Subject: DataWarrior 6.10 in windows: heap-memory Xmx limit?
Posted by juliocoll on Wed, 19 Jun 2024 10:31:07 GMT
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I am trying the Building Evolutionary Libraries (EL) DW method using the new DW6.1 version in windows 10. The DW16 program launches Ok and seems to be working very well, including the size of the lettering improvements (many thanks for that detail!).

However, I may have fallen into small heap-memory for EL.
If I am right, according to the new Datawarrior.exe/.rsrc/VMOPTIONS/5000, the maximum Xmx heap-memory is set to Xmx3600m, which could explain my abundant failures....

Is it possible to set Xmx to use as much heap-memory as available?
I though to have read something like may be posible, but I may be mistaken.

Alternatively, is there another way to increase heap-memories in DW6.1 windows?.
As thomas suggested more than a year ago, I have been sucessfully using windows DW5.5 with 100g heap-memory set by a Linus/windows.exe bypass (enclosed startJarWin.bat).
Is there something similar for DW6.1?.
I tried different alterations of that bat file but I got an extensive pile of failures to launch the WP6.1.....

Any ideas would be most welcome
Thanks for your attention!
julio

File Attachments

1) startJarWin.bat, downloaded 520 times

Subject: Re: DataWarrior 6.10 in windows: heap-memory Xmx limit?
Posted by thomas on Fri, 21 Jun 2024 08:43:46 GMT
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In DW6 a few things are different. On Windows DataWarrior.exe does not contain the main code anymore. It just contains a small launcher that may download an update and then launches the newest datawarrior.....jar. You can launch the same jar from the command line with e.g.:

"C:\Program Files\DataWarrior\jre\bin\java" -Xmx16g -Xms8g --add-exports java.base/jdk.internal.module=ALL-UNNAMED -jar C:\ProgramData\DataWarrior\datawarrior_v06.02.01.jar

As before, you can change Xmx (max memory) and Xms (memory at start) to your needs. You could also change these settings in the DataWarrior.exe using a hex editor, but that would be a kind of a hack...

Subject: Re: DataWarrior 6.10 in windows: heap-memory Xmx limit?
Posted by juliocoll on Fri, 21 Jun 2024 12:57:21 GMT
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Thank you very much Thomas!
I put the code you send me into a bat file and: IT WORKED !!! :)
cheers
julio

Subject: Re: DataWarrior 6.10 in windows: heap-memory Xmx limit?
Posted by juliocoll on Tue, 06 Aug 2024 12:50:03 GMT
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To compare the evolution of Evolutionary library (EL) heap memories on Windows using DW5 (java's 8) and DW6 (recent java), both DW5 (C:\Program Files\DataWarrior5) and DW6(C:\Program Files\DataWarrior) simultaneously installed into the same Windows 10 computer were independently run.

As the initial EL parent molecule, an anti-viral star-like molecule (~ 500 g/mol) were evolved during 6 consecutive EL runs requiring ~100Gb RAM memory in windows 10. Both EL used the same antiviral molecule as parent and targeted the same protein cavity employing the same evolving criteria (MW, logP, toxicity risks and 6 automatic runs).

In the ppt file, the resulting DW5 and DW6 heap memory profiles versus their evolutionary EL times were compared from data monitored from the Java/jdk-19/Jconsole.

Results showed that DW6 (red) periodically peaks up to the ~120Gb Xmx limit and then each time minimizes the memory (garbage collection?) to near the minimal 3Gb Xms.

In contrast, DW5 (blue) keeps increasing the memory with time to reach a ~ 120Gb Xmx limit. Then it slows down before the program crashes !.

This behaviour will favor the new DW6 version, specially since it may allow ~"endless" (?) runs. It may only apply to difficult-to-find EL fit cases, such as when searching for scarce children fitting some viral mutations resistant to drugs…

Hope it may interest to some people at the forum

File Attachments

1) DW5vsDW6.pptx, downloaded 479 times