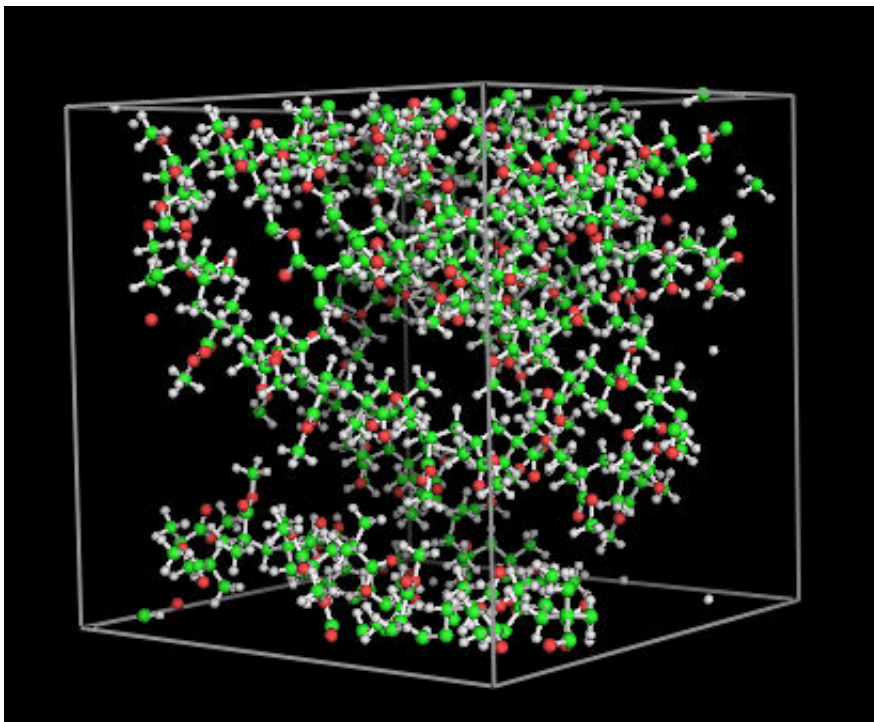


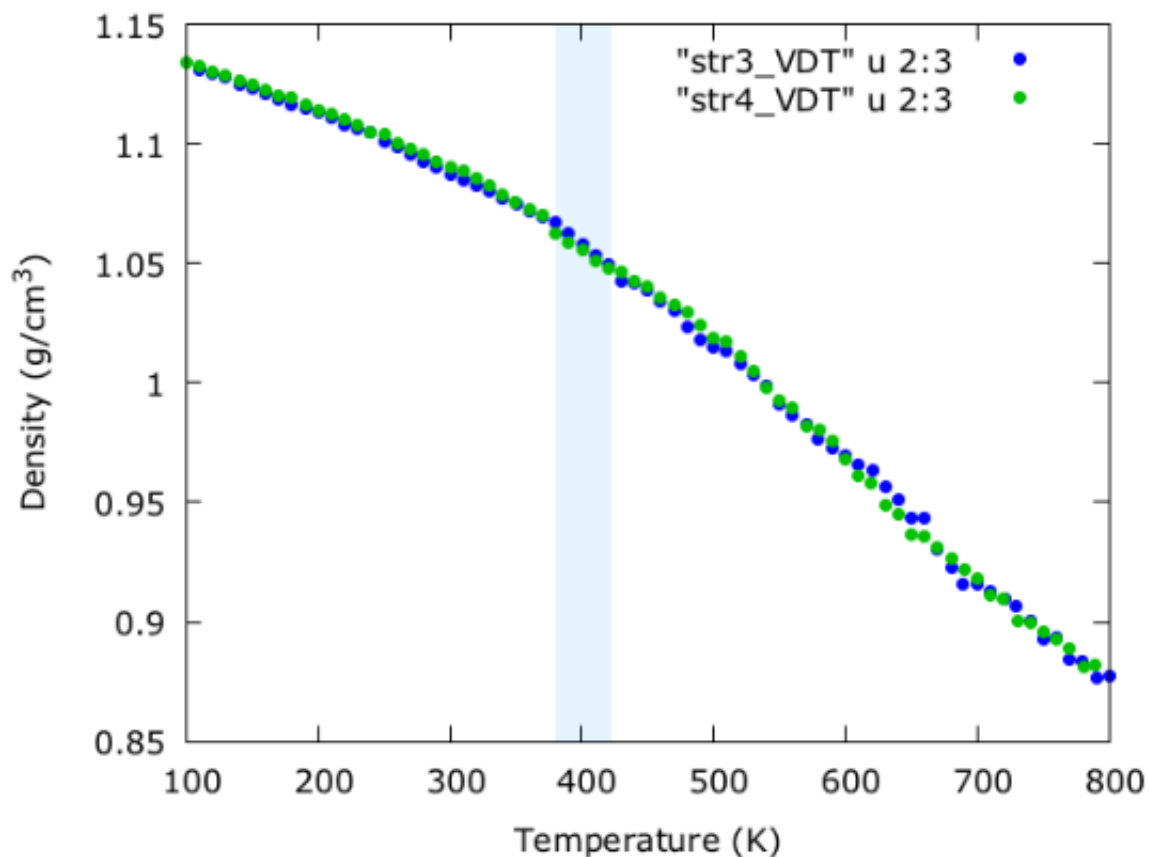
Polymer Service

Calculation of the glass transition temperature of an amorphous system

Overview

- Build the atomistic system (e.g. PolymerModeler)
- Run LAMMPS: cool the system and shrink the box
- Analyze the output from LAMMPS: extract density vs. T





(Image

courtesy Lorena Alzate)

Service proposal

- GET info on available services returns JSON

```
{
  "polybuild": {
    "input": {
      "values": {
        "monomer": {
          "type": "string",
          "desc": "Name of the basic repeating unit",
          "values": ["pmma", "pe", "ps"]
        },
        "chains": {
          "type": "integer",
          "desc": "Number of chains to build"
        },
        "monomers": {
          "type": "integer",
          "desc": "Number of monomers in each chain (polydispersi
```

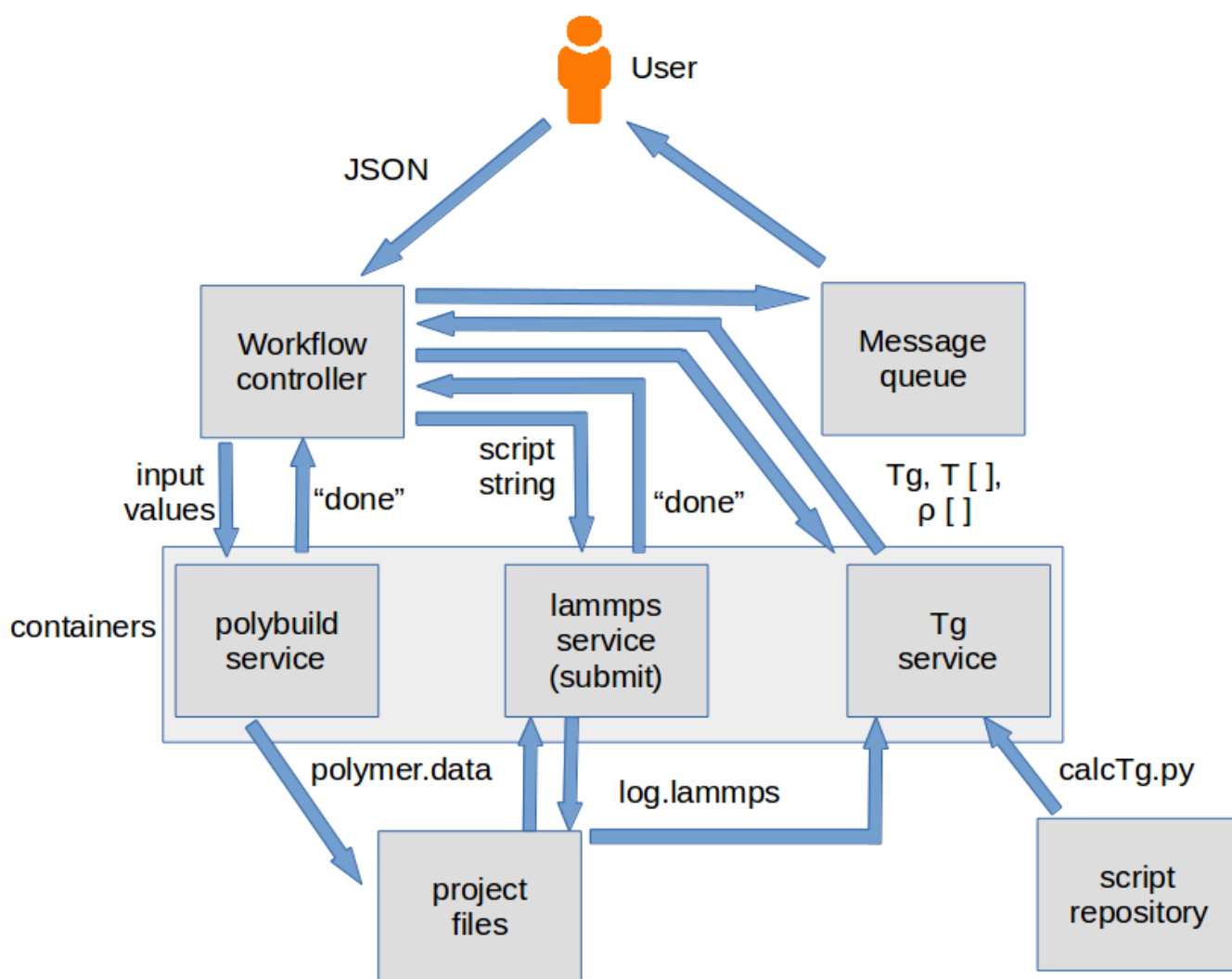
```
ty)"
    },
    "interactions": {
      "type": "string",
      "desc": "Name of interactions between particles",
      "values": ["LJ"]
    },
    "range": {
      "type": "real",
      "units": "Angstroms",
      "desc": "Interaction range between particles"
    },
    "density": {
      "type": "real",
      "units": "g/cc",
      "desc": "Density of the constructed amorphous system"
    },
    "temperature": {
      "type": "real",
      "units": "K",
      "desc": "Temperature of the system while building"
    },
    "configurations": {
      "type": "integer",
