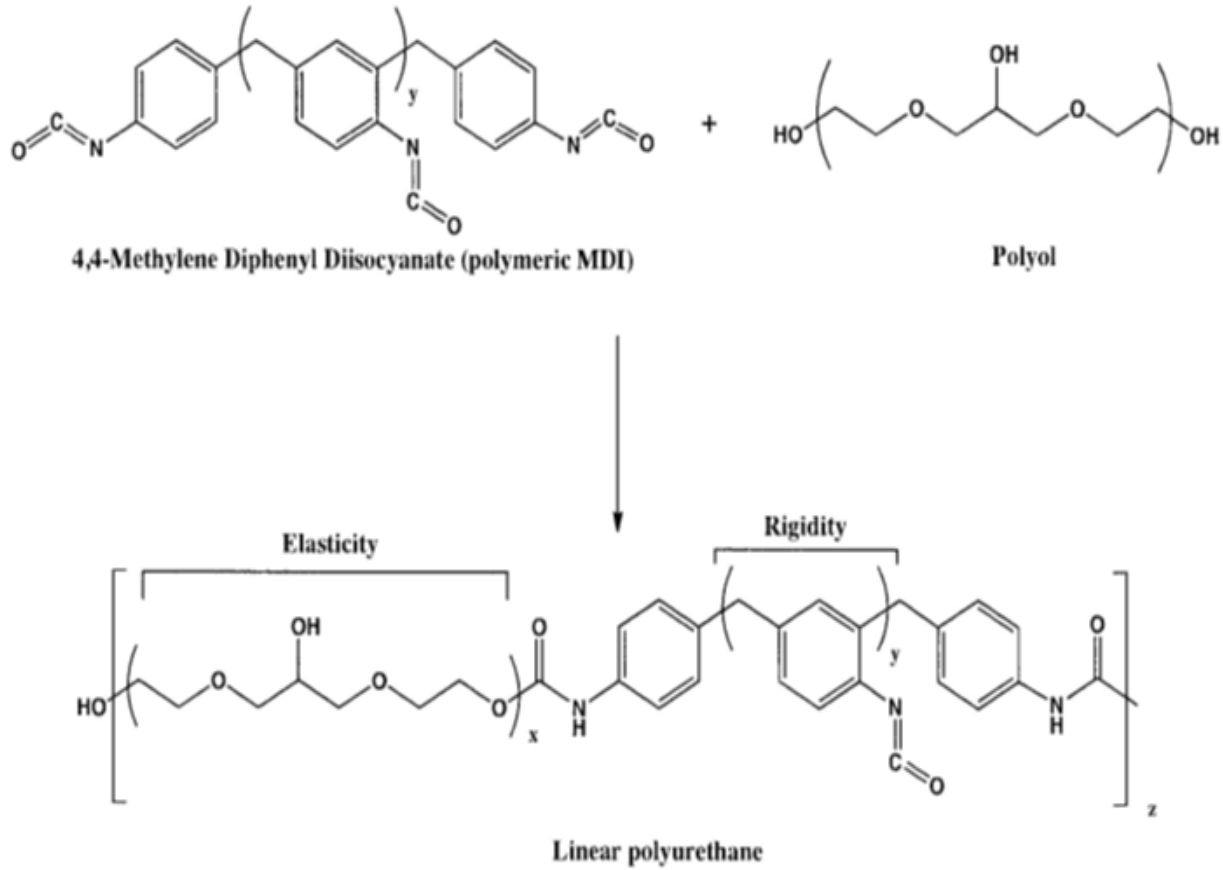
Diffusion Rates of Flame Retardants in Polyurethane Foam

Jeff Parrozzo

Mentor: Dr. Randall Hall

Polyurethane

- Product of step-growth polymerization between a monomer with at least two isocyanate functional groups and another monomer with at least two hydroxyl or alcohol groups in the presence of a catalyst
- Different monomers and additives determine physical properties of material
- Used in insulation foam, suspension bushings, adhesives, print rollers and many other applications



