

TopoICE-X Manual

Abstract: TopoICE-X will

- 1.) Find all rational knots up through 13 crossings that can be obtained from a given rational knot by changing one crossing (see example 1, page 3).
- 2.) Display all topologically different ways to convert a given rational knot to another rational knot via a crossing change (see examples 2a, page and 2b, page).
- 3.) Find all shortest pathways between a given pair of rational knots involving rational knots with less than 14 crossings (see example 3, page). Note there could be shorter pathways than that found by TopoICE-X if non-rational knots were included.

Table of Contents

1.) Introduction to Knots.	1
2.) Downloading KnotPlot and starting TopoICE-X.....	2
3.) To find knots of crossing distance one from $N(A/B)$ using the button marked "Find Now".....	3
4.) To determine if it is possible to convert a given knot into another knot via a crossing change.....	6
5.) Finding Pathways.....	8
6.) References.....	10
7.) TopoICE-X control panel.....	11
8.) KnotPlot summary.....	12
9.) KnotPlot Main control panel.....	13

1.) Introduction to Knots.

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 [4], 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.

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)



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



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



2.) Downloading KnotPlot and starting TopoICE-X.

Download KnotPlot from knotplot.com/download

You may choose PC, Mac, Linux or SGI versions. The free version may be downloaded by selecting the link to the appropriate version for your operating system (about $\frac{3}{4}$ down the webpage). There is also an upgraded version available for \$24.95. The upgraded version has some additional features not directly related to TopoICE. TopoICE is the same for both the free and upgraded versions. If needed, you may obtain additional download instructions on the following websites.

Mac: knotplot.com/download/KPmac_install.html

PC: knotplot.com/download/KPwindows_install.html

To run KnotPlot, double click on the KnotPlot icon (in KnotPlot folder or on Desktop if you created a Desktop KnotPlot icon):



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



At the bottom, you will see some buttons. If you are not already in TopoICE-X, click on the button marked "→TopoICE-X".



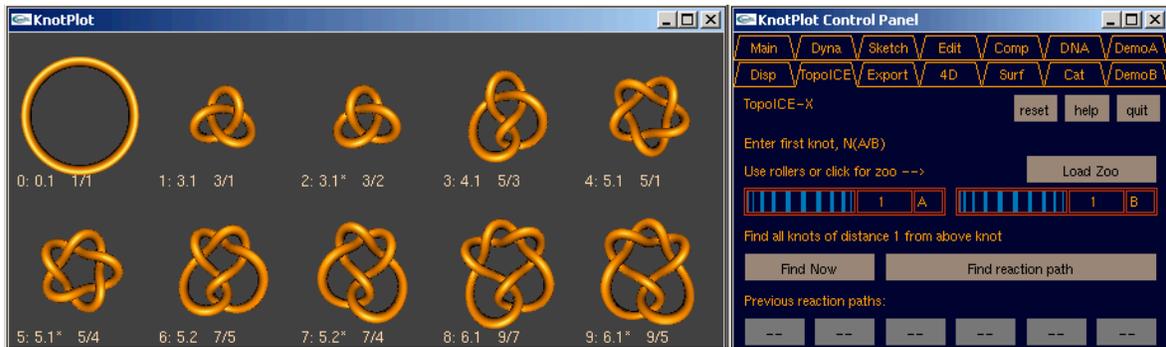
Enter a knot by using the zoo or rollers:



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

A zoo of knots will appear in the KnotPlot Window. On some computers, the zoo may not display properly. If you see only every second knot or nothing at all, you may want to change the setting for the "progressive" zoo feature on the Main control panel (just toggle the radio button located near the top of that panel).

You can enter a knot by clicking on it. The zoo will disappear from the KnotPlot window after a knot has been selected.



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, catalog type pictures of knots [4] 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.

3.) To find knots of crossing distance one from $N(A/B)$ using the button marked "Find Now".

