LAMMPS Build Instructions (Version 22Jul2025)

Introduction

These instructions guide you to build LAMMPS (version 22Jul2025) with MPI and the MOLECULE package, addressing the CMake error due to auto-generated files. The build is tailored for your setup in `/home/gokul/Downloads/lammps_2025/lammps-22Jul2025` and supports running `in.polymers_100x10` in parallel.

Build Steps

1. **Clean Auto-Generated Files**: Remove files from a previous make-based build to resolve CMake conflicts:

```
cd /home/gokul/Downloads/lammps_2025/lammps-22Jul2025/src
make purge
```

2. **Navigate to Build Directory**:

```
cd /home/gokul/Downloads/lammps_2025/lammps-22Jul2025
mkdir -p build && cd build
```

3. **Configure CMake**: Choose user-local or system-wide installation:
   - **User-Local Installation** (no root access needed):

```
cmake -D BUILD_MPI=ON -D CMAKE_C_COMPILER=mpicc -D
   CMAKE_CXX_COMPILER=mpicxx -D PKG_MOLECULE=ON -D
   CMAKE_INSTALL_PREFIX=$HOME/.local ../cmake
```

   - **System-Wide Installation** (requires root access):

```
cmake -D BUILD_MPI=ON -D CMAKE_C_COMPILER=mpicc -D
   CMAKE_CXX_COMPILER=mpicxx -D PKG_MOLECULE=ON -D
   CMAKE_INSTALL_PREFIX=/usr/local ../cmake
```

4. **Build LAMMPS**:

```
make -j$(nproc)
```

5. **Install LAMMPS**:
   - For user-local:

```
make install
```

- For system-wide:

```
sudo make install
```

6. **Update PATH (if User-Local)**: Ensure `/home/gokul/.local/bin` is in your PATH:

```
echo $PATH
echo 'export PATH=$HOME/.local/bin:$PATH' >> ~/.bashrc
source ~/.bashrc
```

7. **Verify Installation**:

```
lmp -h
```

Or use the full path:

```
/home/gokul/Downloads/lammps_2025/lammps-22Jul2025/build/lmp
   -h
```

8. **Test Parallel Run**: Run your script:

```
cd /home/gokul/Downloads/polymers
mpirun -np 4 lmp -in in.polymers_100x10
```

If `lmp` isnt found, use:

```
mpirun -np 4 /home/gokul/Downloads/lammps_2025/lammps-22
   Jul2025/build/lmp -in in.polymers_100x10
```

Check the log file:

```
cat /home/gokul/Downloads/polymers/log.lammps
```

Test Script (test_parallel.in)

If `in.polymers_100x10` fails, use this script to verify parallel execution:

```
# test_parallel.in
units lj
atom_style molecular
region box block 0 20 0 20 0 20
create_box 2 box
create_atoms 1 single 10 10 10
create_atoms 2 single 11 10 10
mass 1 12.0
mass 2 16.0
pair_style lj/cut 10.0
pair_coeff 1 1 0.112 3.4
```

```
pair_coeff 1 2 0.1 3.5
pair_coeff 2 2 0.09 3.6
bond_style harmonic
bond_coeff 1 100.0 1.0
create_bonds single/bond 1 1 2
fix 1 all nve
log log.test
run 100
```

Save in `/home/gokul/Downloads/polymers` and run:

```
mpirun -np 4 lmp -in test_parallel.in
```

Notes

- **CMake Warning**: Ignore the `CMP0109` deprecation warning.
- **Additional Packages**: Add `-D PKG_MANYBODY=ON` or others if needed.
- **Potential Files**: Ensure files like `SiC_1994.tersoff` are in `/home/gokul/.local/share/lammps` (user-local) or `/usr/local/share/lammps/potentials` (system-wide).
- **OpenMP**: To disable 2 OpenMP threads per MPI task:

```
export OMP_NUM_THREADS=1
```

- **Lingering Processes**:

```
ps aux | grep lmp
killall lmp
```

Troubleshooting

- If `make purge` fails:

```
rm /home/gokul/Downloads/lammps_2025/lammps-22Jul2025/src/
   style_*.h
```

- Share errors or log files for further assistance.