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 147 times