Example 1: Find all possible rational knots which can be obtained from a given knot, for

example $3.1 = N(3/1) =$  *, via one round of topoisomerase action:*

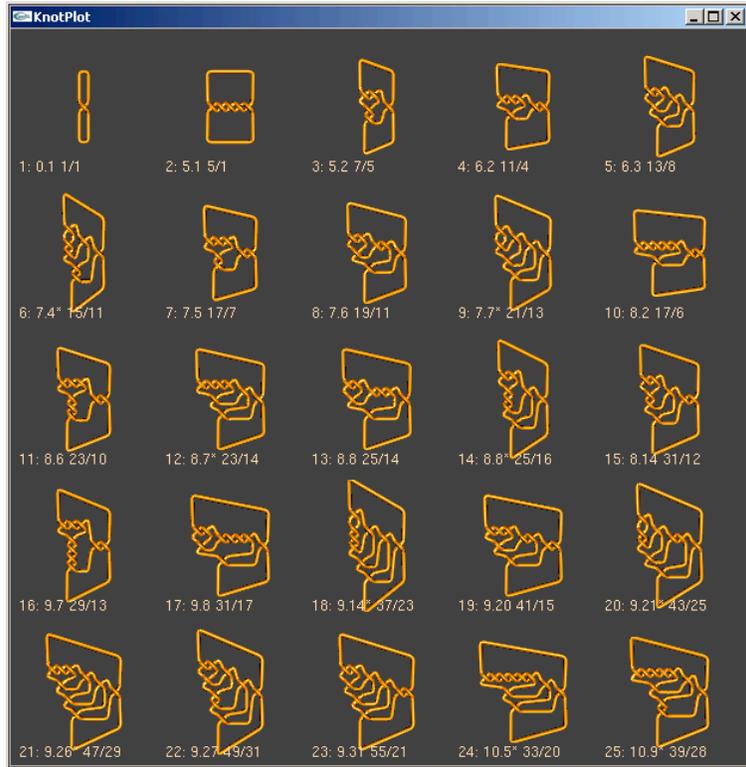
Enter the knot $3.1 = N(3/1)$ by using "Load Zoo" or rollers:



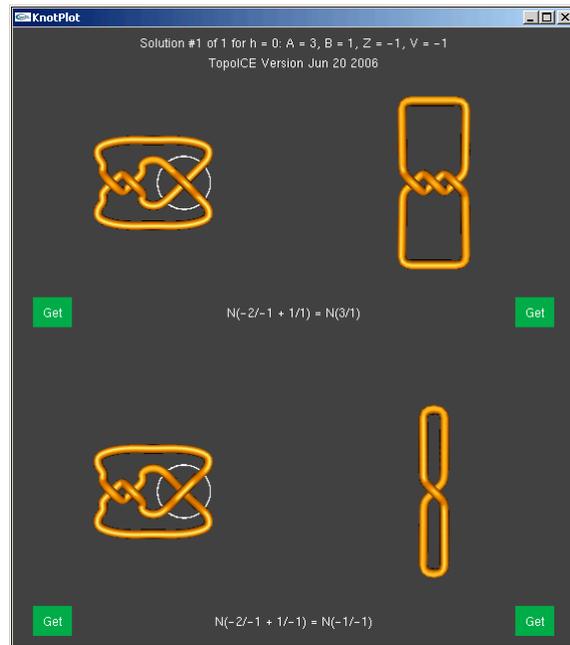
To find knots which can be obtained from the above knot via one round of topoisomerase action, click on "Find Now":



This will find all rational knots up to 13 crossings which can be obtained from the rational knot $N(A/B)$ by changing one crossing. They will be displayed in the KnotPlot window by crossing number with the smallest crossing number knots listed first. For example, the following are knots of crossing distance one from the three crossing knot $3.1 = N(3/1)$:



Click on any of the knots to see how the knot $3.1 = N(3/1)$ can be converted into this knot via a crossing change. For example, if the unknot $0.1 = N(1/1)$ is selected, the KnotPlot window will display the following:



The top two figures show the trefoil knot. In the top left figure, a circle is drawn around the crossing which will be changed to give the knot in the bottom right. In this case an unknot results. The figures on the right are simplified figures of the ones on the left.

To see more solutions:



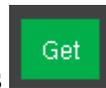
"up" or "down" buttons:

Note there could be more than one way to transform one knot into another knot via a crossing change. Click on the grey box marked "up" or "down" to see the different ways to convert between two given rational knots.

