Lab 4
Installing the correct version of LAMMPS

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1 Installing LAMMPS through `Conda Miniforge`

The version of LAMMPS installed on the Virtual Machine (VM) was not compiled with the `KSPACE` pacakge, which is required to treat long-range interactions in Lab 4.
This document explains how to install a new version of LAMMPS using `Miniforge`. If you run into any issues, feel free to contact us!

Open the terminal and run the following commands:

1. Install the open-source `Conda` implementation (`Miniforge`)

   ```
   wget https://github.com/conda-forge/miniforge/releases/latest\
        /download/Miniforge3-Linux-x86_64.sh

   bash Miniforge3-Linux-x86_64.sh
   ```

   Follow the prompts, then open a new terminal.

2. Create and activate a new environment with LAMMPS from conda-forge.

   ```
   conda create -n lammps-env -c conda-forge lammps -y
   conda activate lammps-env
   ```

3. Test the installation

   ```
   which lmp_mpi
   ```

   This should give you a working `lmp_mpi` command with all the required packages. Make sure to activate the environment every time you open a new terminal using the following command

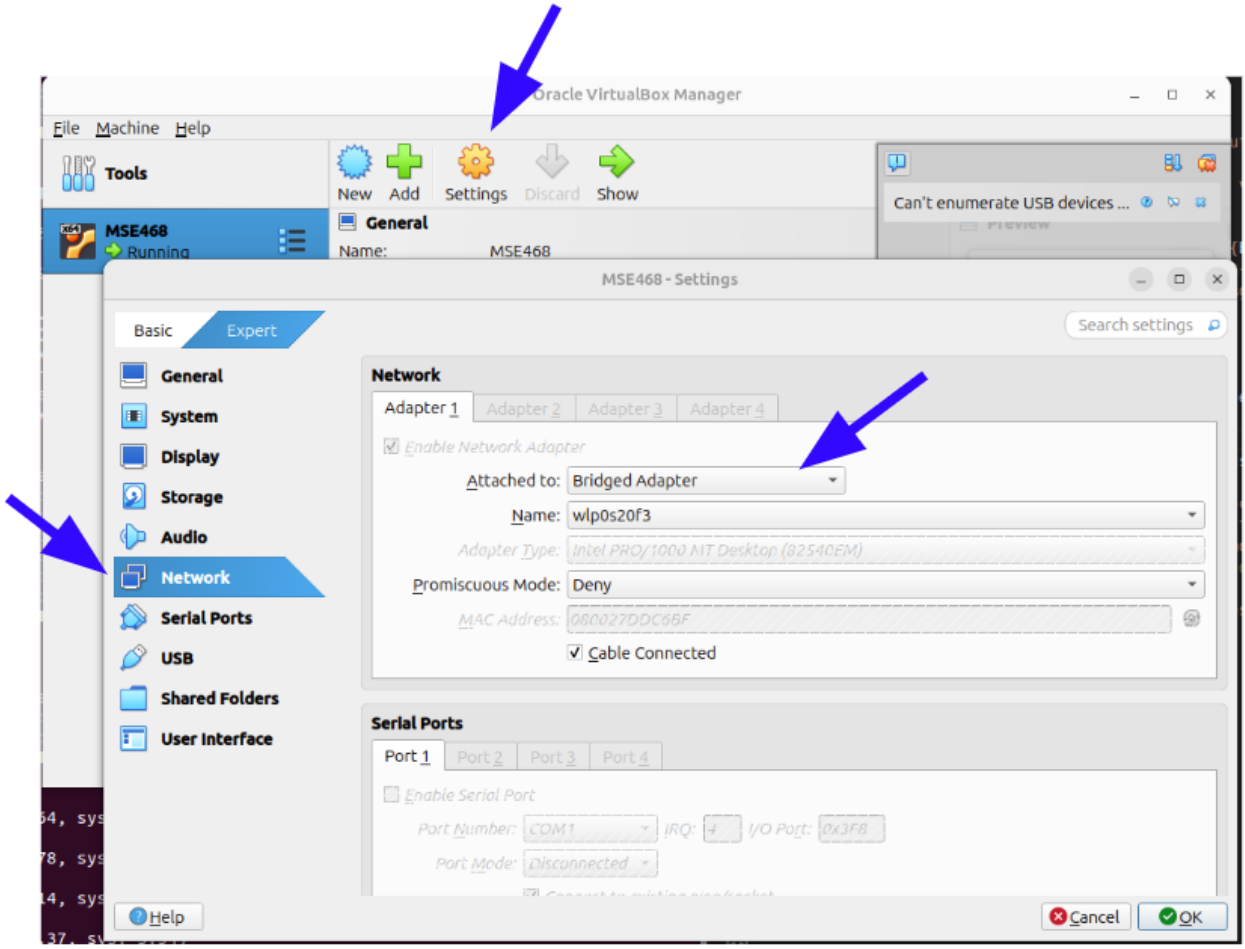
   ```
   conda activate lammps-env
   ```

1.1 Fixing the warning message: "`Unable to find reachable pairing between local and remote interfaces`"

When running LAMMPS with more than one core, you might run into the following warning message:

```
[mse468][[25339,1],0][btl_tcp_proc.c:266:mca_btl_tcp_proc_create_interface_graph]
Unable to find reachable pairing between local and remote interfaces.
```

Although this warning can be ignored, a simple fix consists of changing the "Bridged Adapter" option for the Network in the Settings panel, as shown in Figure 1.1.



If the issue persists, another possible solution consists of adding the following line at the end of your `/home/max/.bashrc` file:

```
export OMPI_MCA_btl_tcp_if_include=lo
```

Then, close and reopen your terminal.