      "desc": "Number of configurations per torsion during MC
sampling",
    },
    "rotate_torsions": {
      "type": "string",
      "desc": "Specify how many torsions in each monomer are
rotated",
      "values": ["all", "only_between"]
    },
    "torsion_probs": {
      "type": "string",
      "desc": "Specify how torsion angles are assigned",
      "values": ["random", "fixed", "sp2", "sp3"]
    },
    "forcefield": {
      "type": "string",
      "desc": "Name of the forcefield to apply for LAMMPS dat
a file",
      "values": ["Dreiding"]
    }
  },
}
```

```
"output": {
  "files": ["lammps_data_file"]
},
"lammps": {
  "input": {
    "files": ["lammps_script", "lammps_data_file"]
  },
  "output": {
    "files": ["lammps_log_file"]
  },
  "submit_options": {
    "cores": {
      "type": "integer",
      "desc": "Number of cores on which to run LAMMPS"
    },
    "walltime": {
      "type": "real",
      "units": "hours",
      "desc": "Requested simulation time for LAMMPS"
    }
  }
}

"Tg": {
  "script": "calcTg.py",
  "input": {
    "files": ["lammps_log_file"]
  },
  "output": {
    "values": {
      "Tg": {
        "type": "real",
        "units": "K",
        "desc": "Glass transition temperature"
      }
    },
    "density": {
      "type": "array",
      "units": "g/cc",
      "desc": "System density over MD steps"
    },
    "temperature": {
      "type": "array",
      "units": "K",
      "desc": "System temperature over MD steps"
    }
  }
}
```

```
}  
  }  
}  
}
```

