Manual

SPICE - a DAS client for protein sequences and structures.

This manual corresponds to SPICE version 0.6. It is still under development.

Author: Andreas Prlić

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What is SPICE?

SPICE is a **DAS client** that allows to browse through the annotations of protein sequences and structures and to investigate sequence and structure relationships of the annotations. The displayed data is retrieved from different sites on the Internet, that make their annotations available using the DAS protocol. It is possible to add new annotations to SPICE, and to compare them with the already available information.

What is DAS?

The **Distributed Annotation System (DAS)** defines a communication protocol used to exchange biological annotations. It is motivated by the idea that annotations should not be provided by single centralized databases, but instead be spread over multiple sites. Data distribution, performed by DAS servers, is separated from visualization, which is done by DAS clients. The original DAS protocol was designed to serve annotation of genomic sequences. We have extended the protocol to be applicable to macromolecular structures. The DAS homepage is located at: http://www.biodas.org

Version

How does SPICE work?

SPICE is a Java program that can be started using Java Web Start by simply following a web link. It accepts either a PDB or a UniProt code as an argument. If the application is started the first time, Web Start will download the program automatically. Once SPICE is running, it connects to the DAS registration service to retrieve a list of available **DAS servers.** SPICE connects to the available servers, retrieves different types of information using the **DAS protocol** and visualizes the data in a display like:
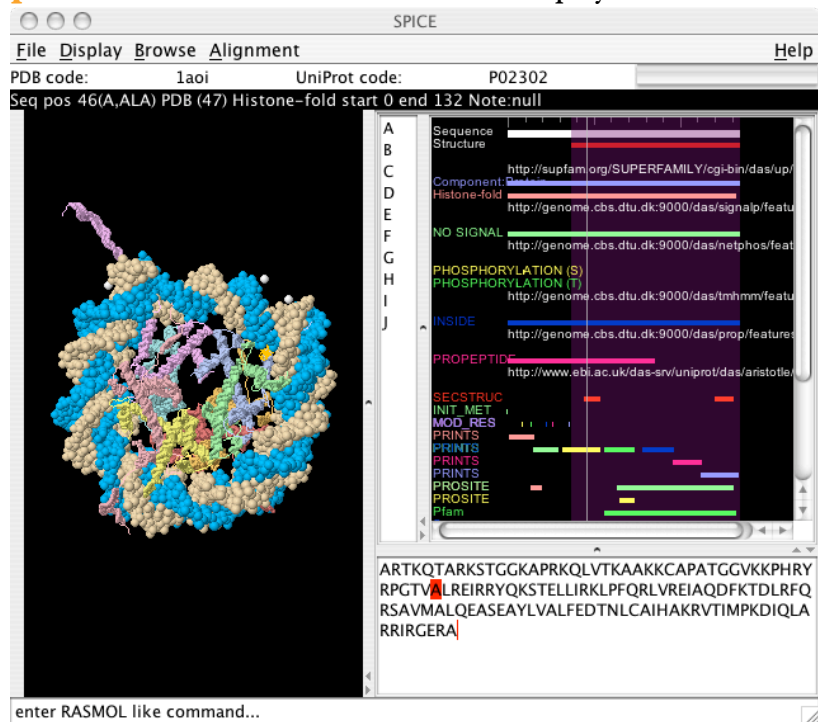
A screenshot of SPICE.

The three main panels of SPICE

SPICE consists of three main panels

- The Structure Panel
- The Sequence Panel
- The Feature Panel

The Structure Panel

The Structure panel provides a 3D visualization of the molecule using the open source [Jmol](#) library. There is a command line that allows to enter [RASMOL](#) like commands.

In this screenshot it displays "enter RASMOL like command..."
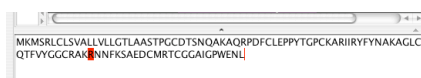
try to enter

select 2-16

This will result in the residues 2-16 of the (PDB file numbering) being selected.

The [RASMOL](#) manual will give you a more detailed description of the scripting commands.

The sequence panel displays the amino acid sequence. If you move the mouse over the sequence, the selected position is displayed in the two other panels. The corresponding position in the feature panel is highlighted in grey.

If coordinates for the selected residue are provided it is selected (yellow) in the structure Panel.

The sequence panel allows to **search for motives** in the sequence. e.g. by typing LVLLGTL the corresponding region is selected.

To look for a second occurrence, pressing <Enter> jumps to the second motive (if available) <Home> clears the entered motive. The Feature and Structure panels displays the corresponding regions with grey background.

By pressing the <Right Mouse Button> a popup menu appears, that locks, the selection. Until the selection is unlocked, it will not follow the mouse cursor.

