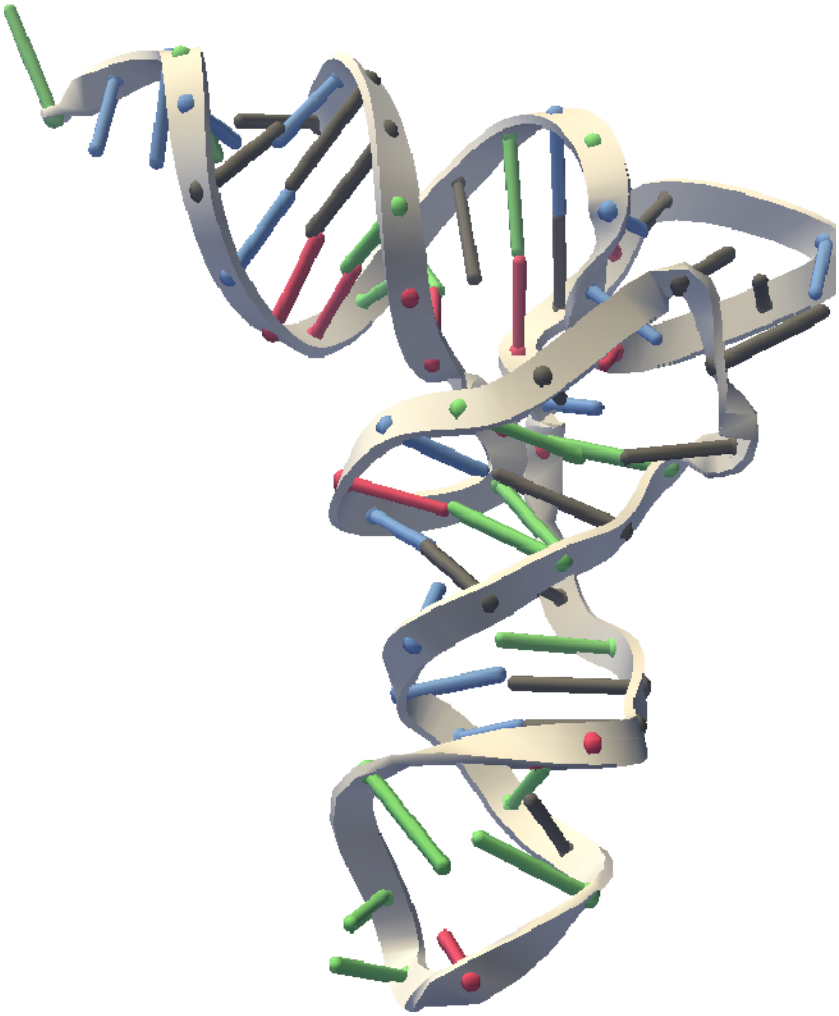
Tornado™



User's Manual

Release 1.0

October 24, 2007

Website: https://simtk.org/home/rna-viz-proto

Copyright and Permission Notice

Table of Contents

Introduction

This document is a work in progress.

What is Tornado?

SimTK Tornado is a dynamic visualization tool for coarse grain (lumped) representations of RNA and/or protein structure. By shifting the focus from individual atoms to higher order structures, such as double helical duplexes, the scientist's attention is naturally focuses toward a larger scale. Biologists will be able to use their intuition to interactively refold RNA structures and produce morphs from one structure to another.

Purpose

Provides an easy to use application for animating and visualizing RNA and other macromolecular structures.

Audience

Biomedical and computation researchers interested in RNA, molecular motions, and folding pathways.

Installing and Running

System Requirements

Platforms: Windows, Mac, and Linux
Java 1.5 or higher required (http://java.sun.com/)

Java Web Start

Tornado uses Java Web Start to load and run directly from the download page at SimTK.org. The downloaded files are stored in a special area on your computer called the Java Web Start cache, so Tornado should start more quickly on the second and subsequent runs.

Download Application

1. Find the tornado project page at **SimTK.org** (Fig 1).
2. Click on **Downloads** on the left side menu (Fig 2).
3. Click on **Tornado1.0.527.jnlp** file on the right side of the screen(Fig 3).
4. If you have not already logged in, please do so now.
5. Describe how you expect to use this software and click **Download Now** (Fig 4).
6. ToRNAdo will begin to download automatically.
7. If a window saying **Warning – Security,** appears, "The application's digital signature has been verified. Do you want to run the application", click the **Run** button.