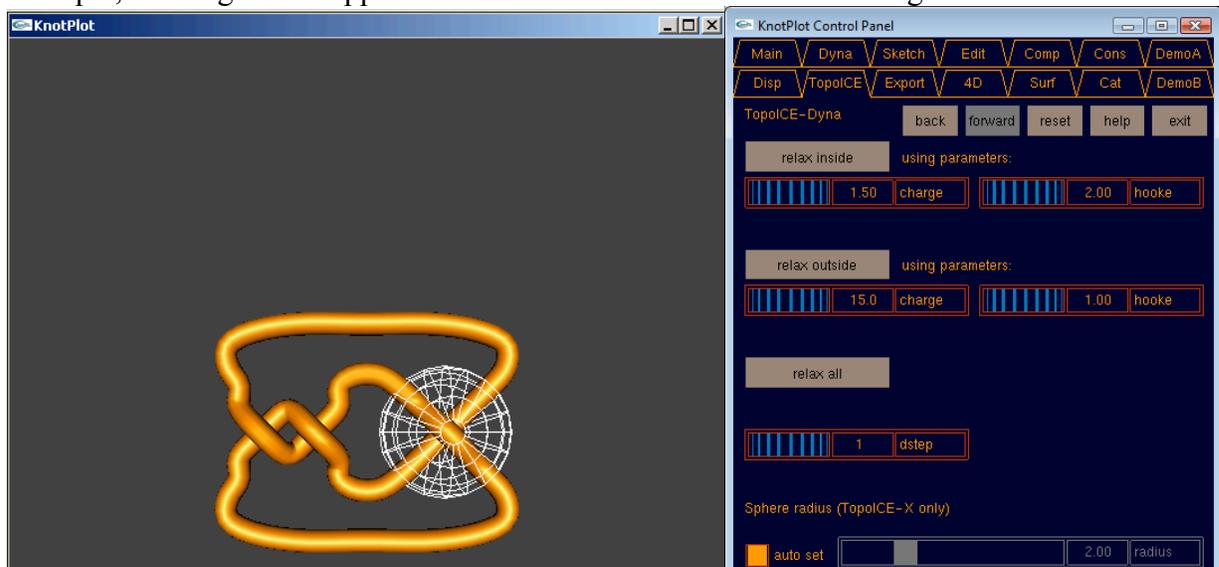
"next" and "prev" buttons:

Click on the grey box marked "next" to see the next knot in the list of rational knots of crossing distance one from the rational knot $N(3/1)$. Click on the grey box marked "prev" to see the previous knot in the list of rational knots of crossing distance one from the rational knot $N(3/1)$.

The notation and mathematics of rational tangles is used to draw these diagrams resulting in diagrams which could be significantly improved for biological modeling. However, one can use the energy functions within Knotplot to simplify diagrams. For more information on these energies, click on the "help" button on the Dynamics panel or see Rob Scharein's thesis, available at knotplot.com/thesis, for more information on these energies.



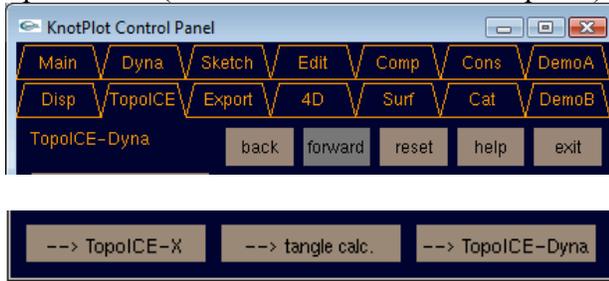
Clicking on one of the green "Get" buttons will choose the diagram closest to the get button that you clicked and take you to the TopoICE -Dynamics page where you can run energies. For example, clicking on the upper left "Get" button results in the following:



Click on "relax inside" to relax the tangle inside the sphere. Click on "relax outside" to relax the tangle outside the sphere. Click "relax all" to relax the entire knot. To speed up the calculations,

change dstep (display step). A redraw of the knot occurs every dstep dynamical step. The radius of the sphere can be changed using the radius slider. Uncheck auto set before attempting to change the radius.

