
Subject: Out of memory

Posted by [Christophe](#) on Tue, 11 Mar 2025 15:10:34 GMT

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Hello everyone,

I am currently working with a quite big dataset (~25000 molecules) and I try to make a UMAP vizualisation after the calculation of some data warrior fingerprints.

Each time I try to create a UMAP vizualization I get the following message:

"Out of memory. Launch DataWarrior with Java option -Xms???m or -Xmx???m"

How can I get around this problem?

I run DW on Intel core i5 at 2.7 GHz with 64 Go RAM

Thank you for any clarification you may be able to provide

Christophe

Subject: Re: Out of memory

Posted by [nbehrnd](#) on Wed, 12 Mar 2025 22:07:27 GMT

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Hello Christophe,

the line you report is very close to the BASH script of DataWarrior's installer and launcher script in Linux. As an example, it can contain the line reading

```
/opt/datawarrior/jre/bin/java -Xms512m -Xmx4096m -splash:/opt/datawarrior/loading.png
--add-exports java.base/jdk.internal.module=ALL-UNNAMED -Dfile.encoding=UTF-8 -cp
$DWJAR/datawarriorlauncher.jar:$DWJAR/capka.jar
org.openmolecules.datawarrior.launcher.DataWarriorLauncher $*
```

This example reads as "allocate DataWarrior 512 MByte RAM to start, provide up to 4 GO/GByte maximum" to allow other programs than DataWarrior to process concurrently. However, if you manage a larger data set on a more powerful computer, it is possible to manually adjust (i.e., increase) these thresholds. Try to work with e.g., `-Xmx60g``.

Best regards,

Norwid

<https://www.star.bris.ac.uk/mbt/stilts/sun256/jvmArgs.html>

Subject: Re: Out of memory

Posted by [thomas](#) on Mon, 17 Mar 2025 19:52:18 GMT

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25'000 Molecules is a rather small file. I am astonished. Do you have hundreds of columns? I just ran a UMAP from SkelSpheres (the largest of the vector descriptors) with 250'000 molecules, which also worked fine with just a few GB of -Xmx.

Which version and which OS do you use? On all platforms except Windows you can increase the -Xmx setting easily.

Subject: Re: Out of memory

Posted by [Christophe](#) on Wed, 19 Mar 2025 14:49:01 GMT

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Hello,

Thank you. Actually I'm running DW 6.04.02 on Windows 10. I can't find the file I have to edit to allocate more RAM on Windows.

Subject: Re: Out of memory

Posted by [nbehrnd](#) on Sat, 22 Mar 2025 16:08:51 GMT

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Hello Thomas,

an answer on stackoverflow describes Windows' control settings to include a category "Java" to set the flags accordingly. Contrasting to my anticipation, on an instance of Windows 10 (64bit) with a working installation of DataWarrior (06.04.02), this however displays only sun's Java engine. Would one have to add `C:\Program Files\DataWarrior\jre\bin\java.exe` (or `javaw.exe`) to monitor (and eventually set the relevant flags) to then address DataWarrior's Java engine?

Best regards,

Norwid

<https://stackoverflow.com/questions/70262178/defining-java-heap-size-for-all-users-on-a-windows-system>

Subject: Re: Out of memory

Posted by [nbehrnd](#) on Sat, 22 Mar 2025 16:26:19 GMT

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Hello Christophe,

a bypass could be to set up a separate Linux partition on your computer because then the file in path /opt/datawarrior/datawarrior would provide you access to these parameters. Either by a

double-boot (right after starting the computer, you will be asked which operating system to be used exclusively), or with a virtualization (for instance windows wsl) as a permanent change to the computer.

It equally is possible to start Linux from a USB/pen drive (e.g., <https://rufus.ie/en/>) provided the BIOS of the computer is set to allow to boot from USB. In principle this would provide a non-permanent access to the parameters (after launch of the OS, installation of DataWarrior, adjustment of the parameters, launch of DataWarrior) without change to the hosting computer. This tends to be a bit less performant than a true installation, though not as much with 64 Go at disposition, than e.g., 8 Go. After disconnection of the USB drive, the computer would boot as it did prior to this excursion. Which could be worth a test, too.

Best regards,

Norwid

https://en.wikipedia.org/wiki/Windows_Subsystem_for_Linux

Subject: Re: Out of memory

Posted by [Christophe](#) on Thu, 27 Mar 2025 14:29:55 GMT

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Thank you for your answers. I will try to run DW under Linux or find another solution.

Best regards,

Christophe