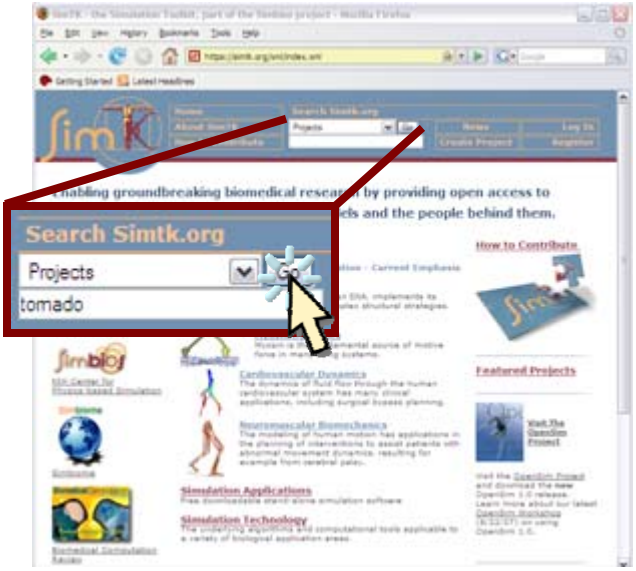


Fig. 1 – Find the Tornado project at SimTK.org

Fig. 2 - Find the Tornado download link at the left of the Tornado project page

Fig. 3 - Select the latest Tornado JNLP file at the right of the Tornado download page

Fig. 4 - Describe how you expect to use this software in the box and click "Download Now"

8. The **Opening Tornado1.0.527.jnlp** will appear, select Open with and click **OK** (Fig 5)
9. Wait a few seconds and the **SimTK ToRNAdo** application will appear (Fig 6).
10. The tornado application is now running on your computer.

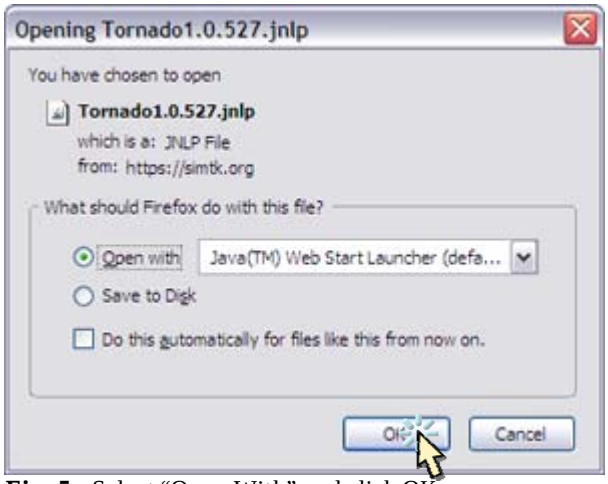


Fig. 5 - Select "Open With" and click OK

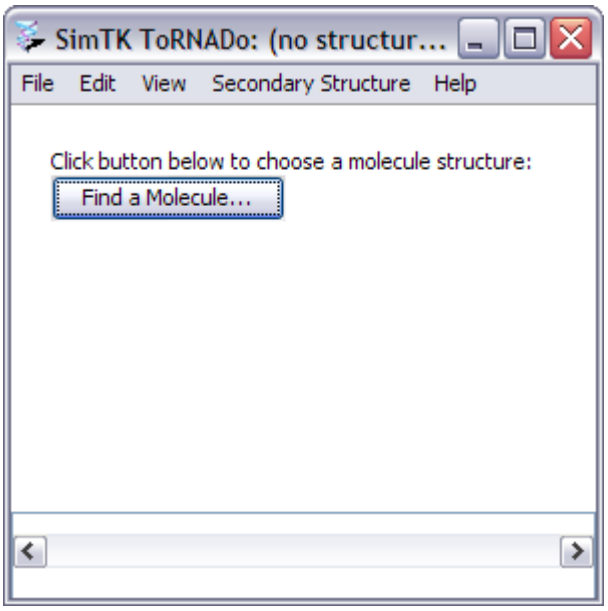
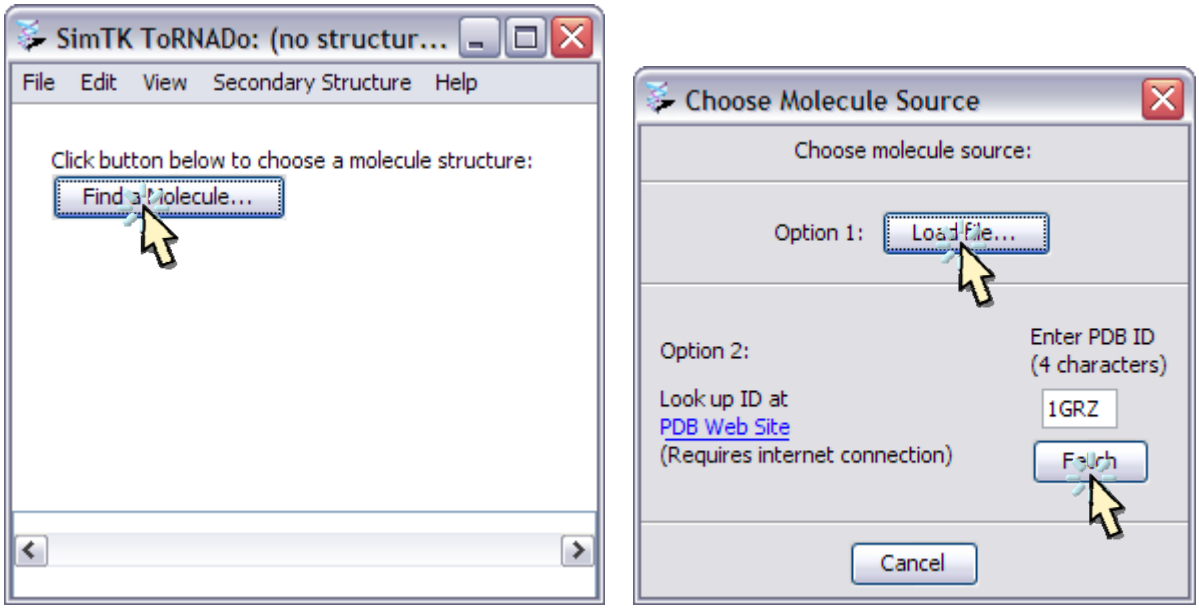