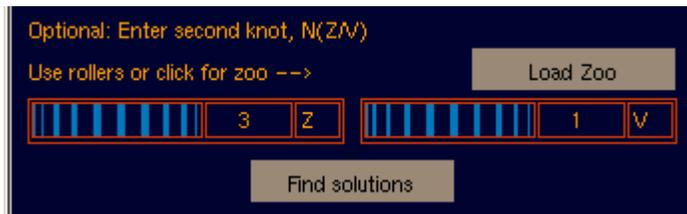
To return to the TopoICE-X panel, click on either the “back” button (top of KnotPlot control panel) or the button marked "→TopoICE-X" (bottom of KnotPlot control panel).



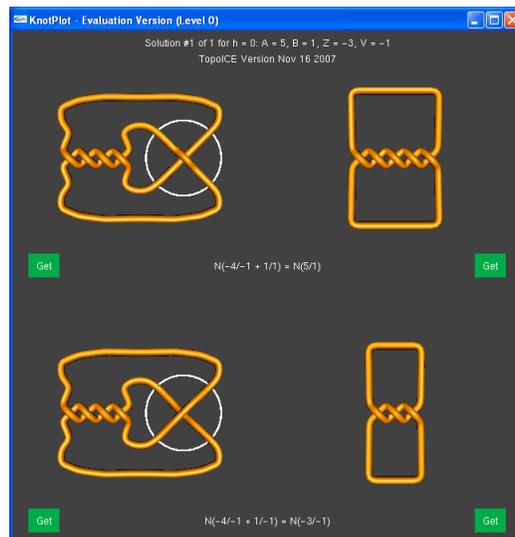
4.) To determine if it is possible to convert a given knot into another knot via a crossing change.

Example 2a: Is it possible to convert $N(5/1) =$  into $N(3/1) =$  ?

Enter first knot as described above. Enter second knot using either the load zoo button or the rollers for the second knot:

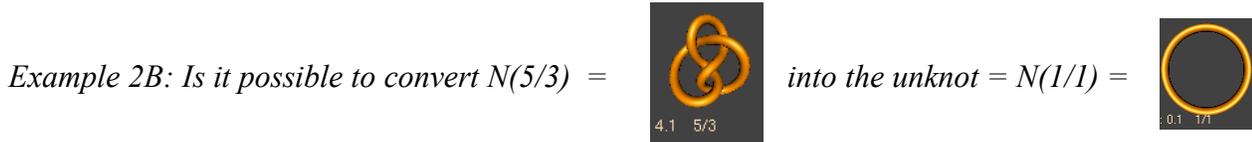


Solution #1 of 1 appears in the KnotPlot window:



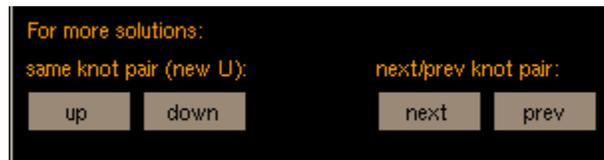
By one solution, we mean that there is exactly one way, topologically speaking, to convert $N(5/1)$ into $N(3/1)$ via a single crossing change. However, any of the 5 crossings in this drawing of the

knot $N(5/1)$ can be changed 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 if the geometry of the bound crossing is the same. 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:



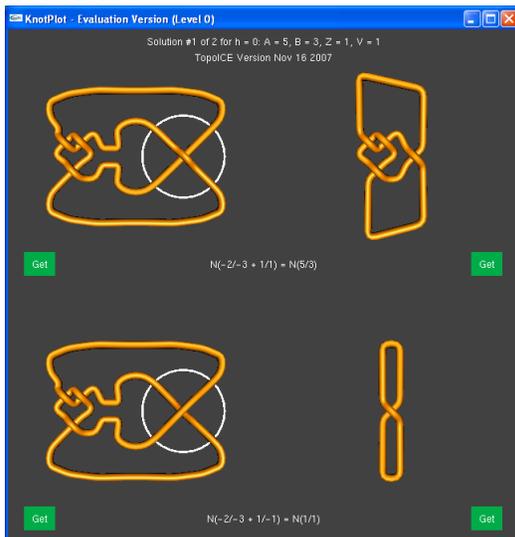
Enter the two knots as described in example 1A.

