Subject: Datawarrior Commandline Option to Use Template
Posted by sbembenek18 on Sun, 22 Dec 2024 19:35:09 GMT
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From the command line, is there a flag that allows one to read a given sdf file with a saved datawarrior template?

Subject: Re: Datawarrior Commandline Option to Use Template
Posted by nbehrnd on Sun, 22 Dec 2024 20:58:43 GMT
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Conceptually, this line of thought is close to let Jmol process data silently (no GUI) by a call of `java -jar ./Jmol.jar -ions my_script.spt` with actions defined in `my_script.spt` -- hence I welcome the feature suggestion.

In case of a native installation in Linux and bypassing the `datawarrior` BASH script the installation provides, I didn't advance further than learning 1) one has to use the Java runtime engine provided by the DataWarrior installation because an other usually used system wide does not. And 2) to reach out for the launcher, i.e.

/opt/datawarrior/jre/bin$ ./java -jar ../../datawarriorlauncher.jar

From here, no successful further advance to either .dwar or .dwam files of tutorial or reference folder (though `datawarrior ./reference/PhysProp.dwar` opens GUI and then file `PhysProp.dwar`).

Norwid

Subject: Re: Datawarrior Commandline Option to Use Template
Posted by sbembenek18 on Mon, 23 Dec 2024 19:41:29 GMT
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Yeah I think this would be a great feature to have as a flag option -->

.../../datawarrior myfile.sdf --template mytemplate.dwat

Our current use case is that we have several SDF models and simply want to script it such that DW opens them all at the end of our run.

This also reminds me of another feature I have been wanting: tabs in DW for multiple data sets.

Then together you could imagine having an existing DW project that you can add aditional SDF file to via the tab approach. And this could be done manually once the project is open or via commandline -->

.../../datawarrior myfile.sdf --template myproject.dwar

where he new SDF would then be added to the project and inherent all the existing features of the original.

I this would really enhance what is already great about DW.

Subject: Re: Datawarrior Commandline Option to Use Template
Posted by nbehrnd on Mon, 23 Dec 2024 22:08:54 GMT
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From your comment, I sense you are comfortable with the command line. Hence I feel comfortable to suggest DataWarrior's mode of action need not to be "file based" only, perhaps additionally could be "stream based" (as so many unix/linux utilities).

An illustration: OpenBabel reads many more file formats than e.g., .sdf DataWarrior accepts as input. While converting these files into a suitable syntax, OpenBabel can apply numeric, or (sub) structure related criteria as a filter. Hence, why not allow openbabel's results (via stdout) as one form of input (stdin) for DataWarrior (in unix' parlance, via a pipe)? Second, if DataWarrior's results are not an illustration, a 2D/3D diagram, they mostly are human readable plain text written into the .dwar file. While often useful, I think a permanent output file needn't be DataWarrior's only mode of operation -- there equally could be an optional output by DataWarrior itself as an output stream to redirect (`>`) or append (`>>`) to a permanent record, or to relay to a subsequent tool living in the command line.

Norwid

https://open-babel.readthedocs.io/en/latest/Descriptors/desc riptors.html
https://en.wikipedia.org/wiki/Pipeline_(Unix)
