

## TopoICE-X examples

A few words about the knots used in the examples below:

The crossing number of a knot is the smallest number of crossings needed to draw the knot. Tables of knots up to 10 crossings are in most knot theory books [1-4] and are also available on the web [5-7]. Knots are frequently referred to by their placement in these table. For example 5.1 refers to the first five crossing knot in the Rolfsen table, while 5.2 corresponds to the second five crossing knot in this table. This table only lists knots up to mirror images. The mirror image of 5.1 is called 5.1\*. Some knots belong to the class of knots called rational. Knots that belong to this class can be represented using rational numbers. The notation  $N(a/b)$  refers to the rational knot corresponding to the fraction  $a/b$ . This notation is not unique. For example  $N(5/2)$ ,  $N(5/3)$ ,  $N(5/7)$  all refer to the same rational knot, 4.1. For more information on rational knots, please see [8-10]. Note, however, that a knowledge of rational knots is not needed for using this program since the user can refer to the pictures of the knots instead of the notation.

Example 1A, 1B, 1C show how to use the "Find solutions" button to determine if it is possible to convert one knot into another knot via exactly one crossing change. If it is possible, these examples also show how to find all different ways of performing this conversion.

Example 2 shows how to use the "Find now" button to find all knots of crossing distance one from a given knot.

Example 3 shows how to find possible reaction pathways starting from a given knot.

In these examples, we will use the following knots:

unknot = 0.1 =  $N(1/1)$  =  
Recall 0.1 stands for first  
(and only) knot with 0  
crossings. Hence it is called the unknot.



Trefoil knot = 3.1 =  $N(3/1)$  =  
(3 crossing right-handed torus knot)



Figure 8 knot = 4.1 =  $N(5/3)$  =  
(4 crossing twist knot)



5.1 =  $N(5/1)$  =  
(5 crossing right-handed torus knot)



5.2 =  $N(7/5)$  =  
(5 crossing twist knot)



[1] [Adams, Colin C.](#) The knot book. An elementary introduction to the mathematical theory of knots. *American Mathematical Society, Providence, RI*, 2004. xiv+307 pp. ISBN: 0-8218-3678-1

[2] [Kawauchi, Akio](#) A survey of knot theory. *Birkhäuser Verlag, Basel*, 1996. xxii+420 pp. ISBN: 3-7643-5124-1

[3] [Livingston, Charles](#) Knot theory. [Carus Mathematical Monographs, 24](#). *Mathematical Association of America, Washington, DC*, 1993. xviii+240 pp. ISBN: 0-88385-027-3

[4] [Rolfsen, Dale](#) Knots and links. [Mathematics Lecture Series, 7](#). Publish or Perish, Inc., Houston, TX, 1990. xiv+439 pp. ISBN: 0-914098-16-0

[5] <http://www.math.toronto.edu/~drorbn/KAtlas/>

[6] <http://www.indiana.edu/~knotinfo/>

[7] <http://www.math.uiowa.edu/~idarcy/TAB/knottable.ps>

[8] [Burde, Gerhard](#); [Zieschang, Heiner](#) Knots. Second edition. [de Gruyter Studies in Mathematics, 5](#). Walter de Gruyter & Co., Berlin, 2003. xii+559 pp. ISBN: 3-11-017005-1

[9] [Darcy, Isabel K.](#) Biological distances on DNA knots and links: applications to XER recombination. Knots in Hellas '98, Vol. 2 (Delphi). [J. Knot Theory Ramifications](#) **10** (2001), [no. 2](#), 269--294

[10] [Goldman, Jay R.](#); [Kauffman, Louis H.](#) Rational tangles. [Adv. in Appl. Math.](#) **18** (1997), [no. 3](#), 300--332.

**Example 1A:** Is it possible to convert the knot  $4.1 = N(5/3) =$



into the knot  $3.1 = N(3/1) =$

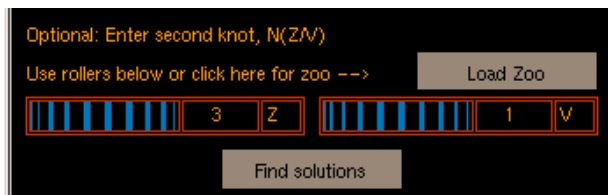


?