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.

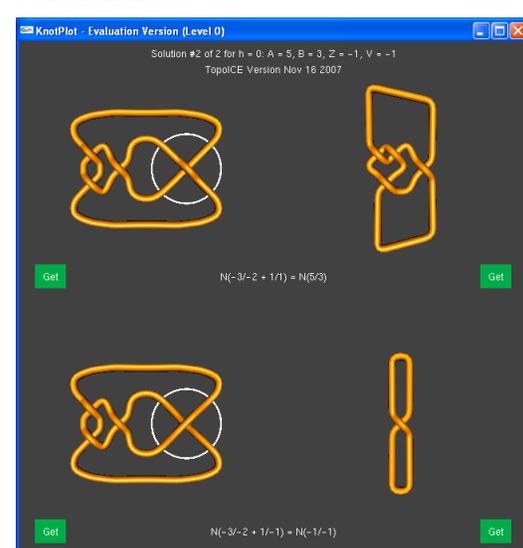


For example, the second solution appears in the KnotPlot window by clicking on "up":

Solution 1:

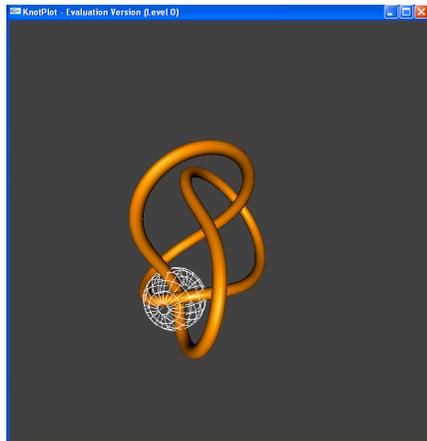


Solution 2:

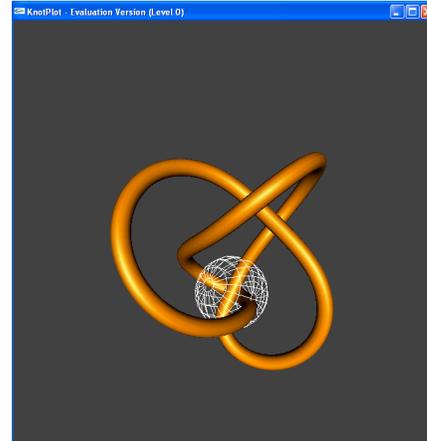


We can mathematically prove that these two ways of converting the figure 8 knot $= 4.1 = N(5/3)$ into the unknot $= N(1/1)$ are topologically different. We can also see that these are topologically different solutions by relaxing the configuration outside of where the crossing change occurs. For example,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

5.) Finding Pathways.

Example 3: Is it possible to convert the knot $3.1 = N(3/1) =$



into the knot $4.1 = N(5/3) =$



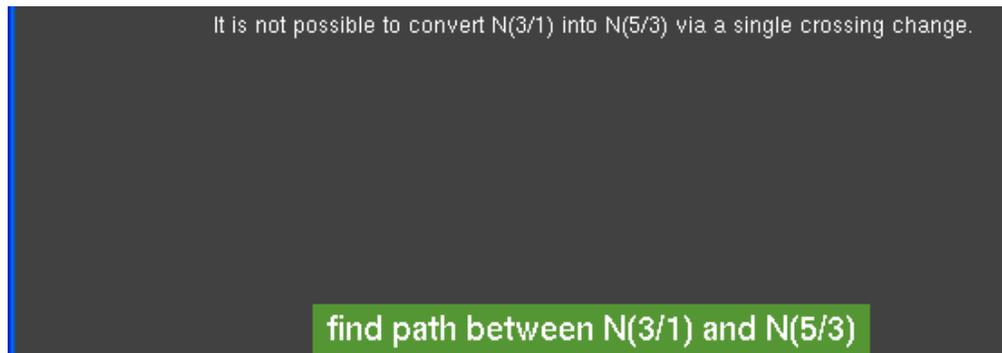
If it is not possible, find pathways between these knots.

