

## TopoIce-R Manual

This software can be used to model the shape of DNA bound by proteins (such as recombinases) which bind 2 segments of DNA and can knot or link circular DNA molecules. For more information regarding this modeling see TopoICE-Rexamples.pdf.

Download KnotPlot from [www.knotplot.com/download](http://www.knotplot.com/download)

**PC.** To download KnotPlot: Click on InstallKnotPlot.exe. This will open a window asking you if you want to run, save, or cancel this file. Click on run (or save if you prefer). After it is downloaded, you will be asked if you wish to run the program. Click on run and follow the KnotPlot Setup Wizard instructions.

**MAC.** Click on KnotPlot.tar.gz. If you have Stuffit, the compressed KnotPlot directory will be automatically uncompressed. Otherwise you can use `tar -xvzf KnotPlot.tar.gz` on any command line terminal (such as X11 or Terminal).

**Linux.** Use gunzip to unzip.

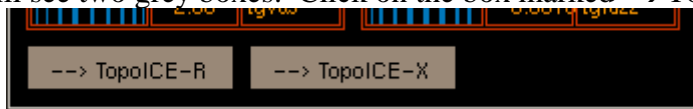
Click on the KnotPlot icon (in KnotPlot folder or on Desktop if you created a Desktop KnotPlot icon) to run KnotPlot:



In the KnotPlot Control Panel window, click on the TopoICE tab (in second column).



At the bottom, you will see two grey boxes. Click on the box marked "→TopoICE-R"



To use the recombinase capability of KnotPlot:  
Enter a knot by using the zoo or rollers:



To enter a knot using the zoo, click on "Load Zoo".

A zoo of knots will appear in the KnotPlot Window. You can enter a knot by clicking on it.



You can display more knots by using the slider to change the zoo size or clicking on "Zoo up" or "Zoo down".



There are two display modes:

If "cat" zoo mode is selected, Rolfsen type pictures of knots will display.

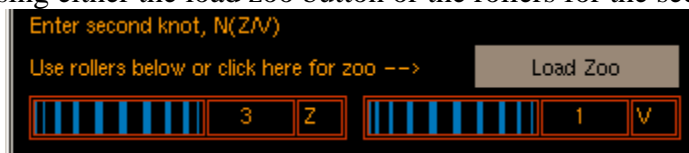
If "rat" zoo mode is selected, the knot is drawn using rational tangle notation.

To enter a knot using the rollers (for those familiar with rational tangle notation):

Enter the fraction corresponding to the rational knot  $N(A/B)$  by using the top two rollers. You can also enter these numbers by double clicking the number, typing in a new number, and hitting return.

Note you can find this number by looking at the table available at <http://www.math.uiowa.edu/~idarcy/TAB/knottable.ps>.

Enter second knot using either the load zoo button or the rollers for the second knot:



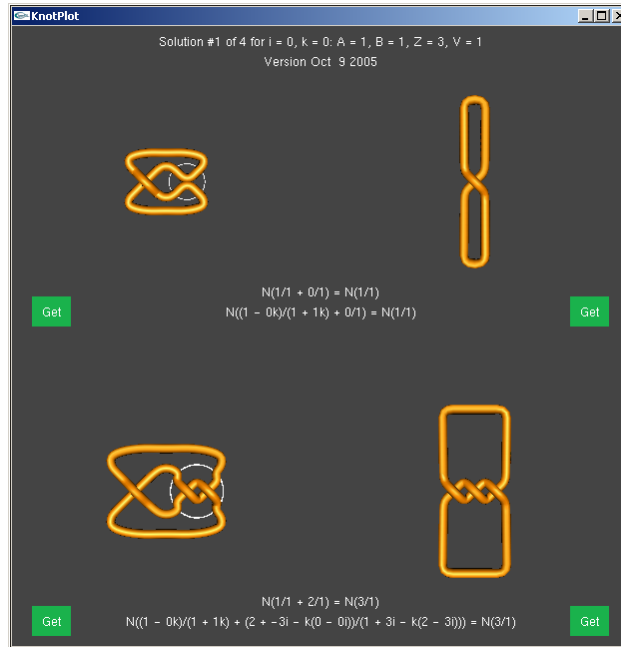
You must also choose the initial DNA shape bound by the protein complex. Enter this using either the load zoo button or the rollers:



You can now click on Solve:

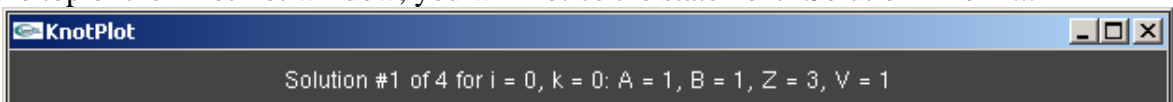


A method of converting the first knot  $N(A/B) = N(1/1)$  into the second knot  $N(Z/V) = N(3/1)$  is shown in the KnotPlot window:



The top two figures shows the unknot. The figure on the left models the protein action. A circle is drawn around the tangle representing the protein-bound DNA. The bottom two figures show the trefoil knot. Note that the protein action has changed the topology of the protein bound DNA. The protein originally bound no DNA crossings (top left diagram). After the protein has acted, it now binds two DNA crossings (bottom left diagram).

At the top of the KnotPlot window, you will notice the statement "Solution #1 of 4..."