Enter the first knot  $N(A/B) = N(5/3)$  by using "Load Zoo" or using rollers (see TopoICE-X manual for more instructions):





Enter second knot  $N(Z/V) = N(3/1)$  using either the load zoo button or the rollers for the second knot and click "Find solutions":



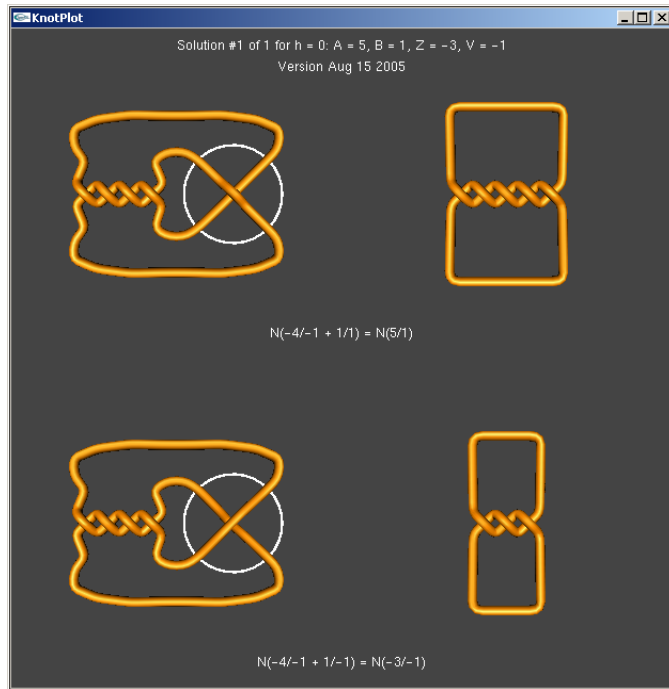
In this case, the words "It is not possible to convert  $N(5/3)$  into  $N(3/1)$  via a single crossing change." appears in the KnotPlot window. Hence the knot  $N(3/1)$  cannot result from a single topoisomerase action starting from  $N(5/3)$ .

(note: currently words only appear in command window, not yet in KnotPlot window)

**Example 1B:** Is it possible to convert  $N(5/1) =$   into  $N(3/1) =$   ?

Enter the two knots as described in example 1A.

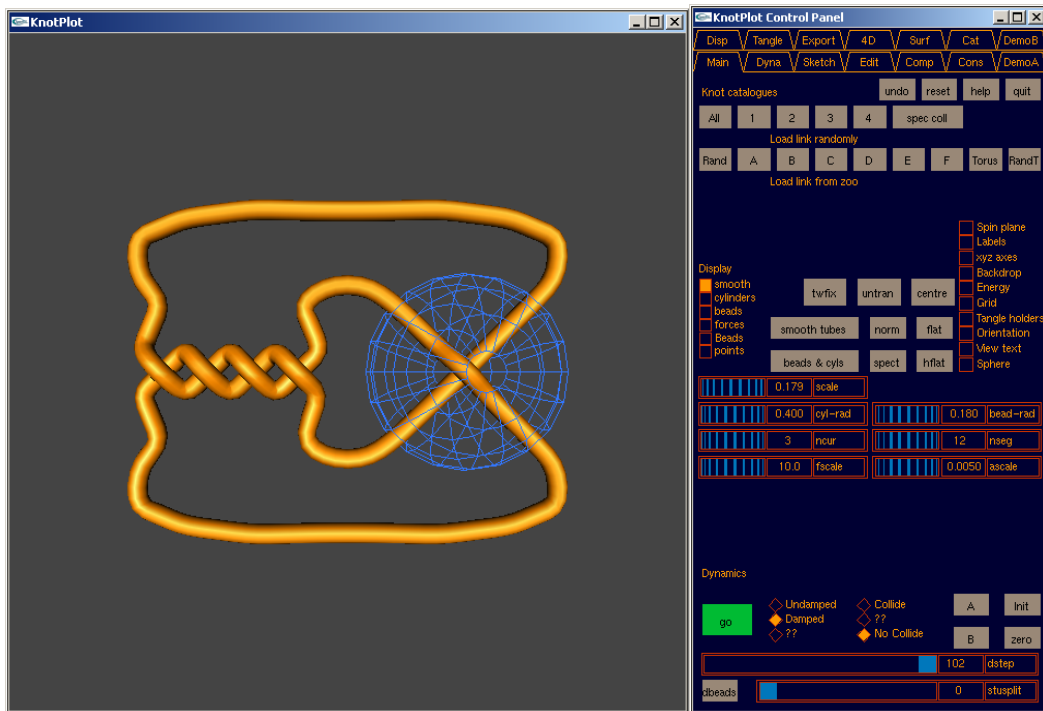
Solution #1 of 1 appears in the KnotPlot window:



