MolPOV Version 2.1.0
January 2012

Installation:

The installation program is provided as a self-extracting executable file MolPOV21_Install.exe. Execute this file from the download location to install MolPOV Version 2.1.

This version is an important update of the previous versions 2.0.0 through 2.0.8. It is made to use with the current Windows 7 operating system - 32 or 64 bit versions - and the most current POV-Ray program (version 3.6). It should work fine on the Windows Vista systems, but has not been tested.

The install package and the MolPOV program are 32-bit. The program installs simply on Windows 32-bit operating systems. It will also install on 64-bit systems, but users need to be aware that running the program in those environments may require knowledge of how to execute some types of 32-bit programs. For example, it may be necessary to use MolPOV via "Run as Administrator" in those 64-bit operating systems. To do that, navigate to the MolPOV installation folder (typically Program Files(x86)), right click on the MolPOV2.exe file, choose Properties, and under the Compatibility tab check the Run as Administrator box. The program should then execute when run from that folder.

Prior to installing MolPOV 2.1, the latest POV-Ray program (currently version 3.6) must be installed. Earlier versions of POV-Ray *are not supported* by MolPOV 2.1 as the POV-Ray 3.6 rendering control files are different from those of version 3.5 and lower. ***MolPOV 2.1 will only load and render files in POV-Ray 3.6***. If you are using an older version of POV-Ray (not recommended!), you will need to use MolPOV version 2.08.

When installing POV-Ray 3.6, note the location of the bin\ folder that contains the pvengine executable file. If you prepare modified include files, they must be in the default locations to be used by MolPOV (unless you are willing to edit the POV input files directly). Please be aware that the current version of POV-Ray (3.6) places these items in different folders by default compared to earlier versions. For example, the include folder and the bin folder are installed in completely different default locations (e.g., the pvengine.exe or pvengine64.exe file is normally in C:\Users*your_ username*\AppData\ Roaming\POV-Ray\v3.6\bin). The pvengine executable file may be installed in a hidden folder, so the Folder View option to show hidden files and folders may need to be enabled. If this is not done, it may not be possible to browse to the location from the MolPOV program.

Once the POV-Ray pvengine location has been entered under Preferences in MolPOV, be sure to click Set As Default to register the entry. Unlike earlier MolPOV versions, you do not need to provide the location of the \include folder the first time you run MolPOV since POV-Ray will use its default location. Finally, after confirming that POV-Ray has been installed correctly, under the POV-Ray Options menu item, check "Keep Single Instance" for the easiest interaction between MolPOV 2.1 and POV-Ray 3.6. If this option is not set, a new POV-Ray program will be launched every time a render job is submitted by MolPOV. For those who

want to know, the Registry location for various MolPOV options is HKEY_CURRENT_USER\Software\VB and VBA Program Settings\MolPOV 2.1.

Executing MolPOV2:

When MolPOV2.exe is first executed, you will be asked to provide the location of the /bin/pvengine.exe (or pvengine64.exe) POV-Ray program file. These must be entered correctly as described above to use POV-Ray directly from MolPOV2.

A Novice mode is available by checking the entry View|Novice Messages on the menu bar. This mode is useful for those who are using MolPOV for the first time. Some sample files are provided to get started- see the Helpfile under Other Resources.

Help:

The help system for MolPOV2 is in Microsoft HTML Help format and normally requires Internet Explorer to be installed on your computer to run. Other necessary files are installed as required. The help file is opened by the Microsoft HTML Help Executable.

Uninstall:

Remove MolPOV2 and its components from the Control Panel|Programs and Features dialog (formerly Add/Remove Programs in Win XP). Any files (pov and bmp) produced after installation are not removed.

MolPOV History:

MOlPOV has been developed since the late 1990's by David E. Richardson, Department of Chemistry, University of Florida. The original version was designed using Visual Basic 5, and later versions were produced using Visual Basic 6/SP6. Many aspects of the program are dated in appearance but remain functional on newer Windows operating systems, including Windows 7.

Please contact the author at der@chem.ufl.edu if you encounter any issues with installation or the program.