Enter the two knots as described in examples 1 and 2a.

Click on "Find solutions". If it is possible to change the first knot into the second knot via a crossing change, a solution showing the crossing change will appear in the KnotPlot window as described above.

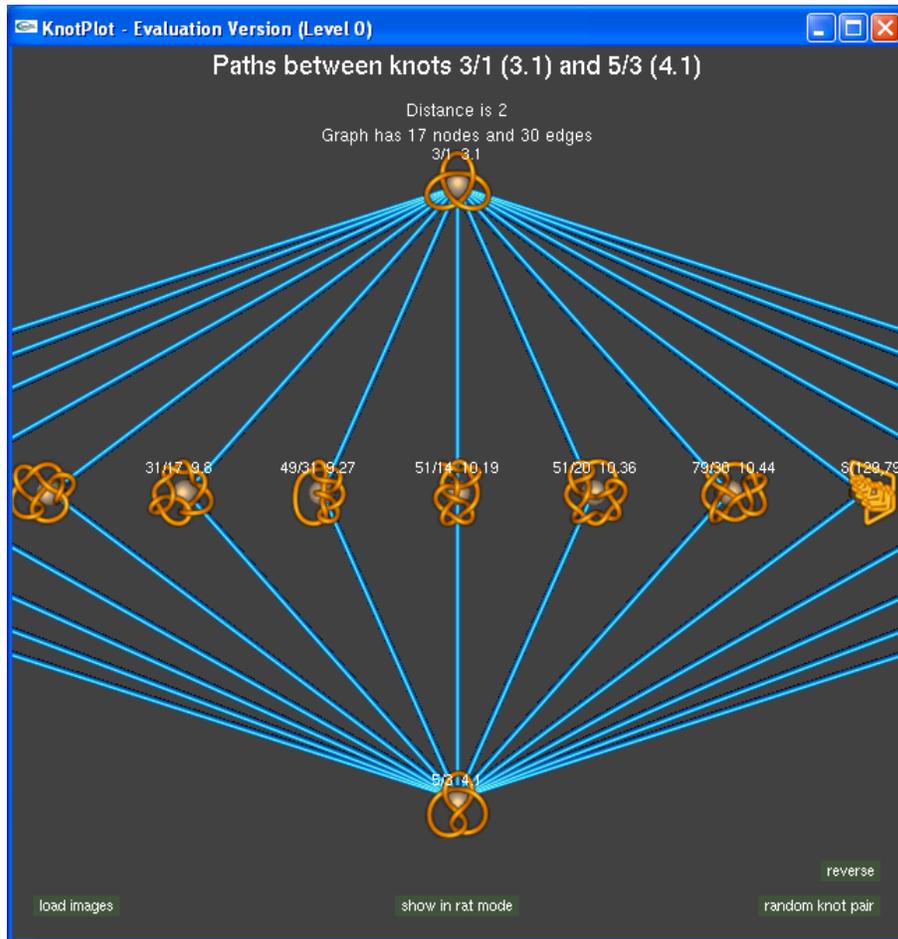
If it is not possible to change the first knot into the second knot via a crossing change, "It is not possible to convert $N(3/1)$ into $N(5/3)$ via a single crossing change." will appear in both the KnotPlot and the KnotPlot Command Windows:

Click on the green "find path between $N(3/1)$ into $N(5/3)$ to obtain all shortest pathways between these knots involving



rational knots with 13 or fewer crossings. Note there could be shorter pathways if nonrational knots were allowed.

If the unknot, $N(1/1)$ was selected as the first knot and if the five crossing knot $N(5.1)$ was chosen to be the second knot, then the following will appear in the KnotPlot window:



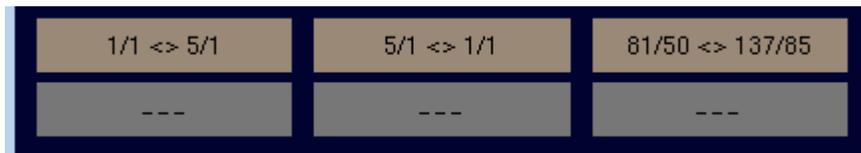
Click on “load images” (bottom right of KnotPlot window) to load knot images.