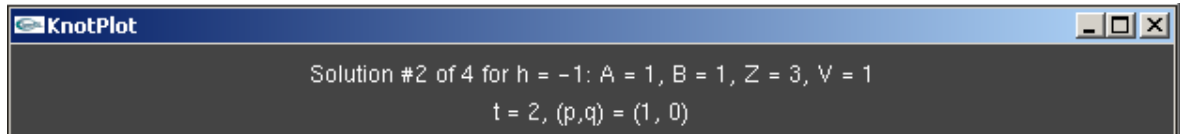


This means there are up to four infinite families of solutions. We will start by exploring the first infinite family of solutions. The statement Solution #1 of 4 for  $i = 0, k = 0$  means that we can change both  $i$  and  $k$  to see more solutions within this family of solutions.

To see more solutions within this family click on "incr i", "decr i", "incr k", "decr k":



To see a different family of solutions click on "up" or "down". In this case for solution #2 of 4, we can only change the variable h to see more solutions within the second family of solutions.

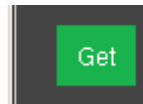


To see more solutions within this family click on "incr h", "decr h":



Note that sometimes a sometimes a solution repeats. This is due to how these solutions are found and hence the repeats may be of interest to mathematicians. See the section "For the mathematician" at the end of the manual for more information on these solutions.

Clicking on one of the green "Get" buttons in the KnotPlot window will choose the diagram closest to the "Get" button that you clicked and take you to the TopoICE -Dynamics page where you can run energies to obtain more 3-dimensional models.

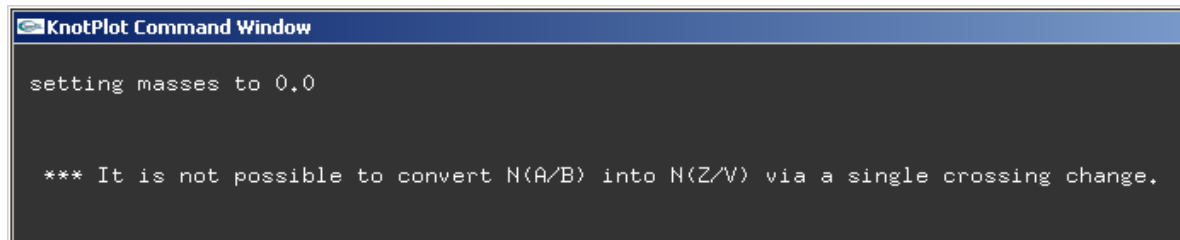


One can also restrict  $f2/g2$  by selecting the filter  $f2/g2$  box and choosing values for  $f2/g2$  (using load zoo or sliders):



Click on "Solve". If it is possible to change the first knot into the second knot via an  $(f1/g1, f2/g2)$  move, solutions showing this move will appear in the KnotPlot window as described above. Use the "up"/"down" buttons to scroll through more solutions.

If it is not possible to change the first knot into the second knot via an  $(f1/g1, f2/g2)$  move, "It is not possible to convert  $N(A/B)$  into  $N(Z/V)$  via this  $(f1/g1, f2/g2)$  move." will appear in the KnotPlot Command Window:



### For the mathematician:

Given  $A, B, Z, V, f_1, g_1$ , TopoICE-R solves the system of two tangle equations

$$N(U + f_1/g_1) = N(A/B),$$

$$N(U + f_2/g_2) = N(Z/V)$$

for  $f_2/g_2$  and  $U$  where  $U$  is assumed to be ambient isotopic to a sum of rational tangles.

There are at most four infinite families of solutions when  $U$  is rational. Hence the first 1-4 sets of solutions correspond to when  $U$  is rational.

The remaining solutions correspond to when the  $(f_1/g_1, f_2/g_2)$  move is equivalent to a  $(0/1, t/1)$  move for some integer  $t$  (see D) and finds both rational solutions for  $U$  as well as solutions when  $U$  is ambient isotopic to a sum of rational tangles.

The double branch cover of a rational knot is a lens space. Replacing the rational tangle  $f_1/g_1$  with  $f_2/g_2$  corresponds to performing surgery on the double branch cover. If  $|f_1/g_1 - f_2/g_2| > 1$ , then by the cyclic surgery theorem [CGLS], the double branch cover of  $U$  is Seifert fibered and one can show that the surgery is performed on a torus knot. By [E],  $U$  must be ambient isotopic to a sum of rational tangles. Hence all solutions are found in this case. The  $(p,q)$  in the KnotPlot window identifies the torus knot. Sometimes different  $(p,q)$ 's correspond to the same solution and hence solutions may be repeated. See [D, DS] for more information.

[CGLS] M. Culler, C. Gordon, J. Luecke, P.B. Shalen, *Dehn surgery on knots*, Bull. Amer. Math. Soc.(N.S.) **13** (1985), no. 1, 43--45.

[DS] Darcy, I. K., Summers, D. W., *Rational Tangle Distances on Knots and Links*, Mathematical Proceedings of the Cambridge Philosophical Society, **128** (2000), no. 3, 497--510.

[D] Darcy, I. K., *Solving unoriented tangle equations involving 4-plats*, J. Knot Theory Ramifications, accepted.

[ES] C. Ernst, D.W. Summers, *A calculus for rational tangles: applications to DNA recombination*, Math. Proc. Camb. Phil. Soc. **108**(1990), 489--515.

[E] C. Ernst, *Tangle equations*. J. of Knot Theory and its Ramifications, **5** no. 2 (1996), 145-159.