

CHR 20 April 1993

Final calculations for Figure 2 in the hydrodynamics paper... I leave the Garcia de la Torre results at the values already calculated (in Figure 2 data-- "Garcia de la Torre Final" or Cricket Graph file) and use my Kirkwood subroutine on radii and intersphere distances calculated for this example, which is particularly simple since the DNA is treated in the rigid limit.

Notice that the Yamakawa and Fujii equation for the sedimentation behavior in the limit of an infinite persistence length (rigid rod) reduces to 3.620 (log[masstrue]-3.552) For Kovacic and van Holde's fit to the DNA data.

```
t=.;
NAvo=6.02 10^23;
ro=1.003; (* density, g/cm^3 *)
visc=0.01016; (* viscosity, g/(cm s) or "Poise" *)
persistenceLength=34000 10^-8; (* persistence length, cm *)
el=3.4 10^-8; (* height of basepair, cm *)
lx={0,0,1}; (* chain vector for a basepair *)
ctorsion=2.4 10^-19; (* not used-- ergs/radian? *)
mhistone=108500; (* octamer mol. weight, g/mole *)
mbp=660; (* basepair mol. weight, g/mole *)
vdna=0.55; (* specific volume of DNA, cm^3/g *)
vhistone=0.75; (* same but of protein, cm^3/g *)
score=10.7 10^-13; (* core sedimentation coeff, sec *)
dDNA=27 10^-8; (* Yamagawa-Fujii (Y-F) diam, cm *)
switchbp=50; (* point at which we switch from *)
(* Y-F to ellipsoid model, bp *)

doKirkwoodG:=Block[{i,j,sum,sumradii},
  (* Calculates friction and sedimentation coefficients, f1 and
  s1, according to the standard Kirkwood-Riseman theory. *)
  sumradii=Sum[radii[[i]],{i,ntot}];
  sum=0;
  Do[ Do[ rirj=N[radii[[i]] radii[[j]]];
    If[ rirj>0,
      delsum=rirj/rij[[i,j]],
      delsum=0
    ];
    If[ test,
      Print[" i,j,rij(cm): ",i," ",j," ",N[rij[[i,j]]]
    ];
    sum=sum+delsum,
    {j,i+1,ntot}];
  {i,ntot}];
  (* Notice we only counted the distance of each pair once,
  but we multiplied by two to make up for it. Now calculate
  frictional coeff and convert from basepairs to cm: *)
  ffree=6 Pi visc sumradii g/s;
  f1=6 Pi visc sumradii/(1 + 2 sum/sumradii) g/s;
  Print[" Kirkwood results: {f free-draining,f1}"];
  Print[" ",N[{ffree,f1}]]
];

snaked[i_]:=Module[{j},
  s1=3.620 (Log[10,i 660]-3.552) 10^-13;
  rstokes=((i 660) (1-vdna ro)/(NAvo s1))/(6 Pi visc)
];
```

*Define radii of rigid-model DNA spheres and of globular region in cm:*

```
r1=57 10^-8;
r2=16.534 10^-8; (* Equal volume achieved
by r2=Sqrt[3/2] 13.5 A *)
```

*Values of the ratio  $L = \text{length}/r1$  to use in the comparison.*

```
(* Values of length/r1 to use in comparison and corresponding
numbers of basepairs: *)
lengthp={3,4,5,6,8,10,12,14,16};
nbasepairs=(lengthp r1)/(3.4 10^-8);
```

