Hackathon & Tutorials

Materials Available:

https://github.com/openchemistry/avogadro-ugm2018

Current & Future APIs

- RPC: Your program => “visualize this file”
- C++ Plugins
- Python
- File Formats
- Input Generators
- Workflows
- *Force Fields / Energies*
- *Charge Models*

Plugin Directory / Ecosystem

- Register GitHub repo
- Search for plugin (author?)
  - “Splash” icon for plugin?
- Reviews / feedback on repo
  - How do we help file bugs on plugins?

Generator Ideas

Chemistry:
GAMESS
Gaussian
Mopac
Orca
Q-Chem
NWChem
Turbomole
Psi4
???

Solid-state:
VASP
~~CP2K~~
Abinit
Quantum Espresso
Crystal
Wien2k
(etc.)

Molecular Dynamics:
Amber
~~OpenMM~~
Gromacs
Tinker
~~LAMMPS~~

Needed:

- Add job types (TS, Saddle, IRC, NMR, TDDFT, *etc.*)
- Update methods (ωB97X-D, SCAN, *etc.*)
- Update basis sets (def2-X, pc-X, *etc.*)
- Add solvation
- Syntax highlighting

Workflow Ideas

Avogadro

- get / modify selection (e.g., enlarge by x Å)
- create enantiomer
- “Random alloy” - Replace x% atom X -> atom Y

Scikit-nano https://docs.scikit-nano.org

- MWNT
- Graphene or TMDC multilayers?

Pymatgen https://github.com/materialsproject/pymatgen

- create a slab
- nanoparticle with Wulff

STK https://lukasturcani.github.io/stk/docs/build/html/

- polymers
- cages
- COF
  - hexagonal, honeycomb, kagome, square

Workflow Ideas

RDKit http://www.rdkit.org/docs/GettingStartedInPython.html

- get ETKDG conformer

ASE

- Generate MoS2 https://wiki.fysik.dtu.dk/ase/ase/build/surface.html#ase.build.mx2
- Generate TIP water box: https://wiki.fysik.dtu.dk/ase/tutorials/tipnp_equil/tipnp_equil.html

GenIce - https://github.com/vitroid/GenIce/

- Generate ice unit cell

PackMol https://github.com/choderalab/openmoltools/blob/master/openmoltools/packmol.py

- Pack current molecule http://timvdm.blogspot.com/2010/03/avogadros-packmol-plugin.html

Glycam(?)

- Sugar / oligosaccaride builder?

Avogadro Demos

Avogadro Demo: Small Molecule Building

- Draw Tool: Click & Drag
- Click on bond: Single, Double, Triple
- Change Element, Click on atom: Alchemy
- Auto-Adjust Hydrogens
- Manually Add H after drawing
- **Keyboard Shortcuts:**
  - Type element symbol to change
  - Type 1, 2, 3, 4 to change bond order
  - Control + 1, 2, 3 to change tools

Avogadro Demo: Larger Molecules

- Copy/paste & Undo
- Insert Fragments
  - Select h-atom to “grow” fragment (v 1.1)
- Insert SMILES
  - Useful for polymers
- “Sculpting” using Auto-Optimization
- Adjusting angles, bond lengths, dihedrals
  - Bond-Centric Manipulate Tool
  - View ⇒ Properties …

Avogadro Demo: Peptides

- Custom Sequences
- Helix, Sheets, Custom Conformations
- Multiple Chains
- Visualization methods

Avogadro Demo: Building Crystals

- New Interface in v1.1
- Still in development: feedback welcome
  - Build slabs and nanoparticles (soon)
  - Edit cell parameters
  - Build supercells (simple slabs)
  - Edit Fractional Coordinates (v1.1)
  - Detect / Set Space Group (v1.1)

Avogadro Demo: Visualization Modes

- Standard Representations
  - Balls & Sticks, Labels, etc.
- Forces
- Hydrogen-Bonding
- Color Modes

Avogadro Demo: Force Fields / Conformers

- Auto-Optimize Tool
- Extension / Menu Item
- Setting Constraints
  - Fixed / Frozen Atoms
  - Ignored Atoms
  - General Constraints (bonds, angles, …)
- Finding & Generating Conformers

Avogadro Demo: More Extensions

- Spectra Viewer (IR, UV/Vis, NMR)
  - Import experimental data
- Vibrations & Orbitals
- Molecular Surfaces
- External Packages
  - Gaussian, GAMESS, Q-Chem…
  - Abinit
  - Packmol, XtalOpt (3rd party)