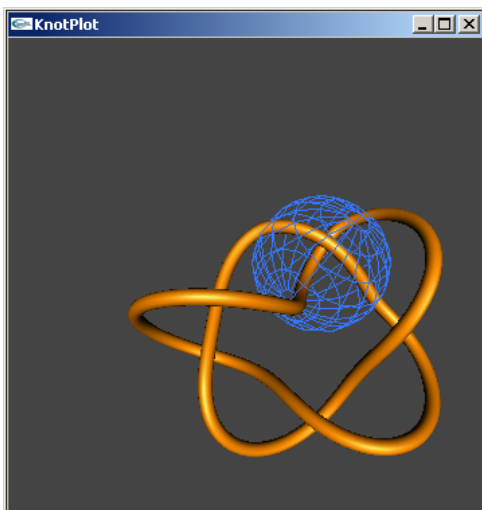
The notation and mathematics of rational tangles is used to draw these diagrams resulting in diagrams which could be significantly improved for biological modeling. To obtain more 3-dimensional configurations, click on "get UL" or "get UR", etc. For example clicking on get UL will select just the upper left diagram in the above KnotPlot window.



This will also take you to the Main KnotPlot control panel where you can run knot energies to obtain better 3D diagrams:



Click on the go button to relax this knot:  
 By default, the region bound by the topoisomerase (represented by the blue sphere) is fixed ...  
 (right now just the 4 endpoints).  
 After running a knot energy we obtain:



By one solution, we mean that there is exactly one way, topologically speaking, to convert  $N(5/1)$  into  $N(3/1)$  via a single crossing change. However, any of these 5 crossings can be changed in this drawing of the knot  $N(5/1)$  to obtain  $N(3/1)$ . Hence it might look like there are 5 different ways to convert  $N(5/1)$  into  $N(3/1)$  via a crossing change. However, they are all topologically equivalent in that no matter which crossing is changed, the configuration outside of where the crossing change occurs are all topologically equivalent. In fact, if knot energies were run to minimize the energy of the outside configuration while keeping the crossing fixed, then they would all minimize to identical configurations no matter which crossing is fixed:

**Example 1C:** Is it possible to convert  $N(5/3) =$

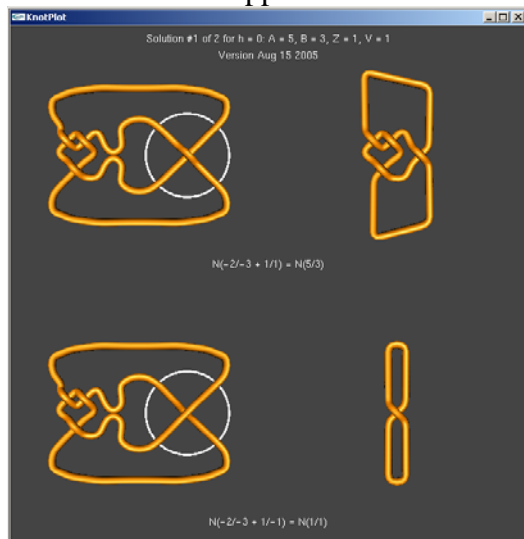


into the unknot  $= N(1/1) =$

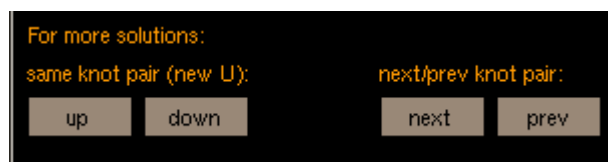


Enter the two knots as described in example 1A.

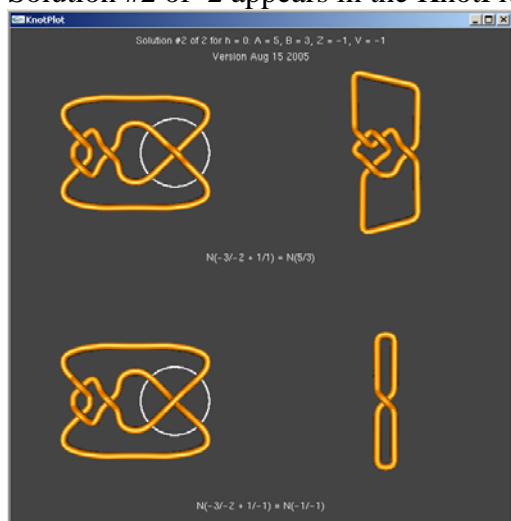
Solution #1 of 2 appears in the KnotPlot window:



In this case there are two topologically distinct ways to convert  $N(5/3)$  into  $N(1/1)$ . Click on "up" or "down" buttons to see more ways of converting  $N(5/3)$  into  $N(1/1)$  via a single crossing change.