Fig. 6 - The tornado application is now running on your computer.

Note: If you do not see the window in Figure 8, please consult the section "Troubleshooting Java Web Start" on page 9.

Tutorial

After downloading and running Tornado as described in the previous section of this document, you should see the Tornado application window, as shown below:



Loading Molecules

- Click on **Find a Molecule** button to choose a molecule structure.
- Option 1: click on the **Load file** button to choose a molecule saved locally.
- Option 2: enter the molecule ID **(PDB ID)** and click the **Fetch** button to load molecule from the PDB Web Site (requires internet connection).
- Molecule will appear on the screen with default view **Residue Balls**.
- To load a new molecule, go to the **File** menu and click **Load PDB Molecule** and choose option 1 or 2.

Change Molecule Views

- Go to the **View** menu, click on **Molecule Style**.
- A menu of various view styles will come up.
- Choose desired style. See the subsection “representations” under Molecular Visualization for more information.

Save Current Molecule View as an Image

- Go to the **File** menu, click on **Save PNG Image**.
- Under **File Name**, choose a desired name followed by **.png**
- Save the file in the desired location.

Rotating, Zoom In/Out Molecules

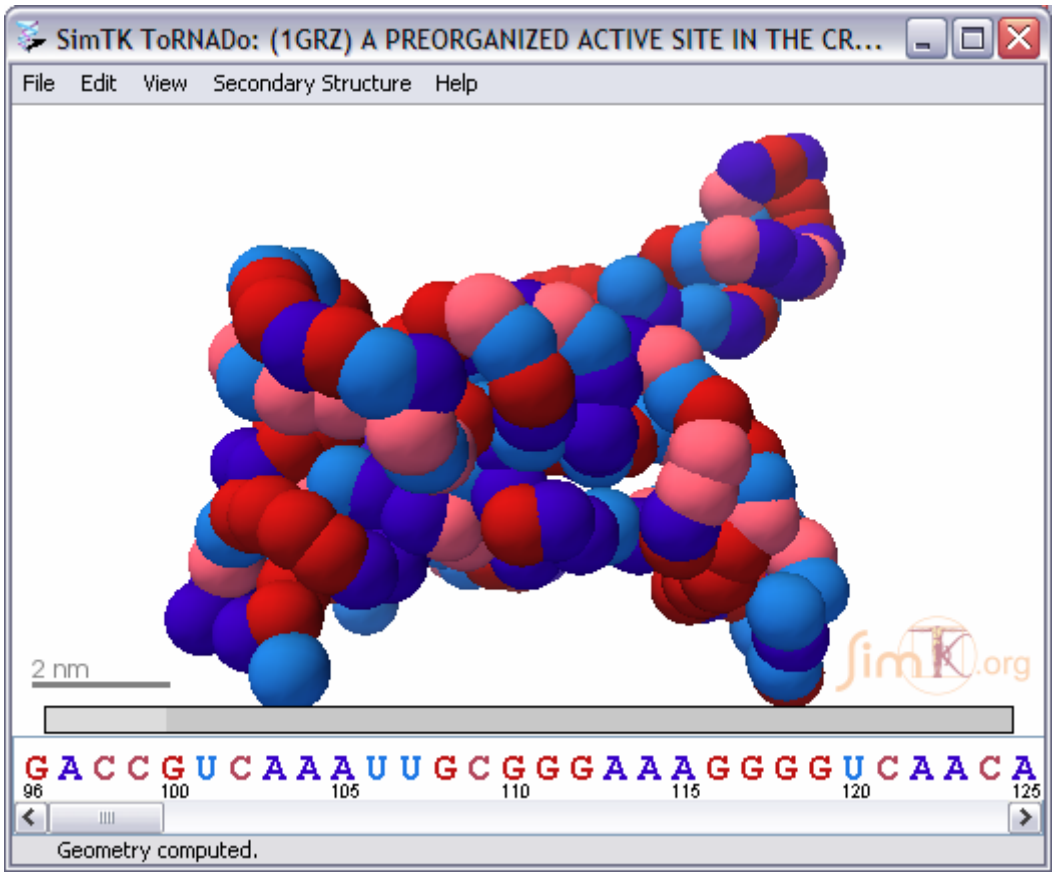
- Go to the **View** menu, click on **Rotation**.
- A menu of various rotation styles will come up.
- Choose desired rotation.

