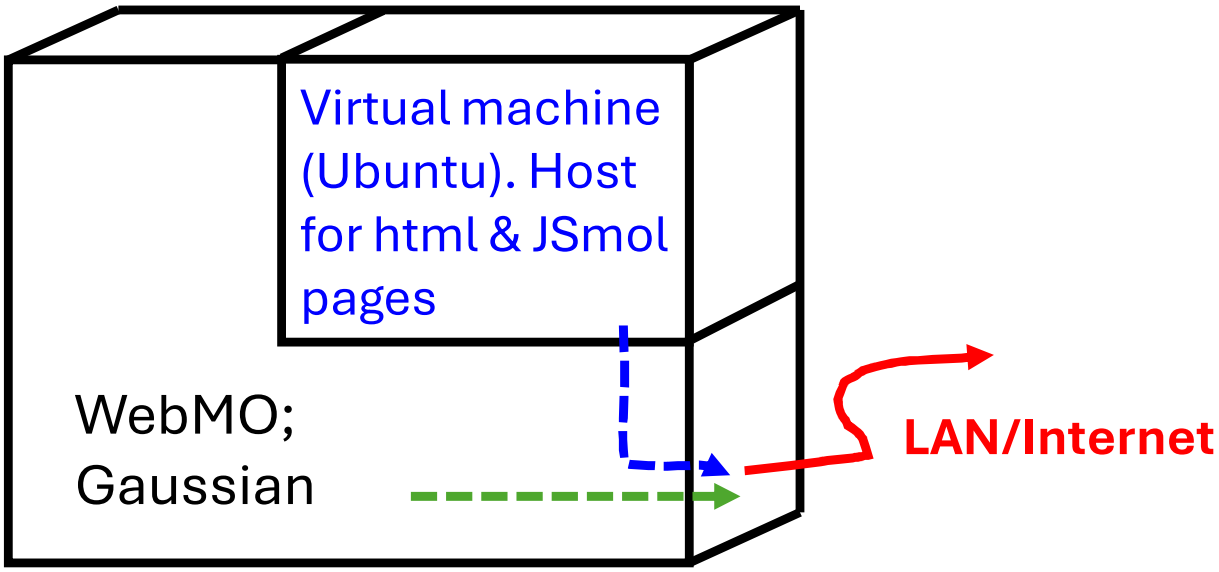
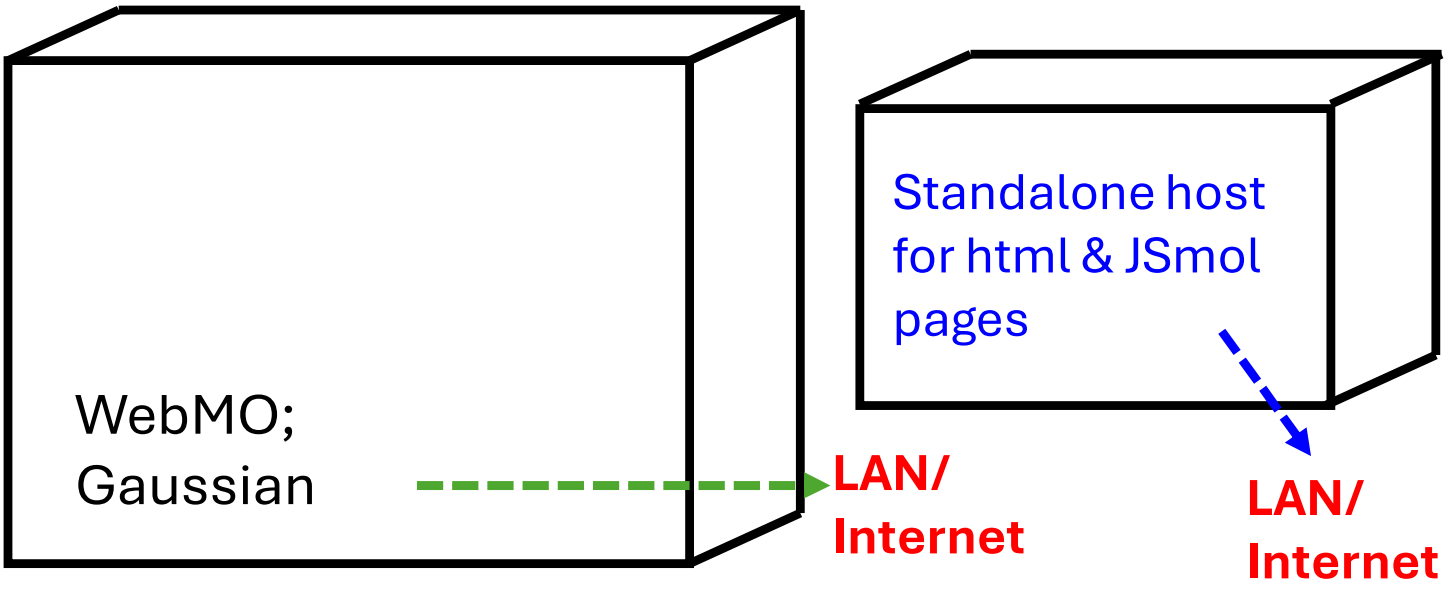



A Linux/Apache instance running WebMO cannot also host normal html websites (in my experience). One solution is to install a small virtual machine and have the two Linux OS's share the network interface.




Or, a separate server can host the Jsmol webpages.