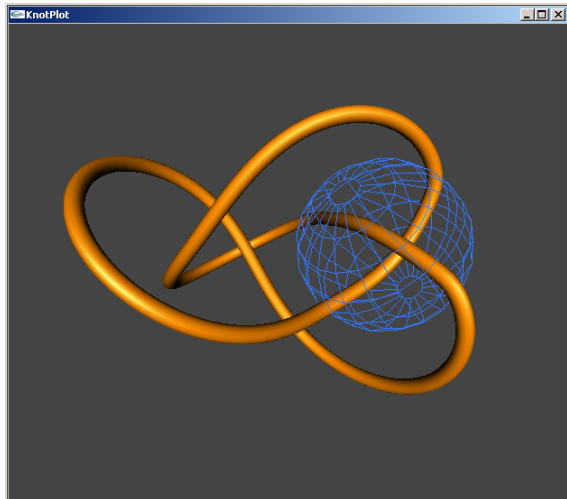


For example, the second solution appears in the KnotPlot window by clicking on "up":  
Solution #2 of 2 appears in the KnotPlot window:

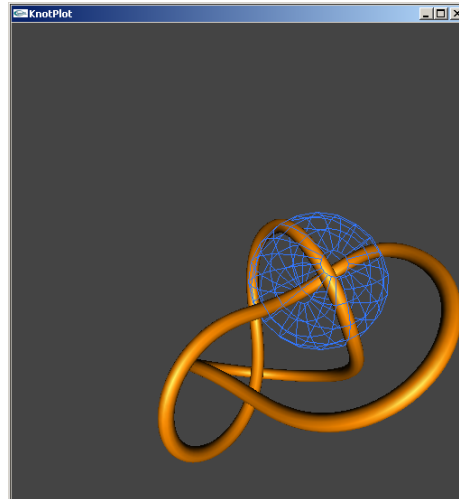


We can mathematically prove that these two ways of converting the figure 8 knot =  $4.1 = N(5/3)$  into the unknot =  $N(1/1)$  are topologically different. We can also see that these are topologically different solutions by relaxing the configuration outside of where the crossing change occurs. For example, for each of these two solutions, if we click on "get UL" and "run", we obtain the following:

Solution 1:



Solution 2:



Note that the configuration outside the sphere for solution 1 looks different than the configuration outside the sphere for solution 2. This is not a mathematical proof that they are different, but a proof does exist whenever KnotPlot finds more than one solution.

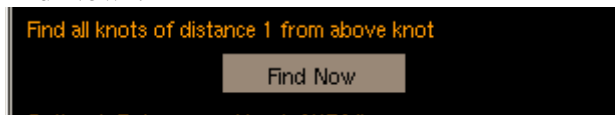
**Example 2:** Find all possible rational knots which can be obtained from a given knot, for example  $5.1 = N(5/1) =$  , via one round of topoisomerase action:



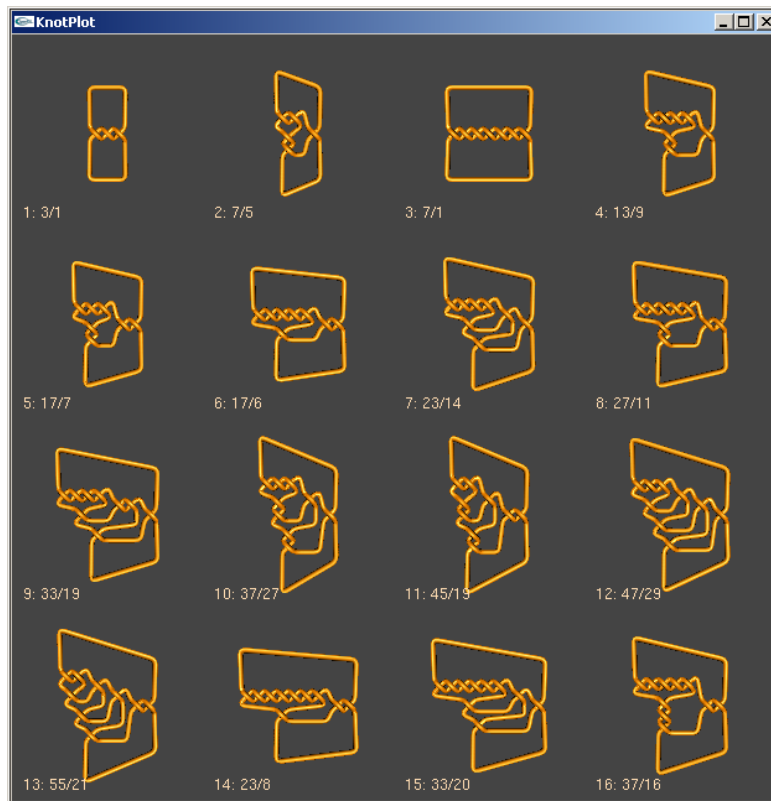
Enter the knot  $5.1 = N(5/1)$  by using "Load Zoo" or rollers (see TopoIce Manual for more directions):



