

CHR 2 November 1994

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

CHR started 18 Feb 2020. Test of reproducibility for the ReScience 10-year reproducibility challenge (<https://rescience.github.io/ten-years/>). Chosen paper is Robert, C.H. (1995) Estimating Friction Coefficients of Mixed Globular/Chain Molecules, such as Protein/DNA Complexes. Biophys J. 69, 840-48.

The code in this file came from the 1995 notebooks "Example 2 1-over-r.nb" and "Example 2 dinucleosomes.nb", extracted into Figure4_1995.nb preserving the original results. Reproduction trials were run using *Mathematica* 5.2 and 12.0.

Changes from original code:

- added dependence on library s6.1 (Get[...])
- changed boolean variable MonteCarlo to montecarlo (MonteCarlo became a reserved word in *Mathematica*)
- modified call from doKirkwood to original doKirkwood0 from library s6.0
- added comments

Results to compare to originals are indicated by blue text boxes.

```
In[1]:= Get["ReScience/" <> "s6.1_repro.m"];
```

```
In[2]:= Off[General::spell];  
Off[General::spell1];
```

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.

```
In[4]:= 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.

```
In[6]:= linker[length_,t_]:=length-t wrapbp;  
ns[length_,t_]:=2+linker[length,t];  
chain[length_,t_]:={ns[length,t],{1,ns[length,t]}};
```

```
In[9]:= template=354;  
nnukes=2;
```

```
In[11]:= turns=1.75;
         chain[template,nnukes]
```

```
Out[12]= {64, {1, 64}}
```

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.

```
In[13]:= template=354;
         nnukes=2;
         collective=True;
         test=True;
         progress=True;
         montecarlo=False;
```

```
In[19]:= 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	510.	A
length		
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 corrected:174.114
```

```
i,j,rij:*1 3 328.72 corrected:324.393
```

```
i,j,rij:*2 3 177.669 corrected:177.027
```

```
{np, nchain, mass1, vbar1}
```

```
{{106, {1, 106}}, 354, 450 640, 0.646307}
```

```
Kirkwood results: {f free-draining,f1,s1}
```

$$\left\{ \frac{3.21167 \times 10^{-7} \text{ g}}{\text{s}}, \frac{2.08541 \times 10^{-7} \text{ g}}{\text{s}}, 1.26264 \times 10^{-12} \text{ s} \right\}$$

```
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	510.	A	
	length			
	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 corrected:151.318
```

```
i,j,rij:*1 3 291.824 corrected:289.001
```

```
i,j,rij:*2 3 154.673 corrected:154.265
```

```
{np, nchain, mass1, vbar1}
```

```
{{90, {1, 90}}, 354, 450 640, 0.646307}
```

```
Kirkwood results: {f free-draining,f1,s1}
```

$$\left\{ \frac{3.11871 \times 10^{-7} \text{ g}}{\text{s}}, \frac{1.96101 \times 10^{-7} \text{ g}}{\text{s}}, 1.34274 \times 10^{-12} \text{ s} \right\}$$

```
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 510.      A
  length
  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 corrected:128.588
```

```
i,j,rij:*1 3 241.539 corrected:239.932
```

```
i,j,rij:*2 3 131.786 corrected:131.547
```

```
{np, nchain, mass1, vbar1}
```

```
{{74, {1, 74}}, 354, 450 640, 0.646307}
```

```
Kirkwood results: {f free-draining, f1, s1}
```

$$\left\{ \frac{3.02182 \times 10^{-7} \text{ g}}{\text{s}}, \frac{1.81873 \times 10^{-7} \text{ g}}{\text{s}}, 1.44778 \times 10^{-12} \text{ s} \right\}$$

```
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 510.      A
  length
  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 corrected:103.521
i,j,rij:*1 3 182.455 corrected:181.748
i,j,rij:*2 3 106.546 corrected:106.433
{np, nchain, mass1, vbar1}
{{56, {1, 56}}, 354, 450 640, 0.646307}

Kirkwood results: {f free-draining, f1, s1}

$$\left\{ \frac{2.90757 \times 10^{-7} \text{ g}}{\text{s}}, \frac{1.6367 \times 10^{-7} \text{ g}}{\text{s}}, 1.60881 \times 10^{-12} \text{ s} \right\}$$

n = 20 ; dl = 26.5533
Chain of 40 segments,
with displacements at segments {1, 40}
Stokes offset 3.00764 A at 50 bp

$$\left( \begin{array}{lll} \text{el0} & 3.4 & \text{A} \\ \text{persistence} & 510. & \text{A} \\ \text{length} & & \\ \text{repeat0} & 10.4 & \text{bp/turn} \\ \text{repeat1} & 10.15 & \text{bp/turn} \\ \text{radius} & 44.916 & \text{A} \\ \text{turns} & 1.9 & \text{turns} \\ \text{pitch} & -28.571 & \text{A/turn} \end{array} \right)$$

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 corrected:82.6754
i,j,rij:*1 3 138.442 corrected:138.165
i,j,rij:*2 3 85.4716 corrected:85.4246
{np, nchain, mass1, vbar1}
{{40, {1, 40}}, 354, 450 640, 0.646307}