The Feature Panel
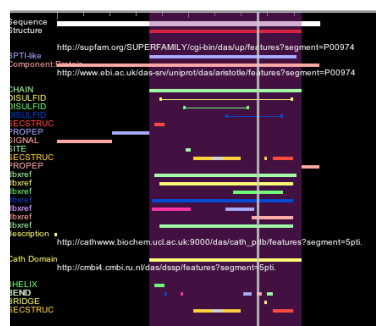
Annotations provided by the distributed servers are displayed in the Feature panel, no matter if is provided in **sequence positions or PDB residue coordinates**, since SPICE can project one onto the other. This is required for the interaction between the sequence and structure panels.

The feature panel contains a listing of available annotations making it easy to compare the annotations made by different methods.

The first line contains a ruler indicating every ten amino acid positions. The second (white) line represents the sequence itself. The third line (red) shows regions of the sequence that are covered with **3D structure information**. If structure information is available the whole column is shaded red in the background.

By moving the mouse over the panel, the column belonging to the sequence position is selected and also shown in both the 3D Structure and the Sequence panel.

If the mouse is over a feature, the annotated information will be displayed in the status window. after approx. one second, a popup window will occur, providing the same information in a popup window. By clicking on a feature, the whole features becomes the current active selection.

Clickingon the background selects a single position in the structure display in spacefill mode.

By pressing the <Right Mouse Button> a popup menu appears, that locks, the current selection. Until the selection is unlocked, it will not follow the mouse cursor.

Configuring SPICE

SPICE can be configured by proceeding to the *File-> Properties* menu
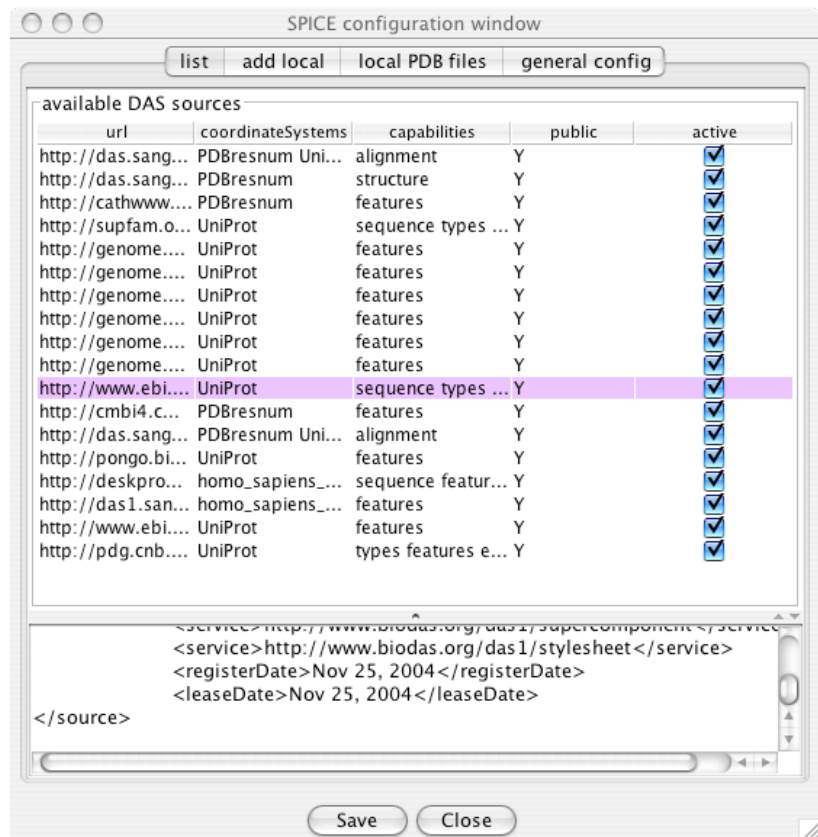
The Configuration window will appear that contains several Tabulators:

- list
- add local
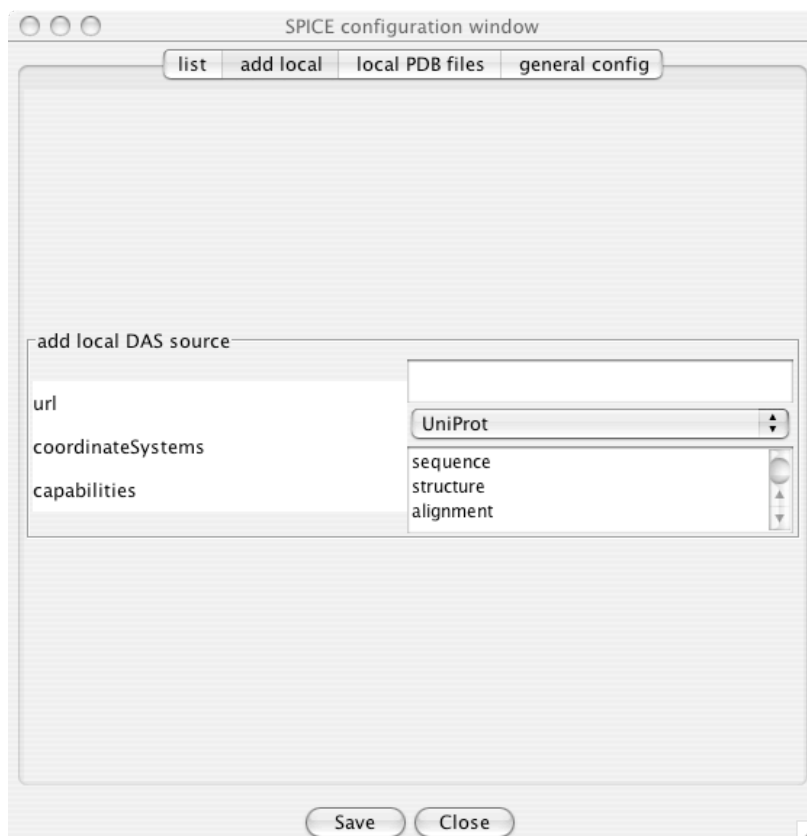- local PDB files
- general config

