

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.

All code in this file came from the original notebook "Example 3 3x208.nb" and was run using Mathematica versions 5.2 and 12.0.

Changes:

- added dependence on library s6.1_repro.m*
- added dependence on additional routines I had written in other libraries and gathered into "extra.m"*
- removed terminal semicolons to see graphical output*

```
In[38]:= Get["ReScience/" <> "s6.1_repro.m"];
         Get["ReScience/" <> "extra.m"];
```

```
In[40]:= Off[General::spell];
         Off[General::spell1];
```

■ **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.

```
In[42]:= ClearAll[A0];
         A0=IdentityMatrix[3];
```

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

```
In[44]:= turns=1.75;
         definebasepair;
         definenuke;
         definephysicalnuke;
         chaininitialize;
         wrapbp

n = 20 ; dl = 24.5119
```

```
Out[49]= 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.

```
In[50]:= ntemplate=624;          (* total length, bp *)

In[51]:= species={{1},{2},{3},{1,2},{1,3},{2,3},{1,2,3}};
         nt[spots_]:=ntemplate - Length[spots] wrapbp + Length[spots];
         Map[nt,species]

Out[53]= {479, 479, 479, 334, 334, 334, 189}
```

```

In[54]:= chain={ {479,{1}},
                 {479,{209}},
                 {479,{417}},
                 {334,{1,64}},
                 {334,{1,272}},
                 {334,{209,272}},
                 {189,{1,64,127}}    };

In[55]:= persistence = 150 e10;
         definebasepair;

In[57]:= collective=True;
         test=True;
         progress=True;
         montecarlo=False;

In[61]:= 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

( e10      3.4      A
  persistence 510.    A
  length
  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

{np, nchain, mass1, vbar1}

{{479, {1}}, 624, 520340, 0.591704}

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

{  $\frac{4.21008 \times 10^{-7} \text{ g}}{\text{s}}$ ,  $\frac{3.69942 \times 10^{-7} \text{ g}}{\text{s}}$ ,  $9.49818 \times 10^{-13} \text{ s}$  }

Chain of 479 segments,

with displacements at segments {209}

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      1.75    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
```

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

```
{{479, {209}}, 624, 520340, 0.591704}
```

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

```
{  $\frac{4.88263 \times 10^{-7} \text{ g}}{\text{s}}$ ,  $\frac{3.44271 \times 10^{-7} \text{ g}}{\text{s}}$ ,  $1.02064 \times 10^{-12} \text{ s}$  }
```

Chain of 479 segments,

with displacements at segments {417}

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      1.75    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

{np, nchain, mass1, vbar1}

{{479, {417}}, 624, 520340, 0.591704}

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

{  $\frac{4.69551 \times 10^{-7} \text{ g}}{\text{s}}$ ,  $\frac{3.39772 \times 10^{-7} \text{ g}}{\text{s}}$ ,  $1.03416 \times 10^{-12} \text{ s}$  }

Chain of 334 segments,

with displacements at segments {1, 64}

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        1.75     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

{np, nchain, mass1, vbar1}

{{334, {1, 64}}, 624, 628840, 0.619016}

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

{  $\frac{5.03067 \times 10^{-7} \text{ g}}{\text{s}}$ ,  $\frac{2.86755 \times 10^{-7} \text{ g}}{\text{s}}$ ,  $1.38108 \times 10^{-12} \text{ s}$  }

Chain of 334 segments,

with displacements at segments {1, 272}

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      1.75    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
```

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

```
{{334, {1, 272}}, 624, 628840, 0.619016}
```

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

```
{  $\frac{5.03067 \times 10^{-7} \text{ g}}{\text{s}}$ ,  $\frac{3.25362 \times 10^{-7} \text{ g}}{\text{s}}$ ,  $1.2172 \times 10^{-12} \text{ s}$  }
```

Chain of 334 segments,

with displacements at segments {209, 272}

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      1.75    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

{np, nchain, mass1, vbar1}

{{334, {209, 272}}, 624, 628840, 0.619016}

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

{  $\frac{5.46506 \times 10^{-7} \text{ g}}{\text{s}}$ ,  $\frac{2.58136 \times 10^{-7} \text{ g}}{\text{s}}$ ,  $1.53419 \times 10^{-12} \text{ s}$  }

Chain of 189 segments,

with displacements at segments {1, 64, 127}

Stokes offset 3.00764 A at 50 bp

(
  el0          3.4      A
  persistence  510.     A
  length
  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

{np, nchain, mass1, vbar1}

{{189, {1, 64, 127}}, 624, 737340, 0.63829}

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

{  $\frac{5.6131 \times 10^{-7} \text{ g}}{\text{s}}$ ,  $\frac{2.15597 \times 10^{-7} \text{ g}}{\text{s}}$ ,  $2.04401 \times 10^{-12} \text{ s}$  }

```

Calculate sedimentation coefficients

In the preceding doKirkwood loop output, the sedimentation coefficients s1 for each species (3rd value in the brackets) are calculated at the same time as the friction coefficients, but they were not calculated in the original 1995 output. In 1995, before running the loop, I apparently executed the cell defining doKirkwood in my library notebook manually (I did not yet use the "Get" command to load the library functions), and forgot to execute the cell defining the sediment[] function. This is why in the original output the sedimentation coefficients s1 had to be recalculated in this section, and at that point I must have executed the library cell defining the "sediment" function. No trace of this, however. This is an example of the pitfalls of "hidden state" in notebook computing.

First check "sediment" routine for a mononucleosome core particle

