Software Installation Instructions for the KIM Tutorial

A virtual machine (VM) is a computer (including operating system (OS) and applications) that is installed on software that imitates dedicated hardware. We will run all the software needed for the KIM Tutorial in a virtual Linux computer installed on your laptop computer. To install the VM, do the following:

Step 0 – System Requirements

In order to install the necessary software, you will need a laptop computer or workstation with the following capabilities:

- Any recent Intel or AMD processor
- At least 3 GB RAM
- At least 16 GB of free hard disk space (after installation, about 4GB can be freed up).
- Linux, MacOS or Windows operating system, 64 bit.

Step 1 – Download the virtual hard disk drive

The first step is to download a .OVA file containing the virtual machine disk drive. This is a fairly large file (4.1GB), but once you have it, you will have all the software you need for the tutorial. (Depending on your internet connection speed, this can take half an hour or more.)

Download the file (openkim-tutorial.ova) here: https://drive.google.com/file/d/1IT7Um4ws2-Ov13y5P2yVOJDTSXGwHuyx/view?usp=sharing

Once the download completes, proceed to the next step.

Step 2 – Download and Install VirtualBox

We will use an application called VirtualBox (VB). VB provides an easy route to virtualization, or running an entire guest operating system within you host operating system.

Download VB for your computer <u>here</u> and follow the instructions to install it. If you have problems with the installation, see the Troubleshooting section at the end.

Step 3 – Import the Downloaded VM

Start up VB. You will be greeted with a screen that looks similar to that shown below (the machine name in the left panel will not appear): (Note that the screen shots below may look somewhat different depending on the platform on which you are running VB.)



Next, click the "Tools" button to reveal an option to "Import". Choose "Import" and follow the instructions. When asked for a file, choose the .OVA file you downloaded in step 1. It is probably in your "Downloads" folder, unless you saved it somewhere else.

Step 4 – Verify your installation

After the import is complete, the machine should appear in the left column as shown above. Double-click on it to launch the VM.

Open a Linux terminal by clicking on the blue Lubuntu logo in the lower left corner of the screen, select "System Tools" and then "QTerminal". When the terminal opens, enter the following command:

ovito -v

You should see the following:

Ovito Basic 3.1.1

Step 5 – Shut down

Shut down the machine by first clicking the blue Lubuntu symbol in the lower left corner of the screen, then choose "Leave" and "Shutdown". After the machine shuts down, you can quit VirtualBox as well.

You can now delete the .ova file you downloaded to save disk space. (*After* the tutorial, you can remove the large files associated with the installed VM by removing it from inside VB.)

Troubleshooting

Several things can go wrong when installing VirtualBox. Here are some possibilities:

- On a Windows machine, if you see a message like this: "The native API dll was not found... VT-x is not available", this may mean that you need to enable virtualization in the computer's BIOS. To do so, restart the computer and press F2 when it reboots. Look for an option similar to "intel virtualization technology" to toggle on, then reboot and try to install VirtualBox again. (If you cannot find the virtualization toggle, note which BIOS you have search online for instructions on how to turn on virtualization.)
- On Windows machine there can be a problem with network connectivity from inside the VM. (The laptop native OS has a network connection, but the VM does not.) The following sometimes works:
 - Shut down the VM
 - In VirtualBox, click settings for your VM.
 - Select the "Network" tab and click on Advanced.
 - Change the Adapter Type to "PCnet-FAST III"
- On Mac installation of VirtualBox can stall due to security issues. Try to follow the instructions at this link to see if the matter is resolved: https://medium.com/@DMeechan/fixing-the-installation-failed-virtualbox-error-on-machigh-sierra-7c421362b5b5

If you continue to run into problems, contact support@openkim.org for assistance.