  Manual Rotation

  - Left click and hold the mouse on current screen.
  - Move up, down, left, right to rotate as desired.

  Zoom In/Out

  - Right click and hold mouse on current screen.
  - Move up or down to zoom in and out.



Molecular Visualization

Selecting residues

Select one or more residues to highlight those residues in the display.

The following mouse gestures apply to all molecule displays in Tornado, including the linear sequence display, 3D structure display, and secondary structure display.

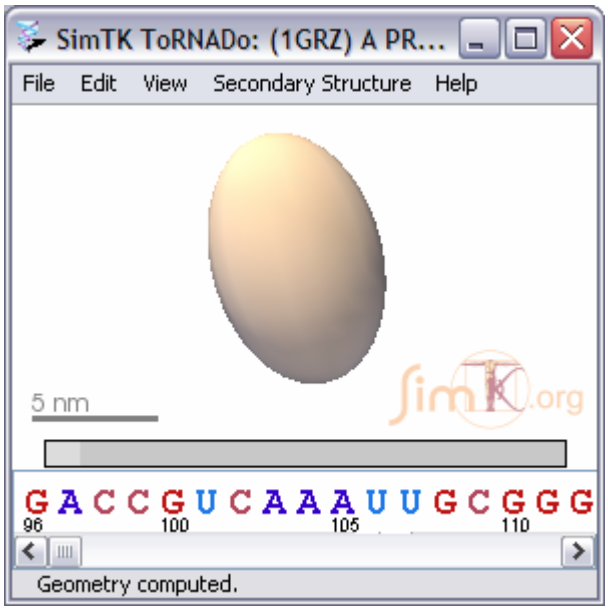
- Click on a residue to select that residue
- Ctrl-click on a residue to add that residue to the list of selected residues.
- Double-click on a residue to center the display on that residue.
- Shift-click to add all residues between the most recently selected residue and the current residue to the list of selected residues.

Representations

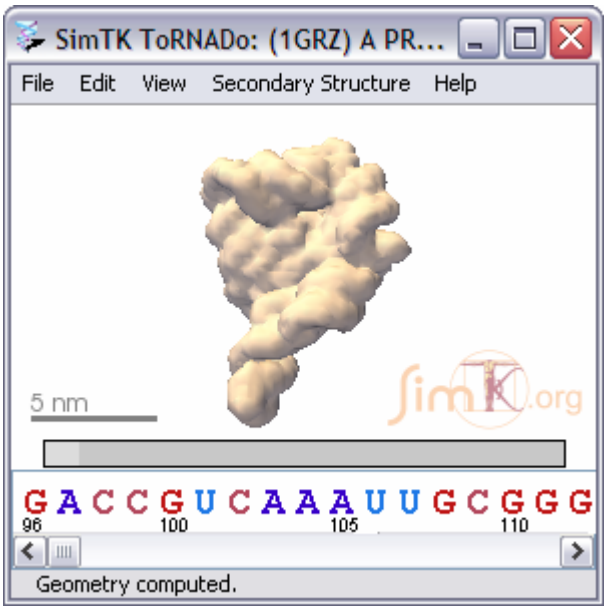
	RNA/DNA	Protein	Ligands	Water
Molecule Ellipsoids	ellipsoid	ellipsoid	ellipsoid	not shown
Molecule Blobs	blob	blob	blob	not shown
Secondary Structure	rope and cylinder	backbone	space filling	not shown
Residue Spheres	residue spheres	residue spheres	ball and stick	not shown
Ribbons	ribbon	ribbon	ball and stick	not shown
Bond Lines	lines	lines	lines	not shown
Atom Balls	atom balls	atom balls	atom balls	not shown
Bonds and Atoms	bonds and Atoms	bonds and Atoms	bonds and Atoms	bonds and Atoms