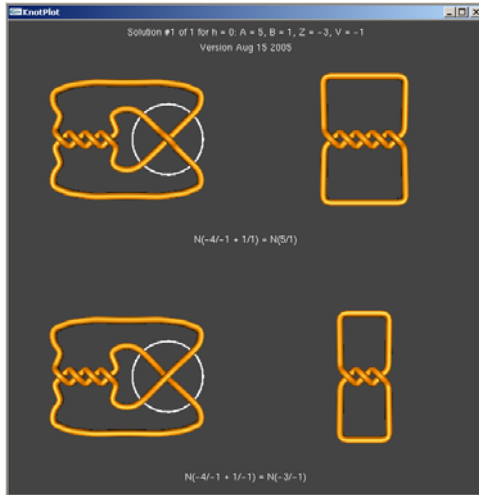
To find knots which can be obtained from the above knot via one round of topoisomerase action, click on "Find Now":



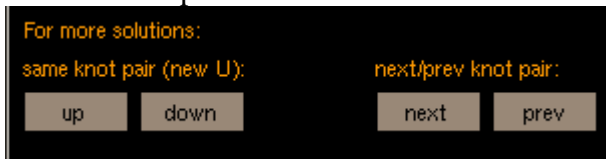
This will find all rational knots up to 13 crossings of crossing distance one from the rational knot  $N(A/B)$ . They will be displayed by crossing number with the smallest crossing number knots listed first.



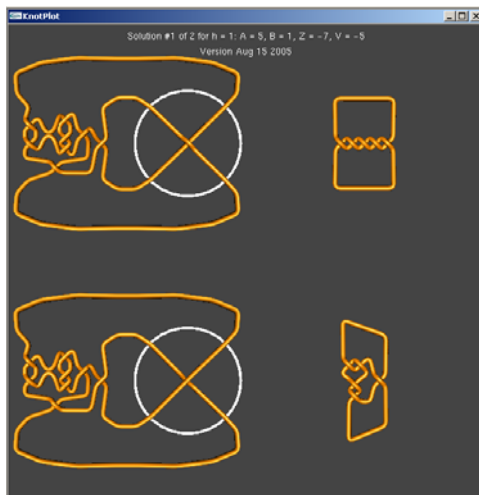
For example, the smallest crossing knot that can result from  $5.1 = N(5/1)$  by one topoisomerase crossing change is the knot  $3.1 = N(3/1)$ . Click on this knot to see this topoisomerase action:



Click on "Find Now" again to get back the list of knots of crossing distance one from 5.1 or click on next/prev to see the next smallest crossing number knot that can result



In this case, it is the five crossing knot  $5.2 = N(7/5)$



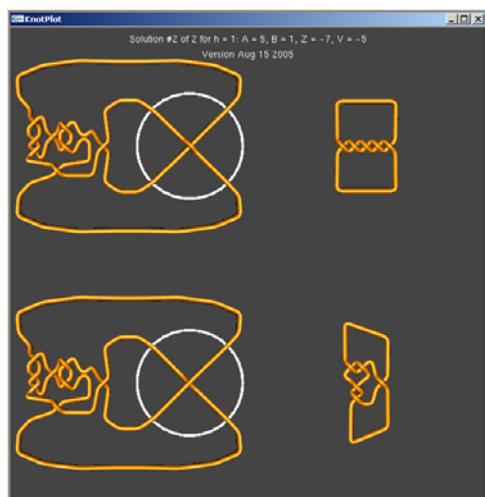
We see that there are two ways of converting 5.1 to 5.2. Click on "up" or "down" buttons to see more ways of converting  $5.1 = N(5/1)$  into  $5.2 = N(7/5)$  via a single crossing change.



For more solutions:

same knot pair (new U):      next/prev knot pair:

up    down      next    prev



To see more knots of crossing distance one from  $5.1 = N(5/1)$ , continue to click on "next".

**Example 3a:** Find all possible pathways starting from the knot  $5.1 = N(5/1) =$  including all knots with the same or fewer crossings.



Enter the knot  $5.1 = N(5/1)$  by using "Load Zoo" or rollers (see TopoIce Manual for more directions):



Click on "R path" or "R path r" (R path r runs an energy to better display the reaction pathway graph).