Click on “show in rat mode” (bottom center) to display images using rational tangle notation or click on “show in cat mode” to display catalog-like images [4] when the crossing number of the knot is less than 11.

Click on “reverse” (bottom left) to reverse the pathway or click on “random knot pair” to see pathways between a randomly chosen pair of knots.

Click on an edge to see the conversion via a crossing change from the upper knot to the lower knot connected by this edge.

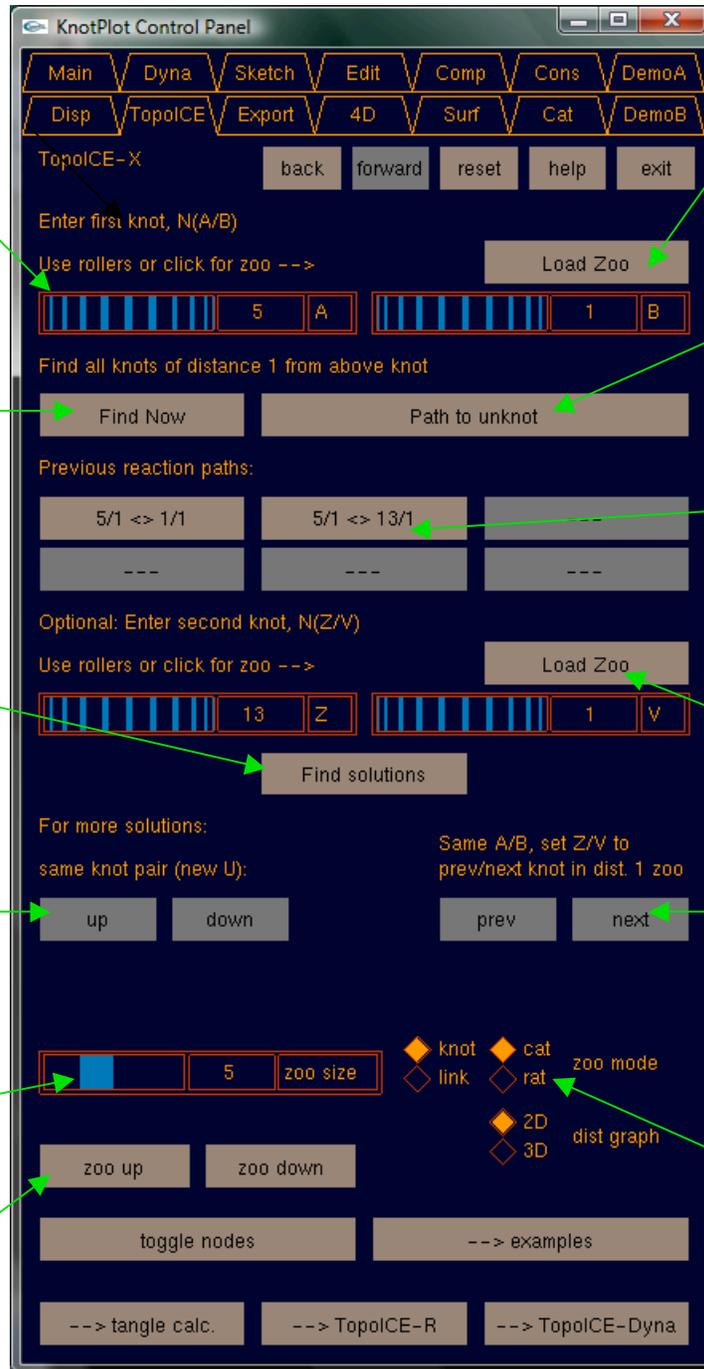
The last six requested reaction pathways are stored and can be easily accessed by clicking on the desired reaction pathway button on the KnotPlot control panel:



6.) Reference.

- [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.

7.) TopoICE-X control panel



You can also load a knot by entering its fraction and hitting return.

Click to find all rational knots of distance 1 from the first knot

Click find solutions to determine if it is possible to convert the first knot into the second knot via one crossing change.

If a solution is found, you can view different solutions using these buttons.