Coarseness (Fineness) of representation

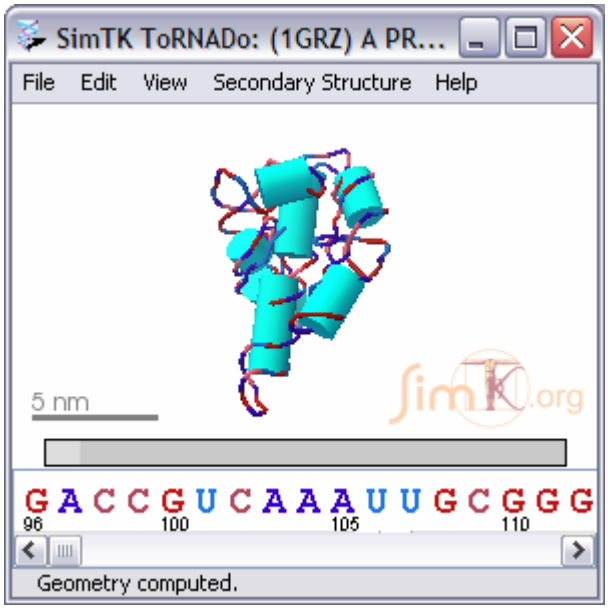
Molecule Ellipsoids



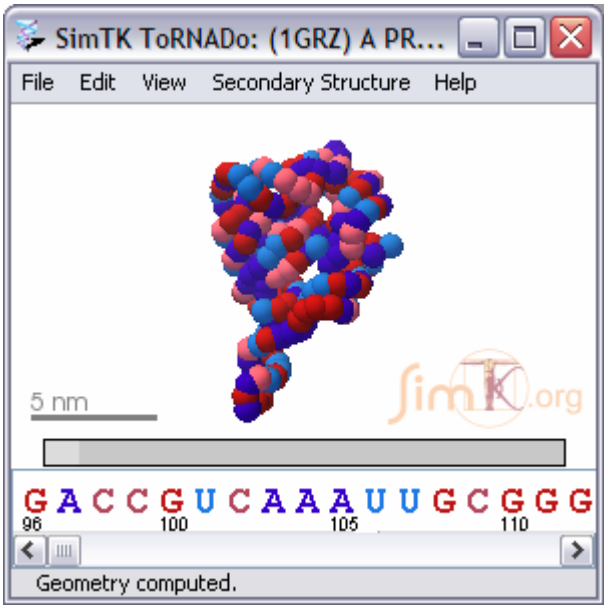
Molecule Blobs



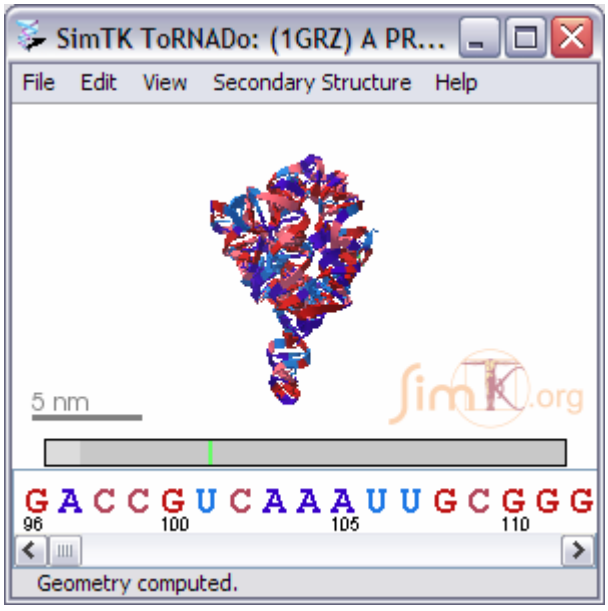
Secondary Structure



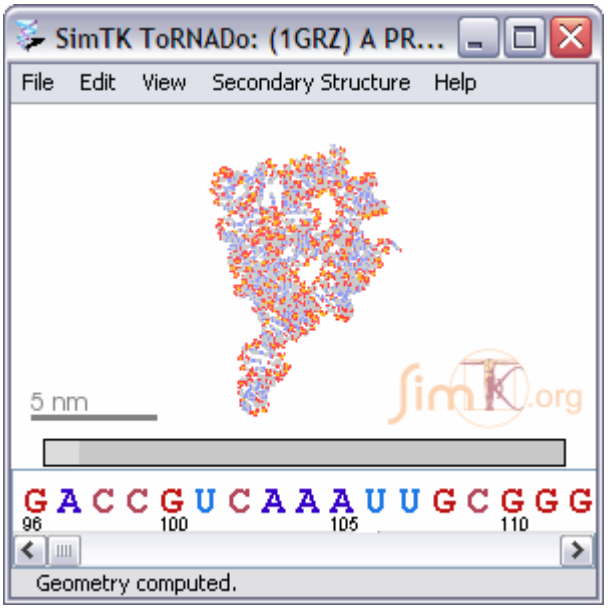
Residue Balls



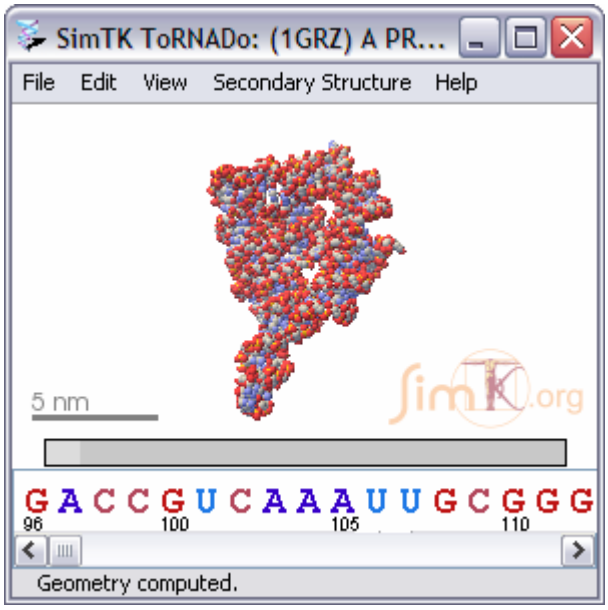
Ribbons



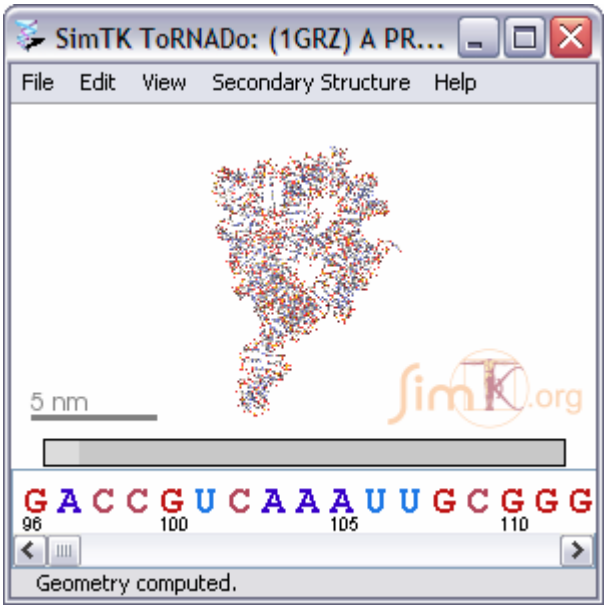
Bond Lines



Atom Balls



Bonds and Atoms



Nucleic Acid Secondary Structure – RNAML files

RNAML is an xml file format for descriptions of RNA structure. Examples of other applications that use and produce RNAML format are RNAVIEW and MFOLD.

You can load an RNAML file (produced for this example by RNAVIEW) for your structure and display the corresponding secondary structure. Select: "Secondary Structure > Load Secondary Structure File". Then select "Secondary Structure > Secondary Structure Source > RNAVIEW".
To view the secondary structure select: "View > Molecule Style > Secondary Structures".
If you select "Secondary Structure > Secondary Structure Source > All", you will see the Tornado secondary and the one in from your RNAML file superimposed.

To just view the secondary structure computed by Tornado select: "Secondary Structure > Secondary Structure Source > Tornado".

For our sample PDB structure 1GRZ an RNAML file (produced by RNAVIEW and obtained from http://ndbserver.rutgers.edu) can be downloaded from the Tornado project by selecting downloads from the left menu and selecting the file named UR0003-rna.xml under Documentation Links (https://simtk.org/project/xml/downloads.xml?group_id=12).

Saving An Image File of the 3D structure

From the menu bar, select "File"->"Save PNG Image".
At the right side of the file save dialog, you can adjust the image magnification, which permits you to save images at a higher resolution than you monitor can display.

Troubleshooting Java Web Start

If downloading stalls, it is possible that a problem is Java Webstart occurred.

Webstart is supposed to fetch the latest version of the program from the simtk server, but sometimes it does not update to the latest version. In this situation, you can get the latest version the next time you run by clearing the webstart cache.

PC Instructions --

Run Java Web Start by itself by typing "javaws -viewer" at the command line, or by finding and clicking Java Web Start on your system.