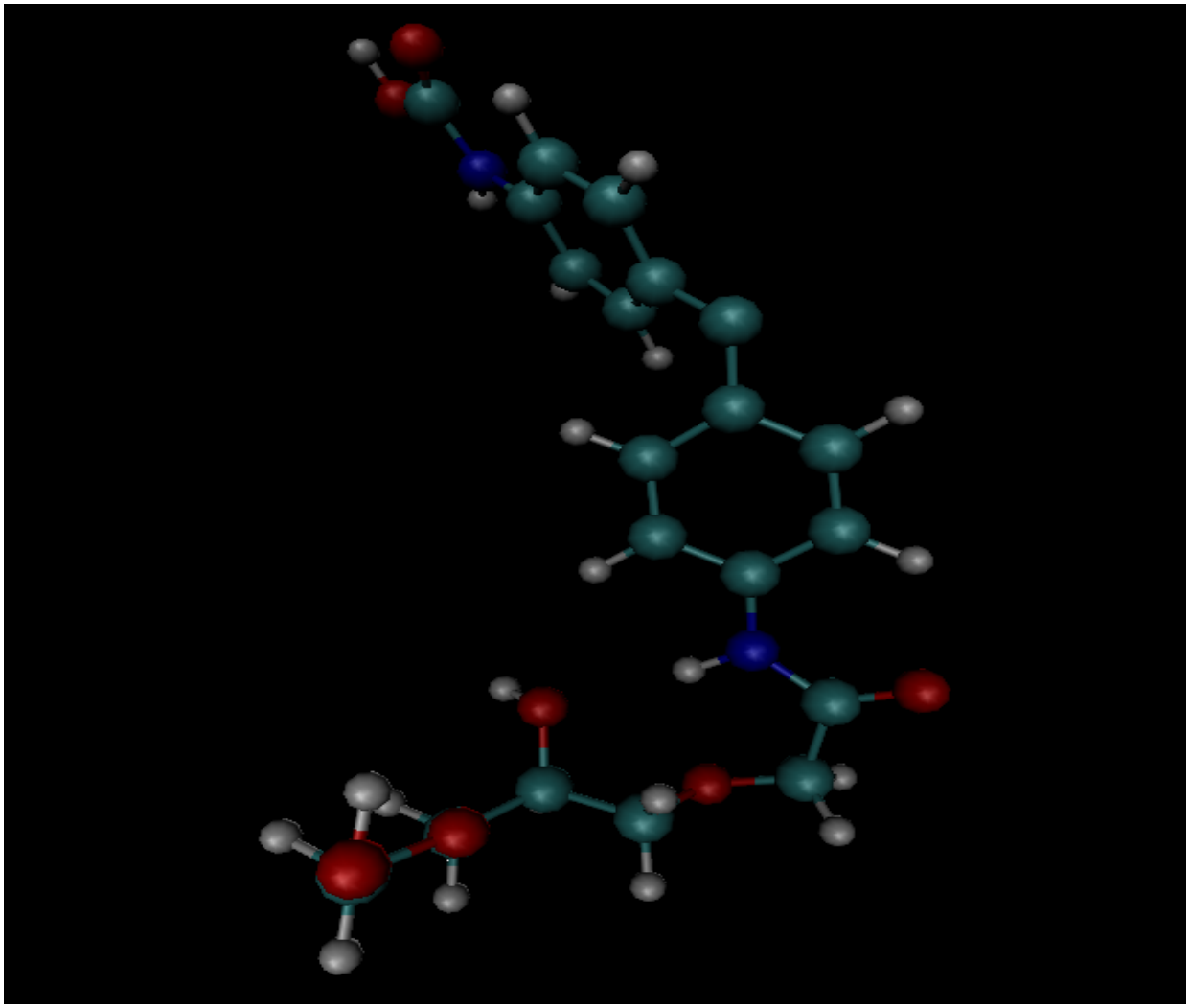
- Synthesized by reacting polymeric MDI with a polyol followed by crosslinking with butane diol to create a polyurethane thermoset
- Most commonly used in automotive seat cushioning and furniture