**nbasepairs**

```
{50.2941, 67.0588, 83.8235, 100.588, 134.118, 167.647, 201.176, 234.706,
 268.235}
```

## LOLLIPOPS

```
f1Kirk={};
f1robert={};
frictionratio={};
rij={};
Do[
  Print[nbasepairs[[k]], " bp spacer"];

  Print["My model:"];
  ntot=2;
  snaked[nbasepairs[[k]]];
  radii={r1,rstokes};
  rij={{0,r1 + lengthp[[k]] r1/2},{r1 + lengthp[[k]] r1/2,0}};
  doKirkwoodG;
  f1robert=Append[f1robert,f1];

  Print["Kirk's model:"];
  ntot=lengthp[[k]]+1;
  radii={r1};
  Do[radii=Append[radii,r2],{i,lengthp[[k]]}];
  rij=Table[0,{i,ntot},{j,ntot}];
  Do[ Do[
    rij[[i,j]]=radii[[i]] + (j-i-1) 2 r2 + r2,
    {j,i+1,ntot}],
    {i,ntot}];
  doKirkwoodG;
  f1Kirk=Append[f1Kirk,N[f1]],

{k,Length[lengthp]}};
```

```
50.2941 bp spacer
My model:
Kirkwood results: {f free-draining,f1}
      -7      -7
1.79634 10 g 1.36724 10 g
{-----, -----}
      s      s
Kirk's model:
Kirkwood results: {f free-draining,f1}
      -7      -7
2.04155 10 g 1.06294 10 g
{-----, -----}
      s      s
67.0588 bp spacer
My model:
Kirkwood results: {f free-draining,f1}
      -7      -7
1.92394 10 g 1.49327 10 g
{-----, -----}
      s      s
Kirk's model:
Kirkwood results: {f free-draining,f1}
      -7      -7
2.3582 10 g 1.10619 10 g
{-----, -----}
      s      s
83.8235 bp spacer
My model:
Kirkwood results: {f free-draining,f1}
      -7      -7
2.04736 10 g 1.61623 10 g
{-----, -----}
      s      s
Kirk's model:
Kirkwood results: {f free-draining,f1}
      -7      -7
2.67484 10 g 1.15792 10 g
{-----, -----}
      s      s
100.588 bp spacer
My model:
Kirkwood results: {f free-draining,f1}
      -7      -7
2.16701 10 g 1.73621 10 g
{-----, -----}
```

```

      s      s
Kirk's model:
Kirkwood results: {f free-draining,f1}
      -7      -7
      2.99149 10 g 1.21429 10 g
      {-----, -----}
      s      s
134.118 bp spacer
My model:
Kirkwood results: {f free-draining,f1}
      -7      -7
      2.39706 10 g 1.96829 10 g
      {-----, -----}
      s      s
Kirk's model:
Kirkwood results: {f free-draining,f1}
      -7      -7
      3.62478 10 g 1.33378 10 g
      {-----, -----}
      s      s
167.647 bp spacer
My model:
Kirkwood results: {f free-draining,f1}
      -7      -7
      2.61743 10 g 2.19157 10 g
      {-----, -----}
      s      s
Kirk's model:
Kirkwood results: {f free-draining,f1}
      -7      -7
      4.25807 10 g 1.45695 10 g
      {-----, -----}
      s      s
201.176 bp spacer
My model:
Kirkwood results: {f free-draining,f1}
      -7      -7
      2.83031 10 g 2.40771 10 g
      {-----, -----}
      s      s
Kirk's model:
Kirkwood results: {f free-draining,f1}
      -7      -7
      4.89136 10 g 1.58096 10 g
      {-----, -----}
      s      s
234.706 bp spacer
My model:
Kirkwood results: {f free-draining,f1}
      -7      -7
      3.03719 10 g 2.61794 10 g
      {-----, -----}
      s      s
Kirk's model:
Kirkwood results: {f free-draining,f1}
      -7      -7
      5.52465 10 g 1.70467 10 g
      {-----, -----}
      s      s
268.235 bp spacer
My model:
Kirkwood results: {f free-draining,f1}
      -7      -7
      3.2391 10 g 2.82316 10 g
      {-----, -----}
      s      s
Kirk's model:
Kirkwood results: {f free-draining,f1}
      -7      -7
      6.15794 10 g 1.82757 10 g
      {-----, -----}
      s      s