Determines number of knots displayed per row

To display more knots

Load first knot

Find shortest paths to unknot involving rational knots (note there could be shorter paths involving non-rational knots).

Up to six pathways are stored and can be viewed by clicking one of these boxes.

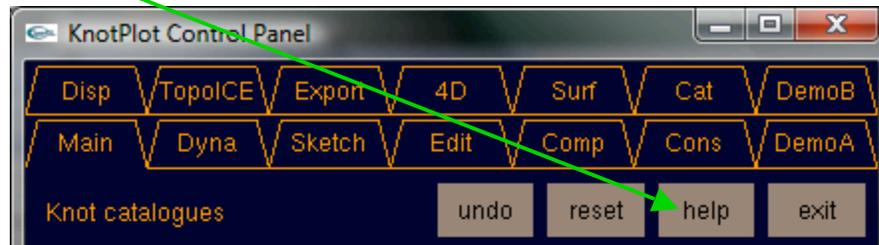
Enter second knot using load zoo or fraction

These buttons allow one to toggle through solutions for knots of distance 1 from first knot.

One can display knots using rational tangle notation or as in Rolfsen's catalog.

8.) KnotPlot summary. TopoICE-X is part of KnotPlot which has a variety of tools for manipulating and visualizing knots. A brief summary of the control panels available in KnotPlot is given below. For more information about these control panels, click on that control panel's help button

Control
Panels:



Main: See p. 13

Display: to change display settings.

Dyna: can change settings for various forces that affect the dynamical behaviour of knots when the “go” button is clicked. The “go” button changes the conformation of a knot based upon the selected dynamics. Frequently used to simplify a knot diagram.

TopoICE: Includes TopoICE-X for modeling topoisomerase action, TopoICE-R for modeling recombinase action, TopoICE-Dyna for running dynamics on tangle solutions found by TopoICE. The tangle calculator is not part of TopoICE, but can be accessed from this panel. The tangle calculator can be used to draw a variety of tangles including rational tangles.

Sketch: For sketching a knot.

Export: To export figures in a variety of formats including eps, bitmap, and 3D surface models.

Edit: To edit a knot. For example, one can delete/add/move vertices and edges.

4D: 4-dimensional knots.

Comp: For computing physical properties, topological invariants, etc of knots.

Surf: To change coloring of knots.

Cons: To construct a torus knot, Lissajous knot, chains, braids.

Cat: To load a knot from catalogues of knot

DemoA: A number of demos are available. ACN and rat tang may be of particular interest.

DemoB: More demos.

9.) Main Control Panel

The image shows the KnotPlot Control Panel interface with several callout boxes providing instructions:

- undo --- often can be used to undo an operation.** (points to the 'undo' button)
- reset - useful to get KnotPlot into its initial state. If there are problems, click this button.** (points to the 'reset' button)
- To display a help page for this control panel. Click for info on buttons not explained here.** (points to the 'help' button)
- quit KnotPlot. you can also use the ESC key at any point.** (points to the 'exit' button)
- load knots from the standard catalogues included with KnotPlot. Click on help for more information about these catalogues.** (points to the 'Knot catalogues' section)
- progressive - Try changing the setting of this if the knot zoos don't display properly (either every second knot or none at all).** (points to the 'progressive' checkbox)
- Knots are display either as 'smooth tubes' (the default), or as 'beads & cyls', which are the vertices and edges representing the knot.** (points to the 'smooth tubes' and 'beads & cyls' options)
- To scale the scene. Can also use right mouse button** (points to the 'scale' slider)
- radius of the smooth tube or cylinder** (points to the 'cyl-rad' slider)
- Change radius of beads.** (points to the 'bead-rad' slider)
- Dynamics Section** (points to the 'Dynamics' section)
- This is a subset of what is displayed on the 'Dyna' control panel. Click on the 'Dyna' tab and read the help provided there for more info.** (points to the 'Dynamics' section)

Use the following mouse buttons to change the view (click down and drag):

left --- rotate the scene with this button using a 'virtual trackball'

middle --- translate the scene

right --- scale the scene (move mouse to left to reduce, move mouse to right to enlarge)

None of these operations change the knot itself, just how it is viewed. You can undo any of these operations using the 'untran' button.