John Keller University of Alaska Fairbanks 2024

# Set up a Linux guest VM on a Linux host using VirtualBox

## Install VirtualBox

- Download VirtualBox for Linux (VirtualBox-7.0-7.0.18_162988_el8-1.x86_64.rpm)
- As root,

  $ dnf install gcc make SDL qt5 kernel-headers* -y

  $ dnf localinstall [path_to_rpm_file]

## Install Ubuntu and configure as web server

- Download ubuntu-24.04-desktop-amd64.iso
- Start VB
- Machine, New
- Select the above iso file in its download location.
- Check “skip unattended”
- Choose username, password, hostname, and domain name. (These are VB’s reference to the guest machine. The actual Linux OS username, password hostname and domain are set from inside Ubuntu)
- Memory and processors (8 Gb and 2 procs are plenty).
- Hard disk (recommend a minimum of 50 GB). Check pre-allocate. Should be plenty of room if your host system as a 1- or 2-TB SSD or NVME drive.
- Finish

---

- Ubuntu Install dialog starts. Check download updates. Choose username and password. Ubuntu automatically partitions the disk.
- Log in
- Activate the root user.

  $ sudo –i

  $ (your password )

  $ passwd

  $ (enter root password)

  $ (retype root password)
- As root: $ apt install apache2 openssh-server

- Turn on the firewall and open it to ssh and html connections
  $ ufw enable
  $ ufw allow ssh
  $ ufw allow http
  $ ufw allow https
  $ ufw status
- Create webmasters group and add the ubuntu user to the group
  $ groupadd –g 499 webmasters
  $ usermod –aG webmasters <ubuntu user>
- Restart VM
  $ reboot now
- log back in as ubuntu user, then
  $ su
- Adjust permissions on website directory /var/www/html per https://gist.github.com/stefanbc/9956ed211cd32571e73f
- Log off

---

SSL certificate. If your WebMO server has an SSL certificate installed, then use the same procedure to obtain and install SSL and the SSL certificate on the VM.

---

To connect the VM to the network, in VirtualBox Manager, select the VM, click Settings; Network, Attached to…Bridged Adapter. Name..choose the name of the working ethernet adapter on the host machine, most commonly, eno1.

---

- Lastly create and test Jsmol and other html pages on your local machine, then upload to the VM.
- Download and install xampp for windows.
- The c:/xampp/htdocs folder is analogous to the /var/www/html directory on the webserver. Save .html files within the file structure in xampp, then upload same folders and files with Filezilla or WinSCP.

John Keller University of Alaska Fairbanks 2024

# JSmol webpages

JSmol is a web-enabled version of Jmol where the Jmol commands are contained in script sections within the html page. A typical JSmol page contains a 2-column table with a molecular display area and programmable buttons in the second column.

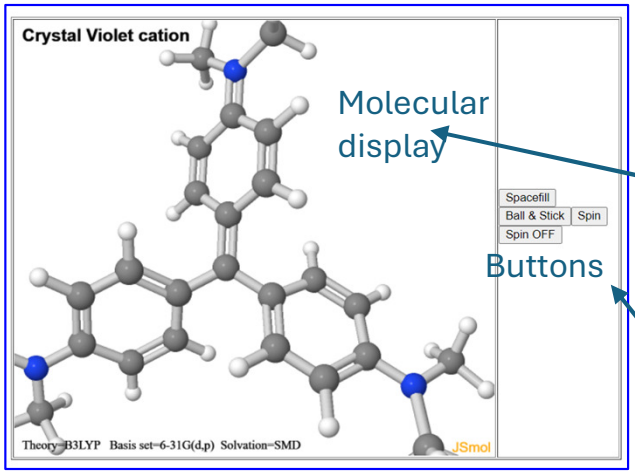
Importantly, the subject .mol file must be located in the same directory as the .html file.

Also, the Jsmol program files must be present on the server and the JSmol page must reference its location. Two levels up here (`"../../JSmol.min.js"`)

```
/var/www/html
    /jsmol-etc
        JSmol.min.js
        /j2s
        /folder
            /molecule
                cv.mol
                cv.html
```

From downloaded and expanded jmol

## Visible web page




## Html code for JSmol web page

```
<!DOCTYPE html>
<html>

<head>
<title>Crystal violet cation</title>
<meta charset="utf-8">
<script type="text/javascript" src="../../JSmol.min.js"></script>
<script type="text/javascript">

$(document).ready(function(){

Info = {
    width: 550,
    height: 500,
    debug: false,
    j2sPath: "../../j2s",
    disableJ2SLoadMonitor: true,
    disableInitialConsole: true,
    addSelectionOptions: false,
    use: "HTML5",
    readyFunction: null,
    script: "load cv.mol; background white; set antialiasdisplay on; wireframe 0.15;
    spacefill 22%; set cameradepth 0.4; select *; set multiplebondradiusfactor 0.75;
    set multiplebondspacing -0.5; color bond gainsboro; rotate z -12; zoom 100; set
    echo top left; font echo 20 sansserif bold; color echo black; echo Crystal Violet
    cation; set echo bottom left; font echo 14 serif plain; echo Theory=B3LYP   Basis
    set=6-31G(d,p)  Solvation=SMD;"
    }

$("#mydiv").html(Jmol.getAppletHtml("jmolApplet0",Info))
$("#btns").html( Jmol.jmolButton(jmolApplet0,  " spacefill 90% ","Spacefill")
  +Jmol.jmolButton(jmolApplet0, " isosurface off; wireframe 0.15; spacefill 22%; set
  cameradepth 0.4; set multiplebondradiusfactor 0.75; set multiplebondspacing -0.5; "
  ,"Ball & Stick")
  +Jmol.jmolButton(jmolApplet0, "spin y 30","Spin")
  +Jmol.jmolButton(jmolApplet0, "spin off","Spin OFF")
)
});

</script>
<style type="text/css">
.auto-style1 {
    font-size: small;
}
</style>
</head>
```

Make your own Jsmol page by **saving this one** and replace the Jmol commands with your own.