Partial List of Features and Fixes:

Version 2.1.0 (Jan 2012)

-Now works smoothly with POV-Ray 3.6 (*required* to use all MolPOV features). Check "Keep Single Instance" in POV-Ray Options for best results. When a file is sent to POV-Ray from MolPOV 2.1, a special "povray.ini" file is written in the current directory to pass options to

POV-Ray renderer. This file in temporary and changes based on selected options in MolPOV each time a file is sent for rendering.

-the WinZip Installer package is fully 32-bit and will install the program on 32- and 64-bit Windows operating systems. Windows 7 is recommended.

- The POV scene files written by MolPOV 2.1 are much more compact and easy to read than those from earlier versions (in the atom and cylinder parts of the file).

- Some minor clean up and fixes of the main window and other dialogs have been done to accommodate the Vista/Win 7 interface.

- The default preview and render size is increased to 400x300 pixels.

Version 2.0.8

- MolPOV can now read files with >32,000 atoms

- Bug in POV Style read/write fixed

- Animation option added under Render. When POV-Ray is executed from MolPOV the number of frames entered in the dialog will be rendered with sequential numbering. The molecule will be rotated 360/(n+1) degrees per frame around the axis or axes checked, where n is the number of frames (see POV-Ray documentation for more information). The resulting n files can be combined into an animated movie of the rotating molecule using appropriate software.

Version 2.0.7

- Initial light positions and camera position are determined by the size of the molecule

- Protein data bank files downloaded from the PDB Web site are now read correctly despite the Unix format. A temporary PDB file is written with the ASCII format line terminators.

- Molecules with large numbers of atoms no longer produce a read error.

- Once closed, the preview window does not reopen if camera position is changed. This makes it faster to change the camera positions for very large molecules without rendering the preview window for each modification. A similar function is available by unchecking View|Auto Update Previewer.

- Auto Update Previewer menu item now functions correctly.

- For very large molecules (>5000 atoms) the program offers to skip the find bonds routine, which can be time consuming. If find bonds is not run, Cylinders mode and Ball and Stick

mode are not available for POV-Ray rendering and Stick mode is not available in the previewer.

Version 2.0.0:

- If new covalent radii are entered in Atom Edit dialog, running Find Bonds correctly alters the internal bond table and refreshes preview accordingly

- Larger preview windows available

- Previously saved bond table can be used or bond search is run every time a pdb is loaded depending on option chosen in Preferences

- Other minor fixes

Beta 2:

- The 3D previewer now can be in spacefill or cylinder mode.

- The size of the 3D previewer window can be fixed to one of several sizes or set to be the same as the POV-Ray render width and height set in MolPOV.

- Area lights are available as optional lighting to cast more realistic, diffuse shadows. Note: this feature can increase rendering time if turned on.

- A No Shadow mode prevents any shadows from being cast in the scene.

Beta 1:

- A 3D viewer has been provided for lining up the camera position before writing POV-Ray file. It is loaded by default when a PDB file is read. This viewer can be disabled by the Edit|Preferences dialog. Use View|Auto Update Viewer to control auto update feature (useful for huge molecules).

- POV schemes (camera position, lights, etc.) can be saved from the toolbar or File menu (*.par files)

- Atom schemes can also be saved (color, radii) from the File menu or Atom Edit tab (*.ats files)

- An Atom List function is available for perusing the parsed atom data in MolPOV for errors.

- All options for rendering and atom appearance are on a single form

- Handy toolbar for common functions and many tool tips

- Bond table generated and saved for cylinder and ball/stick renders

- Expanded control of camera ("look at" coordinates and "sky" vector). Also advanced properties accessible, including angle of view

- Easy slider control of camera coordinates

- Expanded color lists for atoms, lights (grey scales especially useful for controlling light intensity)

- Status bar for info, date, time, files used

- Under Edit one can load PDB and POV files for viewing (PDB editing not updated in MolPOV unless PDB file reloaded)

- Auto increment of POV filenames an option (see Preferences dialog)

- Windows 32-bit program, long file names supported, Registry used for program settings, uninstall from Control Panel|Add/Remove Programs

- Better looking, easier to use, and faster due to modest improvement in programming skill

- Several standard finishes, metallic highlights, and atom sphere transparency option available under Atom Finish

- Atoms and bonds can be set to one color under Atom Edit

- Preferences dialog sets default folders for PDB files, POV files, image files, and others

- Optional warnings before overwriting various file types (under Preferences)

- Expanded Help resources, including context sensitive help