

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

```
In[27]:= 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[29]:= 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[31]:= linker[length_,t_]:=length-t wrapbp;
ns[length_,t_]:=2+linker[length,t];
chain[length_,t_]:= {ns[length,t], {1, ns[length,t]}};
```

```
In[34]:= template=354;
nnukes=2;
```

```
In[36]:= turns=1.75;
chain[template,nnukes]
```

```
Out[37]= {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[38]:= template=354;
nnukes=2;
collective=True;
test=True;
progress=True;
montecarlo=False;
```

```

In[44]:= 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, 450640, 0.646307}

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

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

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, 450640, 0.646307}
```

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

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

```
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, 450640, 0.646307}

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

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

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, 450640, 0.646307}

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

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

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 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, 450640, 0.646307}
```

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

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

```
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, 450640, 0.646307}

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

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

```

These results, while close, do not exactly match the output in the original notebooks. 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[46]:= 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}

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

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)

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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}

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

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 510.    A
  length
  repeat0    10.4    bp/turn
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  radius     44.916   A
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Array of chain lengths (bp)

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Array of friction element positions (bp)

```

```

{1, 37, 74}

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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}

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

n = 20 ; dl = 25.1939

Chain of 56 segments,

with displacements at segments {1, 56}

Stokes offset 3.00764 A at 50 bp

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  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}

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

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,fl,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

```
(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
```

```
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 "f1ist" 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[48]:= turnlist={1.5,1.6,1.7,1.8,1.9,2.0};
          f1ist={2.0895,1.96407,1.82091,1.63805,1.46442,1.34983};
          Dtlist=10^7 gettrans[f1ist 10^-7,296.15]/.
                {cm->1,g->1,s->1}
```

```
Out[50]= {1.95652, 2.08147, 2.24511, 2.49574, 2.79165, 3.02864}
```