8283

```

```

Chain of 74 segments,
with displacements at segments {1, 74}
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        1.7         turns

pitch        -28.571     A/turn
Array of chain lengths (bp)
{0, 72, 0}
Array of friction element positions (bp)
{1, 37, 74}
Array of Stokes radii (A)
{56.5554, 44.6771, 56.5554}

...doKirkwood...
i,j,rij:*1 2 128.809
i,j,rij:*1 3 241.539
i,j,rij:*2 3 131.786
  Kirkwood results: {f free-draining,f1,s1}
                    -7          -7
                    3.02182 10   g  1.82091 10   g
                    {-----, -----, s1}
                      s              s
n = 20 ; dl = 25.1939
Chain of 56 segments,
with displacements at segments {1, 56}
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        1.8         turns

pitch        -28.571     A/turn
Array of chain lengths (bp)
{0, 54, 0}
Array of friction element positions (bp)
{1, 28, 56}
Array of Stokes radii (A)
{57.0163, 37.7895, 57.0163}

```

```

...doKirkwood...
i,j,rij:*1 2 103.623
i,j,rij:*1 3 182.455
i,j,rij:*2 3 106.546
  Kirkwood results: {f free-draining,f1,s1}
                    -7          -7
      2.90757 10  g  1.63805 10  g
    {-----, -----, s1}
        s          s

```

```

n = 20 ; dl = 26.5533
Chain of 40 segments,
with displacements at segments {1, 40}
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        1.9         turns

```

```

pitch        -28.571     A/turn
Array of chain lengths (bp)
{0, 38, 0}
Array of friction element positions (bp)
{1, 20, 40}
Array of Stokes radii (A)
{57.4198, 31.1152, 57.4198}

```

```

...doKirkwood...
i,j,rij:*1 2 82.7165
i,j,rij:*1 3 138.442
i,j,rij:*2 3 85.4716
  Kirkwood results: {f free-draining,f1,s1}
                    -7          -7
      2.7952 10  g  1.46442 10  g
    {-----, -----, s1}
        s          s

```

```

n = 20 ; dl = 27.9063
Chain of 24 segments,
with displacements at segments {1, 24}
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       2.          turns

pitch       -28.571     A/turn
Array of chain lengths (bp)
{0, 22, 0}
Array of friction element positions (bp)
{1, 12, 24}
Array of Stokes radii (A)
{57.8177, 23.7954, 57.8177}

...doKirkwood...
i,j,rij:*1 2 65.094
i,j,rij:*1 3 125.456
i,j,rij:*2 3 67.388
  Kirkwood results: {f free-draining,f1,s1}
                    -7          -7
      2.67026 10   g  1.34983 10   g
    {-----, -----, s1}
        s          s

turnlist={1.5,1.6,1.7,1.8,1.9,2.0};
f1list={2.0895,1.96407,1.82091,1.63805,1.46442,1.34983};
Dtlist=10^7 gettrans[f1list 10^-7,296.15]/.
      {cm->1,g->1,s->1}

{1.95652, 2.08147, 2.24511, 2.49574, 2.79165, 3.02864}

```