Kirkwood results: {f free-draining, f1, s1}

$$\left\{ \frac{2.7952 \times 10^{-7} \text{ g}}{\text{s}}, \frac{1.46368 \times 10^{-7} \text{ g}}{\text{s}}, 1.79897 \times 10^{-12} \text{ s} \right\}$$

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	510.	A	
	length			
	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 corrected:65.0828

i,j,rij:*1 3 125.456 corrected:125.366

i,j,rij:*2 3 67.388 corrected:67.3743

{np, nchain, mass1, vbar1}

{{24, {1, 24}}, 354, 450 640, 0.646307}

Kirkwood results: {f free-draining, f1, s1}

$$\left\{ \frac{2.67026 \times 10^{-7} \text{ g}}{\text{s}}, \frac{1.34956 \times 10^{-7} \text{ g}}{\text{s}}, 1.9511 \times 10^{-12} \text{ s} \right\}$$

These results, while close to the output in the original notebooks, do not exactly match it. The reason was a small chain-statistics correction applied to the doKirkwood function after the figure was made; here is the calculation with the original function, here named doKirkwood0, which has been added to the library file s6.1.

```
In[21]:= definebasepair;
Do[ turns=turns0;
  definenuke;
  definephysicalnuke;
  assembleelements[chain[template,nnukes]];
  makeAs[chain[template,nnukes]];
  doKirkwood0[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	510.	A	
	length			
	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}

$$\left\{ \frac{3.21167 \times 10^{-7} \text{ g}}{\text{s}}, \frac{2.0895 \times 10^{-7} \text{ g}}{\text{s}}, 1.9511 \times 10^{-12} \text{ s} \right\}$$

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	510.	A	
	length			
	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}
```

$$\left\{ \frac{3.11871 \times 10^{-7} \text{ g}}{s}, \frac{1.96407 \times 10^{-7} \text{ g}}{s}, 1.9511 \times 10^{-12} \text{ s} \right\}$$

```
n = 20 ; dl = 23.8283
```

```
Chain of 74 segments,
```

```
with displacements at segments {1, 74}
```

```
Stokes offset 3.00764 A at 50 bp
```

e10	3.4	A
persistence	510.	A
length		
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}
```

$$\left\{ \frac{3.02182 \times 10^{-7} \text{ g}}{s}, \frac{1.82091 \times 10^{-7} \text{ g}}{s}, 1.9511 \times 10^{-12} \text{ s} \right\}$$

```
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	510.	A
length		
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}

$$\left\{ \frac{2.90757 \times 10^{-7} \text{ g}}{\text{s}}, \frac{1.63805 \times 10^{-7} \text{ g}}{\text{s}}, 1.9511 \times 10^{-12} \text{ s} \right\}$$

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	510.	A
length		
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}

$$\left\{ \frac{2.7952 \times 10^{-7} \text{ g}}{\text{s}}, \frac{1.46442 \times 10^{-7} \text{ g}}{\text{s}}, 1.9511 \times 10^{-12} \text{ s} \right\}$$

n = 20 ; dl = 27.9063
Chain of 24 segments,
with displacements at segments {1, 24}
Stokes offset 3.00764 A at 50 bp

$$\left( \begin{array}{lll} \text{el0} & 3.4 & \text{A} \\ \text{persistence} & 510. & \text{A} \\ \text{length} & & \\ \text{repeat0} & 10.4 & \text{bp/turn} \\ \text{repeat1} & 10.15 & \text{bp/turn} \\ \text{radius} & 44.916 & \text{A} \\ \text{turns} & 2. & \text{turns} \\ \text{pitch} & -28.571 & \text{A/turn} \end{array} \right)$$

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}

$$\left\{ \frac{2.67026 \times 10^{-7} \text{ g}}{\text{s}}, \frac{1.34983 \times 10^{-7} \text{ g}}{\text{s}}, 1.9511 \times 10^{-12} \text{ s} \right\}$$


```

In the article, the f1 values calculated as above were stored in "f1list" and converted to Dt values in the file "Example 2 dinucleosomes.nb" for Figure 4 using the following code. The calculated values are identical to those stored here (and plotted in that figure).

```

In[23]:= turnlist={1.5,1.6,1.7,1.8,1.9,2.0};
         flist={2.0895,1.96407,1.82091,1.63805,1.46442,1.34983};
         Dtlist=10^7 gettrans[flist 10^-7,296.15]/.
           {cm->1,g->1,s->1}

```

```

Out[25]= {1.95652, 2.08147, 2.24511, 2.49574, 2.79165, 3.02864}

```

```

In[39]:= "a" && "b"

```

```

Out[39]= a && b

```

```

In[48]:= xlabel = "Superhelical\nturns";
         ylabel = Row[{"Dt x", Superscript[10, 7], Superscript["", cm", 2], "/s"}];
         ListPlot[
           Transpose[{turnlist, Dtlist}],
           PlotJoined -> True,
           AxesLabel -> {xlabel, ylabel},
           PlotRange -> {{1.4, 2.07}, {1.8, 3.1}},
           AxesOrigin -> {2, 2},
           AspectRatio -> 9/14.8,
           Frame -> False
         ]

```

```

Out[49]=

```