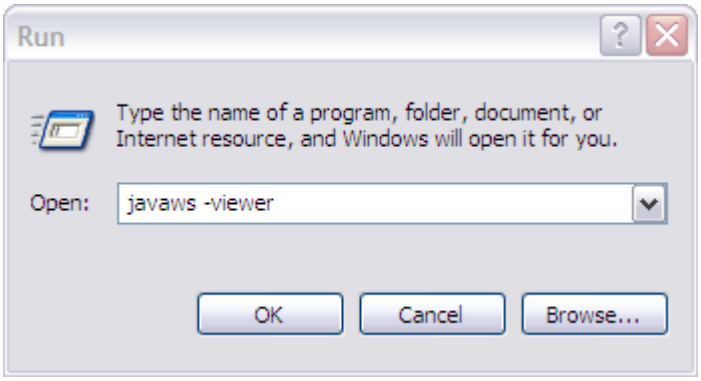


Figure 7: Command line window

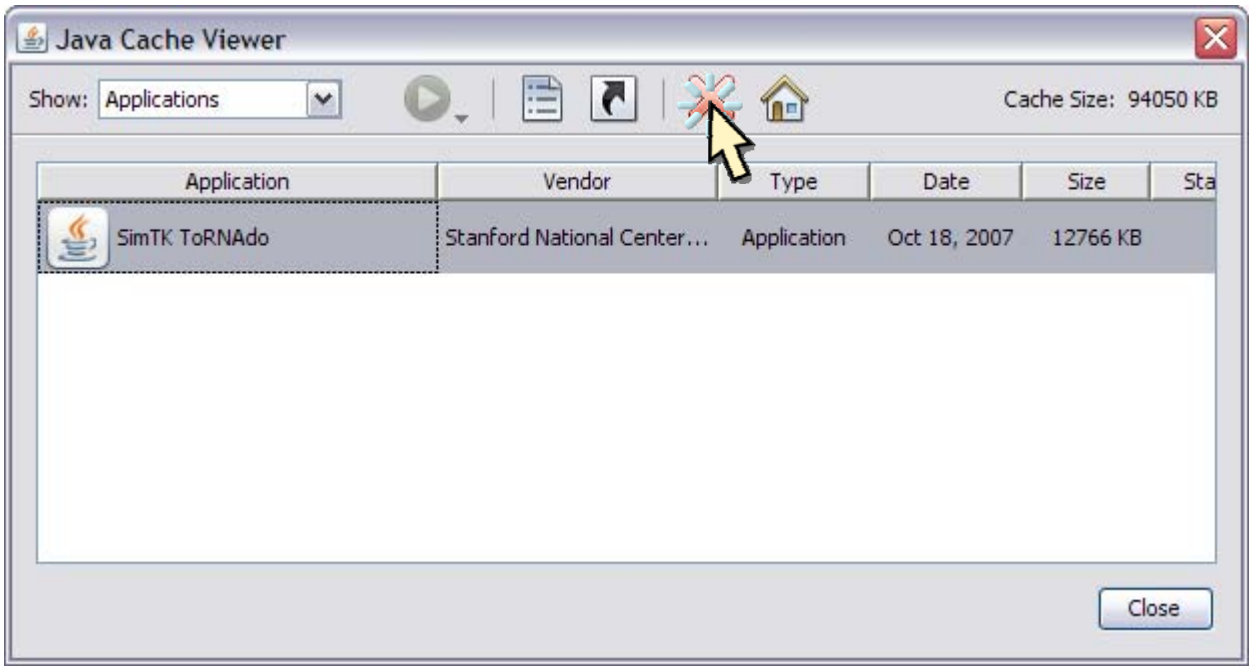


Figure 8: To force an update to the latest version of the program, remove the ToRNADo application and any Shared SimTK Java Classes from the application cache.

Figure 9: If the ToRNADo application is not shown in the Java Web Start Application Manager, you will be unable to remove just the ToRNADo application from the application cache. In this case, close the Java Cache Viewer and using the Java Control Panel, click on the General Tab. Under the General Tab window, go down to Temporary Internet Files-> Click on Settings-> Click on Delete Files-> Click OK. Please note that this will clear the entire application cache.

MAC Instructions –

Run Java Cache Viewer by typing "javaws" in a terminal window, or by finding and clicking Java Cache Viewer on your system, located in the Utilities > Java > J2SE folder which you can find as follows:

- Find the "Utilities" folder by going to the "File" menu, click on "Find" and type "utilities" on the search area.
- In the "Utilities" folder find the "Java" folder and expand it.
- In the Java folder select the J2SE folder
- Double Click on "Java Cache Viewer" to run the application.
- The "Java Web Start Application Cache Viewer" window will come up.