Research Goal

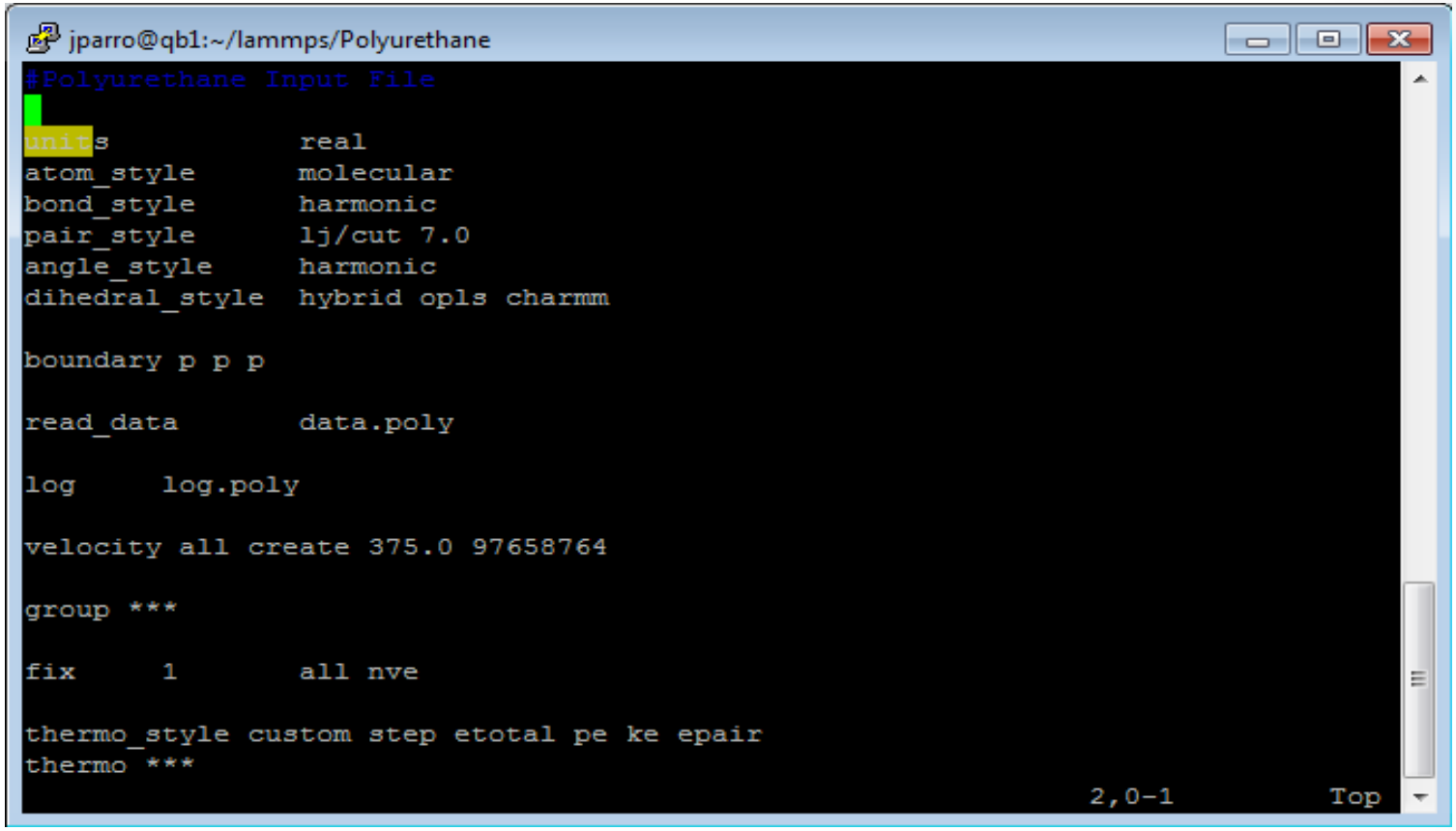
- Polyurethane is highly flammable in its raw state
- Production companies must introduce flame retardant molecules in the form of powders and liquids to make the polymer more stable
- Must know the best temperature and density of the materials for optimal diffusion of the flame retardant