The List Tab

The **List Tab** lists all available DAS sources in the upper regions. In the lower regions details of a currently selected server are being displayed. Servers can be activated and de-activated by pressing the checkbox.

Changing the order of the servers

The order in which servers are being contacted and displayed in the Feature panel can be changed by selecting a server and pressing the *<Up>* and *<Down>* keys. Pressing *<Page-Up>* will move a server to the first position. All changes need to saved by pressing the *Save* button in order to become active.

The Add Local Tab

The **Add Local Tab** allows access to local DAS sources that are still under development, or have not been registered with the DAS registration server.

The Add Local PDB File Tab

The **Add Local PDB File Tab** allows to configure to load PDB files locally. If a local PDB installation is available, SPICE can be configured to check there first when looking for structure data. If a required structure is not found, it is automatically retrieved using the macromolecular structure DAS extension.

All files should be available in a single directory.

General Config Tab sorry, implementation not finished, yet.

The Menus

SPICE has the following Menus:

- File
- Display
- Browse
- Alignment
- Help

TODO: describe the Menus

Downloading and Installing SPICE

It is very easy to download and install SPICE, because of the **Java Web Start** technology. For most users it will be sufficient to follow a link like

http://protodas.derkholm.net/dasregistry/makespicejnlp.jsp?pdb=1a4a

If Java Web Start is installed on your system, SPICE will be downloaded automatically. To learn more about Java Web Start precede to Sun's product pages.

Integrating SPICE into other Web Sites

As easy as to download and install SPICE, it is to integrate SPICE into a other web sites. The program can be launched by **providing a link** like

http://protodas.derkholm.net/dasregistry/makespicejnlp.jsp?pdb=1a4a

The end of this URL looks like:

?pdb=1a4a

This can be used to tell SPICE which PDB structure to display during startup. It is also possible to provide a Uni-Prot code by adding e.g.

?uniprot=P00280

so the complete URL would look like

http://protodas.derkholm.net/dasregistry/makespicejnlp.jsp?uniprot=P0
0280

In the next version it will be also supported to specify which DAS servers should be displayed and in which order they should appear in the Feature Panel.

Getting the Source Code

It is not necessary to download and compile the SPICE source code in order to run it. This is just in case you are a developer or you want to see how SPICE works.

The SPICE **source code is available under the LGPL** license from http://www.derkholm.net/svn/repos/spice/ using Subversion.

Frequently asked questions

Which Java version does SPICE require?

Java 1.4.2 or higher. To install Java please download from http://java.sun.com/j2se/. It will automatically install Web Start on your system as well.

On which platforms is SPICE running?

We are regularly testing SPICE on

- OSX
- Linux (Debian, Red Hat)
- Windows XP

with the following browsers:

- Firefox (our recommendation)
- Internet Explorer 6
- Safari
- Camino

If you have any problems with running SPICE, please contact us.

SPICE does not start when I follow the link that is supposed to start it. Instead I see an .jnlp file (XML file) What is wrong?

You need to tell your browser to use Java Web start, when .jnlp files are downloaded. This is usually automatically configured when Java is installed. If it somehow did not happen, you have to do it manually. E.g. for Mozilla

Start Mozilla and open the Menu

Edit > Preferences > Navigator > Helper Apps

Enter a new helper application:
Description of Type: Java Web Start
File Extension:jnlp
MIME type: application/x-java-jnlp-file
Application To Use: /path/tojavaws

I am using (old version X of browser Y). SPICE is starting correctly, but does not open any of the pages displayed in the Browse menu. What is wrong?

We noticed this behavior e.g with Mozilla 1.5 on Linux. This seems to be an in-compatibility between Java Web Start and the browser, and is beyond our influence. Upgrading the browser e.g. to Firefox (http://getfirefox.com)resolves this problem.

Can I launch SPICE from the command-line?

Yes you can. make sure Java Web Start is you $PATH and do e.g.

javaws
http://protodas.derkholm.net/dasregistry/makespicejnlp.jsp?pdb=1a 4a