```

**MatrixForm[Transpose[{N[nbasepairs,3],N[f1robert,4],N[f1Kirk,4]}]]**

50.3	$\frac{1.367 \cdot 10^{-7} \text{ g}}{\text{s}}$	$\frac{1.063 \cdot 10^{-7} \text{ g}}{\text{s}}$
67.1	$\frac{1.493 \cdot 10^{-7} \text{ g}}{\text{s}}$	$\frac{1.106 \cdot 10^{-7} \text{ g}}{\text{s}}$
83.8	$\frac{1.616 \cdot 10^{-7} \text{ g}}{\text{s}}$	$\frac{1.158 \cdot 10^{-7} \text{ g}}{\text{s}}$
101.	$\frac{1.736 \cdot 10^{-7} \text{ g}}{\text{s}}$	$\frac{1.214 \cdot 10^{-7} \text{ g}}{\text{s}}$
134.	$\frac{1.968 \cdot 10^{-7} \text{ g}}{\text{s}}$	$\frac{1.334 \cdot 10^{-7} \text{ g}}{\text{s}}$
168.	$\frac{2.192 \cdot 10^{-7} \text{ g}}{\text{s}}$	$\frac{1.457 \cdot 10^{-7} \text{ g}}{\text{s}}$
201.	$\frac{2.408 \cdot 10^{-7} \text{ g}}{\text{s}}$	$\frac{1.581 \cdot 10^{-7} \text{ g}}{\text{s}}$
235.	$\frac{2.618 \cdot 10^{-7} \text{ g}}{\text{s}}$	$\frac{1.705 \cdot 10^{-7} \text{ g}}{\text{s}}$
268.	$\frac{2.823 \cdot 10^{-7} \text{ g}}{\text{s}}$	$\frac{1.828 \cdot 10^{-7} \text{ g}}{\text{s}}$

## DUMBBELLS

Here are the dumbbell calculations. We use a linear array that is the same as before, but another subunit is added at the end.

```

f1Kirk={};
f1robert={};
frictionratio={};
rij={};
Do[
  Print[nbasepairs[[k]], " bp spacer"];

  Print["My model:"];
  ntot=3;
  snaked[nbasepairs[[k]]];
  radii={r1,rstokes,r1};
  rij={{0,r1 + lengthp[[k]] r1/2,2 r1 + lengthp[[k]] r1},
        {0,0,r1 + lengthp[[k]] r1/2},
        {0,0,0}};
  doKirkwoodG;
  f1robert=Append[f1robert,f1];

  Print["Kirk's model:"];
  ntot=lengthp[[k]]+2;
  radii={r1};
  Do[radii=Append[radii,r2],{i,lengthp[[k]]}];
  radii=Append[radii,r1];
  rij=Table[0,{i,ntot},{j,ntot}];
  Do[ Do[ If[ j<ntot,
            rij[[i,j]]=radii[[i]] + (j-i-1) 2 r2 + r2,
            rij[[i,j]]=radii[[i]] + (j-i-1) 2 r2 + radii[[j]]
          ],
        {j,i+1,ntot}],
    {i,ntot}];
  doKirkwoodG;
  f1Kirk=Append[f1Kirk,N[f1]],

{k,Length[lengthp]}};

50.2941 bp spacer
My model:
Kirkwood results: {f free-draining,f1}