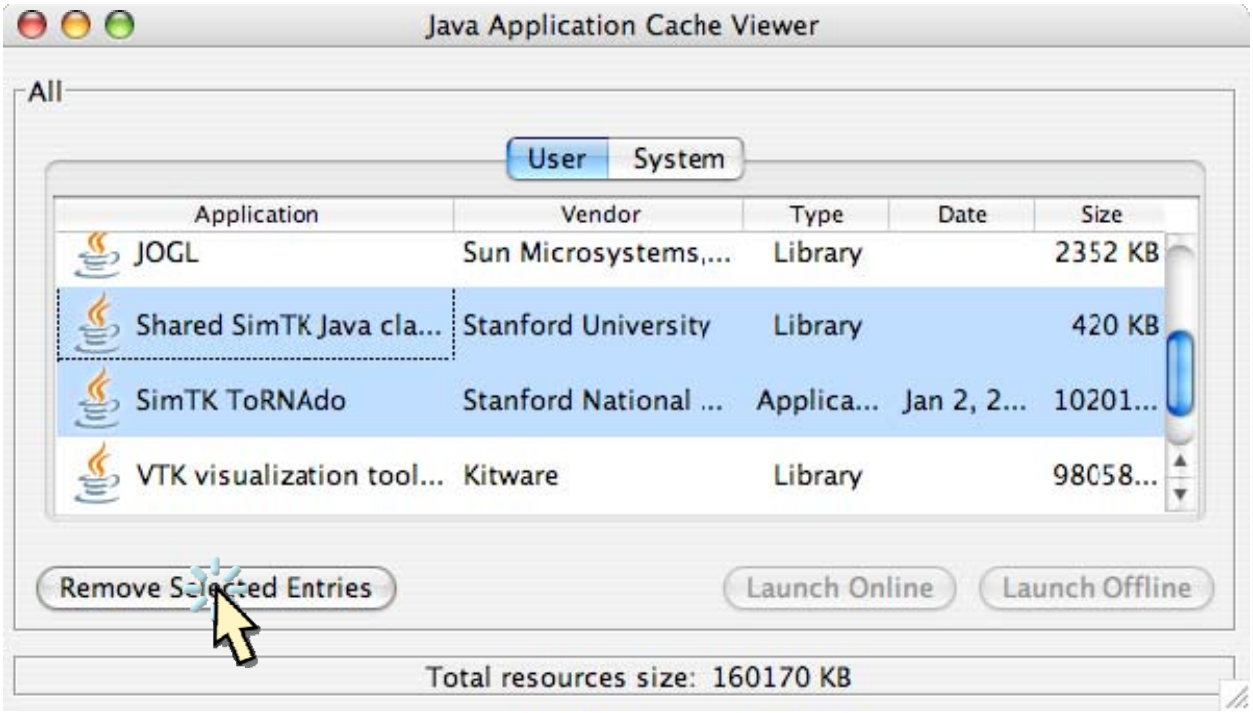


Figure 10: To force an update to the latest version of the program, bring up the Java Cache Viewer, and remove the ToRNADo application and any Shared SimTK Java Classes from the application cache.

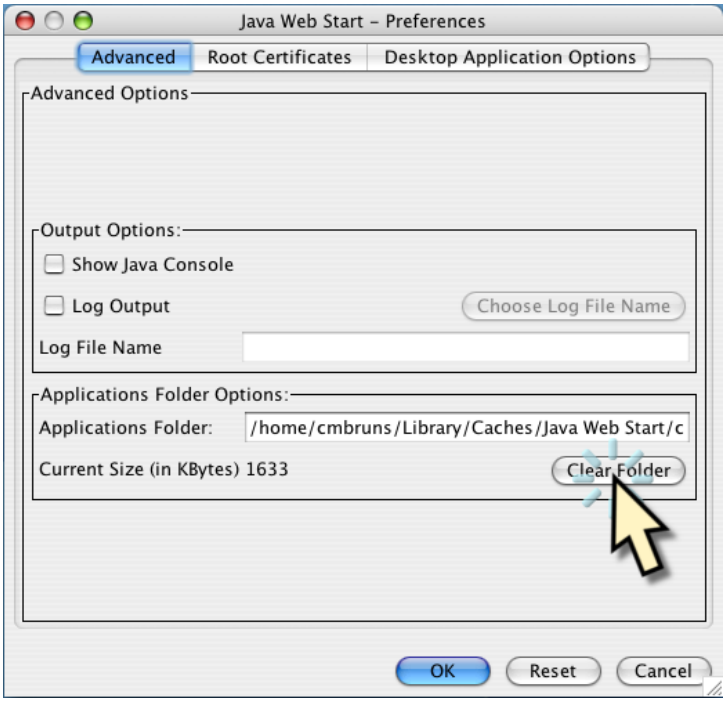


Figure 11: If you cannot find the ToRNADo application, you can clear all applications by running Java Web Start in Utilities > Java > Java Web Start and selecting Preferences from the top menu.

After Clearing the Java Cache reopen the jnpl file.

Submitting Problem Reports and Enhancement Requests

If you observe a problem with the Tornado program, or if you would like to request a new behavior in future versions of Tornado, please file a bug or feature report at SimTK.org. You can do this by selecting "Help > Report a program Problem (bug" or "Help > Request a new program feature" directly from the application.

You can also file a bug or request a feature from the Simtk.org site:

- Go to the ToRNADo project page (https://simtk.org/home/rna-viz-proto), and select Advanced->"Features & Bugs". Then select "Bugs" or "Features" on the main screen and then select "Submit New" from the left menu.
- Fill in the report and click "Submit".

Thank you for helping us to improve Tornado.

References

[RNAVIEW] Yang, H., Jossinet, F., Leontis, N., Chen, L., Westbrook, J., Berman, H.M., Westhof, E. (2003). Tools for the automatic identification and classification of RNA base pairs. *Nucleic Acids Research* **31** (13): 3450-3460.

[MFOLD] M. Zuker, D.H. Mathews and D.H. Turner Algorithms and Thermodynamics for RNA Secondary Structure Prediction: A Practical Guide in RNA Biochemistry and Biotechnology, J. Barciszewski and B.F.C. Clark, eds., NATO ASI Series, Kluwer Academic Publishers, (1999)