```

In[62]:= sediment[{1,{1}},1.09 10^-7 g/s]

{np, nchain, mass1, vbar1}

{{1, {1}}, 146, 204860, 0.655926}

Out[62]= 1.06806 × 10-12 s

```

```

In[63]:= 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}

9.49818×10-13 s
{np, nchain, mass1, vbar1}

{{479, {209}}, 624, 520340, 0.591704}

1.02064×10-12 s
{np, nchain, mass1, vbar1}

{{479, {417}}, 624, 520340, 0.591704}

1.03416×10-12 s
{np, nchain, mass1, vbar1}

{{334, {1, 64}}, 624, 628840, 0.619016}

1.38108×10-12 s
{np, nchain, mass1, vbar1}

{{334, {1, 272}}, 624, 628840, 0.619016}

1.2172×10-12 s
{np, nchain, mass1, vbar1}

{{334, {209, 272}}, 624, 628840, 0.619016}

1.53419×10-12 s
{np, nchain, mass1, vbar1}

{{189, {1, 64, 127}}, 624, 737340, 0.63829}

2.04401×10-12 s

```

■ Hydro MS Example 3: Generate sedimentation distributions for trimer

First use the Kovacic and van Holde to calculate the sedimentation of the free DNA

```

In[65]:= rYF[3 208]

Out[65]= 197.515

```

This function rYF returns the hydrodynamic radius, not the sedimentation coefficient, so part of this calculation was apparently deleted from the notebook. I didn't pursue this further, because calculating the hydrodynamics of free DNA is not part of the novelty of the article. The correct value for 3x208 bp of free DNA is 8.1 S.

The sedimentation coefficients as calculated above are identical to those recopied to the list below, after scaling to Svedburg units of 10^{-13} s.

```
In[66]:= ss={8.1,9.5,10.2,10.3,13.8,12.2,15.3,20.4};

In[67]:= 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}];

In[69]:= Print[MatrixForm[{ss,fcoop[0.5]}]]


$$\begin{pmatrix} 8.1 & 9.5 & 10.2 & 10.3 & 13.8 & 12.2 & 15.3 & 20.4 \\ 0.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0.5 \end{pmatrix}$$


In[70]:= Print[MatrixForm[{ss,frand[0.5]}]]


$$\begin{pmatrix} 8.1 & 9.5 & 10.2 & 10.3 & 13.8 & 12.2 & 15.3 & 20.4 \\ 0.125 & 0.125 & 0.125 & 0.125 & 0.125 & 0.125 & 0.125 & 0.125 \end{pmatrix}$$

```

The two saturation models fcoop (perfectly cooperative saturation) and frand (random saturation) were calculated using elementary statistics (see article text) and used to weight the calculated sedimentation coefficients for the plotted distributions.

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

```
In[71]:= Print[Simplify[Apply[Plus,fcoop[x]]]];
Print[Simplify[Apply[Plus,frand[x]]]];

{1, 1, 1, 1, 1, 1}

{1, 1, 1, 1, 1, 1}

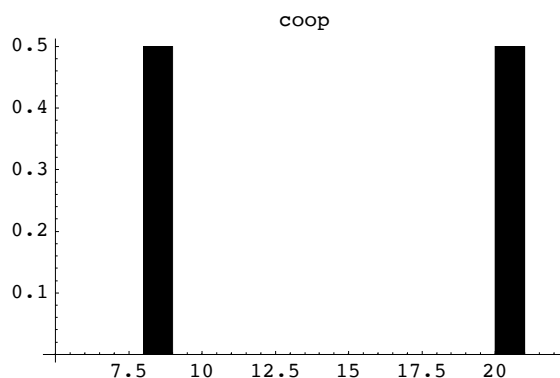
In[73]:= wdistribution[ss,fcoop[0.5],1,0,5,22,0,"coop"]

{17, 1, 8}

binned...

top summed...

Average is 14.25
```



Out[73]= - Graphics -

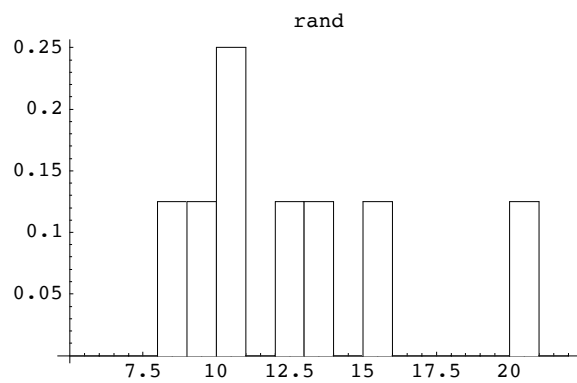
```
In[74]:= wdistribution[ss,frand[0.5],1,0,5,22,1,"rand"]
```

```
{17, 1, 8}
```

```
binned...
```

```
top summed...
```

```
Average is 12.475
```



```
Out[74]= - Graphics -
```

These are the results shown in Figure 5 and Table 1 of my 1995 Biophysical Journal paper.