Simulation Methods

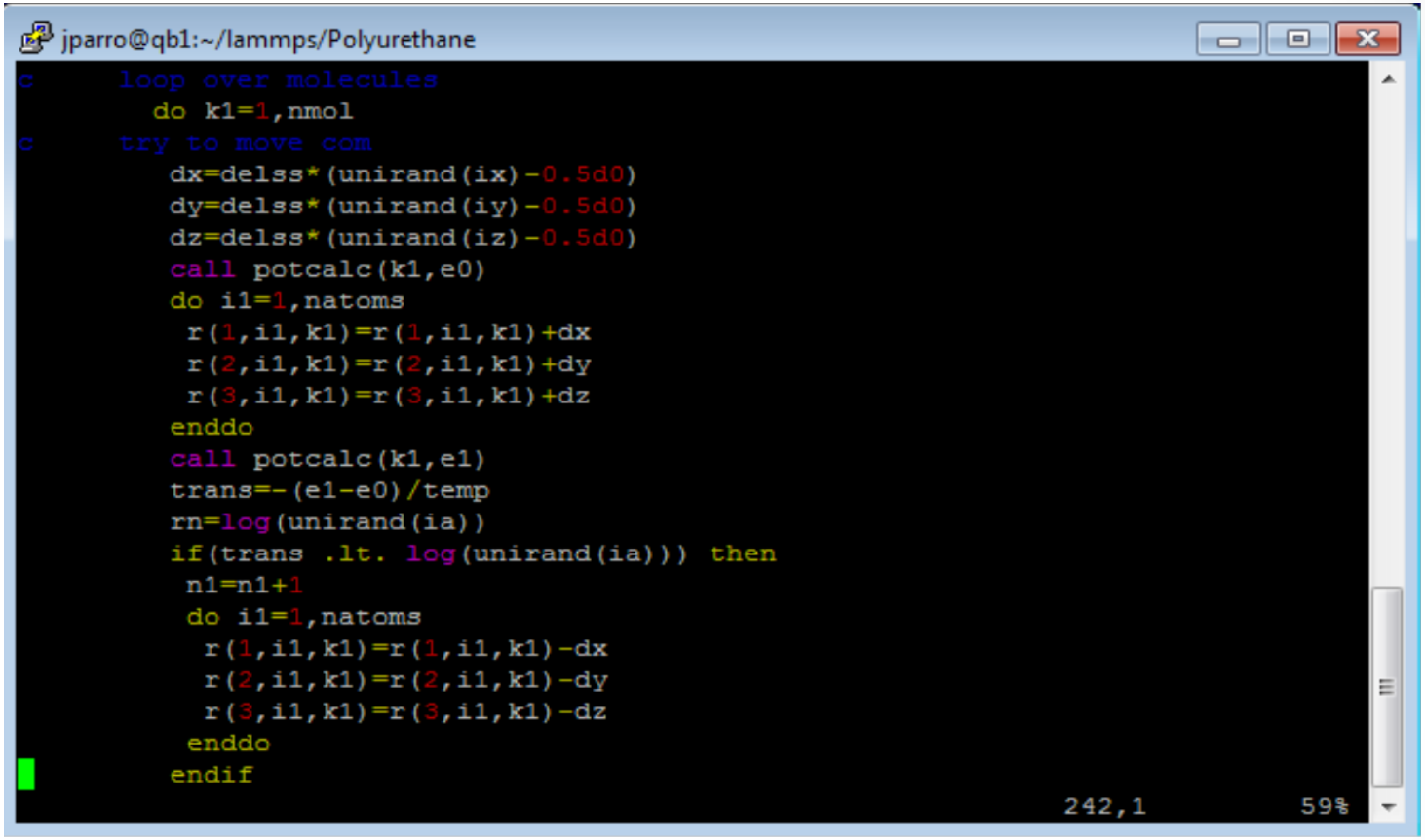
- Polyurethane molecule and flame retardant molecules built in Molden
- Structures optimized on Louisiana Optical Network Initiative (LONI) supercomputers
- Script written for Large Atomic/Molecular Massively Parallel Simulator (LAMMPS) of single molecules
- Fortran code using Monte Carlo algorithm to replicate polyurethane molecule and generate environment for flame retardant diffusion tests
- LAMMPS output can then be visualized in VMD