- Construct JSON input describing a workflow
 - polybuild: build the atomistic system
 - lammps: run LAMMPS to cool and compress
 - Tg: identify Tg from LAMMPS thermo output



```
{  
  "tasks": ["polybuild", "lammps", "Tg"],  
}
```

```
"polybuild": {
  "input": {
    "values": {
      "monomer": "pmma",
      "chains": 10,
      "monomers": 5,
      "interactions": "LJ",
      "range": 6.0,
      "density": 0.5,
      "temperature": 300,
      "configurations": 50,
      "rotate_torsions": "all",
      "torsion_probs": "random"
      "forcefield": "Dreiding"
    }
  },
  "output": {
    "files": {
      "lammmps_data_file": "polymer.data"
    }
  }
},

"lammmps": {
  "input": {
    "files": {
      "lammmps_script": {
        "contents": "units real\natom_style full\nboundary p p p\nspe
cial_bonds lj/coul 0.0 0.0 1.0 dihedral yes\ndielectric 1.0\npair_style lj/c
ut 6.0\nbond_style harmonic\nangle_style harmonic\ndihedral_style harmonic\n
improper_style harmonic\nread_data polymer.data\nneighbor 2.0 bin\nthermo_st
yle custom step etotal ke temp pe ebond eangle edihed eimp evdwl ecoul elong
press pxx pyy pzz pxy pxz pyz lx ly lz\nthermo 50\nthermo_modify flush yes\
nMINIMIZE\ndump 1 all custom 1 polymer.dump id mol type xu yu zu\ndump_modif
y 1 format \"%d %d %d %.10f %.10f %.10f\"\nrun 0\nundump 1\nwrite_restart po
lymer.restart\n"
      }
      "lammmps_data_file": "polymer.data"
    }
  },
  "output": {
    "files": {
      "lammmps_log_file": "log.lammmps"
    }
  }
},
```

POLYMER SERVICE

```
"submit_options": {  
  "cores": 4,  
  "walltime": 12.0  
}
```

```
}
```

```
}
```