```

```

      -7      -7
2.88796 10  g  1.87331 10  g
{-----, -----}
      s      s
Kirk's model:
Kirkwood results: {f free-draining,f1}
      -7      -7
3.13317 10  g  1.4686 10  g
{-----, -----}
      s      s
67.0588 bp spacer
My model:
Kirkwood results: {f free-draining,f1}
      -7      -7
3.01556 10  g  2.02566 10  g
{-----, -----}
      s      s
Kirk's model:
Kirkwood results: {f free-draining,f1}
      -7      -7
3.44981 10  g  1.50246 10  g
{-----, -----}
      s      s
83.8235 bp spacer
My model:
Kirkwood results: {f free-draining,f1}
      -7      -7
3.13898 10  g  2.1688 10  g
{-----, -----}
      s      s
Kirk's model:
Kirkwood results: {f free-draining,f1}
      -7      -7
3.76646 10  g  1.54392 10  g
{-----, -----}
      s      s
100.588 bp spacer
My model:
Kirkwood results: {f free-draining,f1}
      -7      -7
3.25863 10  g  2.30493 10  g
{-----, -----}
      s      s
Kirk's model:
Kirkwood results: {f free-draining,f1}
      -7      -7
4.0831 10  g  1.59033 10  g
{-----, -----}
      s      s
134.118 bp spacer
My model:
Kirkwood results: {f free-draining,f1}
      -7      -7
3.48868 10  g  2.56156 10  g
{-----, -----}
      s      s
Kirk's model:
Kirkwood results: {f free-draining,f1}
      -7      -7
4.71639 10  g  1.69212 10  g
{-----, -----}
      s      s
167.647 bp spacer
My model:
Kirkwood results: {f free-draining,f1}
      -7      -7
3.70904 10  g  2.80287 10  g
{-----, -----}
      s      s
Kirk's model:
Kirkwood results: {f free-draining,f1}
      -7      -7
5.34968 10  g  1.80055 10  g
{-----, -----}
      s      s
201.176 bp spacer
My model:
Kirkwood results: {f free-draining,f1}
      -7      -7
3.92193 10  g  3.03298 10  g
{-----, -----}
      s      s
Kirk's model:
Kirkwood results: {f free-draining,f1}
      -7      -7
5.98297 10  g  1.91227 10  g
{-----, -----}
      s      s
234.706 bp spacer
My model:
Kirkwood results: {f free-draining,f1}
      -7      -7
4.12881 10  g  3.25447 10  g
{-----, -----}
      s      s
Kirk's model:
Kirkwood results: {f free-draining,f1}
      -7      -7
- - - - -

```

```

6.61626 10 g 2.02559 10 g
{-----, -----}
s s
268.235 bp spacer
My model:
Kirkwood results: {f free-draining,f1}
-7 -7
4.33072 10 g 3.46903 10 g
{-----, -----}
s s
Kirk's model:
Kirkwood results: {f free-draining,f1}
-7 -7
7.24955 10 g 2.13958 10 g
{-----, -----}
s s

```

**MatrixForm[Transpose[{N[nbasepairs,3],N[f1robert,4],N[f1Kirk,4]}]]**

50.3	$\frac{1.873 \cdot 10^{-7} \text{ g}}{\text{s}}$	$\frac{1.469 \cdot 10^{-7} \text{ g}}{\text{s}}$
67.1	$\frac{2.026 \cdot 10^{-7} \text{ g}}{\text{s}}$	$\frac{1.502 \cdot 10^{-7} \text{ g}}{\text{s}}$
83.8	$\frac{2.169 \cdot 10^{-7} \text{ g}}{\text{s}}$	$\frac{1.544 \cdot 10^{-7} \text{ g}}{\text{s}}$
101.	$\frac{2.305 \cdot 10^{-7} \text{ g}}{\text{s}}$	$\frac{1.59 \cdot 10^{-7} \text{ g}}{\text{s}}$
134.	$\frac{2.562 \cdot 10^{-7} \text{ g}}{\text{s}}$	$\frac{1.692 \cdot 10^{-7} \text{ g}}{\text{s}}$
168.	$\frac{2.803 \cdot 10^{-7} \text{ g}}{\text{s}}$	$\frac{1.801 \cdot 10^{-7} \text{ g}}{\text{s}}$
201.	$\frac{3.033 \cdot 10^{-7} \text{ g}}{\text{s}}$	$\frac{1.912 \cdot 10^{-7} \text{ g}}{\text{s}}$
235.	$\frac{3.254 \cdot 10^{-7} \text{ g}}{\text{s}}$	$\frac{2.026 \cdot 10^{-7} \text{ g}}{\text{s}}$
268.	$\frac{3.469 \cdot 10^{-7} \text{ g}}{\text{s}}$	$\frac{2.14 \cdot 10^{-7} \text{ g}}{\text{s}}$