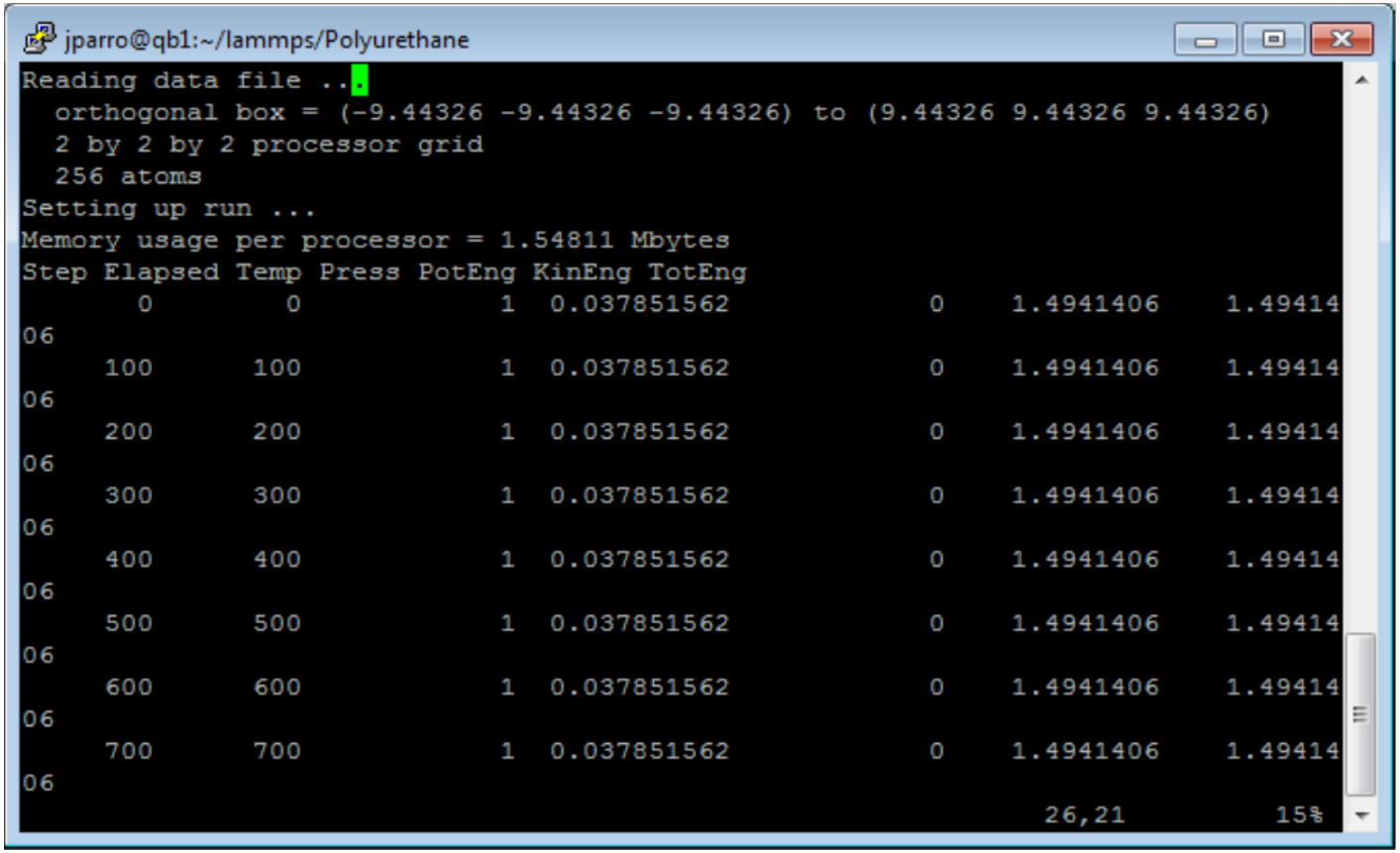
Optimized polyurethane molecule



Input script for polyurethane molecule



Monte Carlo code for creating environment



Output file for simulation

Acknowledgements

- LA-SiGMA, funded by the National Science Foundation (NSF) award number #EPS-1003897
- Dr. Randall Hall, Chemistry Dept., LSU
- Louisiana Optical Network Initiative (LONI)
- Large Atomic/Molecular Massively Parallel Simulator (LAMMPS)
- Humphrey, W., Dalke, A. and Schulten, K., "VMD - Visual Molecular Dynamics", J. Molec. Graphics, 1996, vol. 14, pp. 33-38. (VMD)
- G.Schaftenaar and J.H. Noordik, "Molden: a pre- and post-processing program for molecular and electronic structures", J. Comput.-Aided Mol. Design, 14 (2000) 123-134 (Molden)