INSTRUCTIONS FOR DROIDS v3.0 ON WINDOWS and/or GOOGLE CLOUD PLATFORM

Option 1: running a Linux Mint Virtual Machine (VM) on Windows PC

1. Download and install VirtualBox from this website

   https://www.virtualbox.org/

2. Get a .vdi file (for Linux Mint) from this website

   https://www.osboxes.org/virtualbox-images/

3. Build a Linux Mint VM following instructions from VirtualBox
4. Copy the required files to the VM (i.e. DROIDS-3.0.tar.gz, Amber18.tar.gz, AmberTools18/19.tar.gz, Chimera-1.14-linux_x86_64.bin). These can be obtained from the following websites
   https://people.rit.edu/gabsbi/
   https://ambermd.org/
   https://www.cgl.ucsf.edu/chimera/download.html
   and you'll probably want Modeller enabled on Chimera
   https://salilab.org/modeller/
5. Run the DROIDS+AMBERinstaller.pl script on the VM's desktop terminal

   perl DROIDS+AMBERinstaller.pl

   NOTE: your PC must already have Nvidia GPU hardware, CUDA and Nvidia graphics drivers properly installed.

Option 2: running an Ubuntu Linux VM on GCP (Google Cloud)

https://cloud.google.com/

1. Open GCP account, go to your console and request resource quota to enable building GPU VM instances.
2. Upload the required files to a Google Cloud Storage Bucket (i.e. DROIDS-3.0.tar.gz, Amber18.tar.gz, AmberTools18/19.tar.gz, Chimera-1.14-linux_x86_64.bin). These can be obtained from the following websites
   https://people.rit.edu/gabsbi/
   https://ambermd.org/
   https://www.cgl.ucsf.edu/chimera/download.html
   and you'll probably want Modeller enabled on Chimera
   https://salilab.org/modeller/
3. On your Dashboard, go to 'Compute Engine' and build your VM instance. IMPORTANT: Be sure to add an Nvidia GPU and use Ubuntu 18.04 LTS so that you can install and link to a desktop application.
4. Once the VM appears, connect to it via the SSH link and run the following commands.
   su passwd (to reset root password)
   su passwd yourusername (to reset your user password)
   sudo apt-get install xrdp

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sudo apt-get install xfce4
sudo apt-get xrdp restart
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5. Leave this terminal open and go to your Windows RDP (Remote Desktop) application and enter the external IP address from your VM to open the new xfce desktop you installed with your new passwords.
6. At this point you can transfer your files from your cloud bucket to the VM desktop and proceed with the installation using the DROIDS+AMBERinstaller.pl script at the desktop terminal

```
perl DROIDS+AMBERinstaller.pl
```