Avogadro User's Group Meeting

Welcome, Feedback, Roadmap

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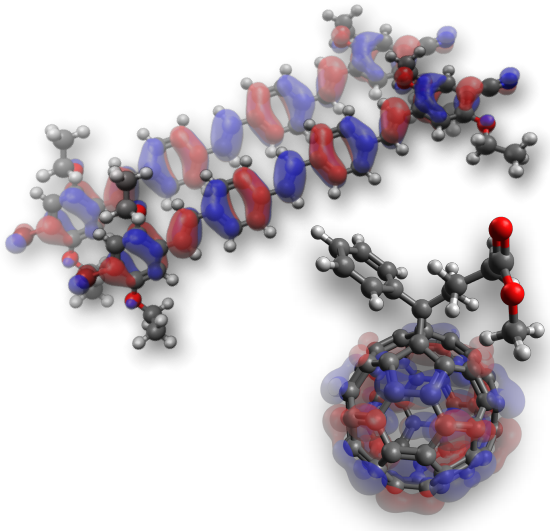
Department of Chemistry

University of Pittsburgh

Avogadro User Meeting

August 25, 2018



What is Avogadro?

Avogadro Project

- Free, open source molecular **editor**
- Cross-platform: Win, Mac, Linux…
- Fast, intuitive, flexible
- Extensible: plugins & scripting
- Molecules, Proteins, DNA, Materials, Nanotubes, …
- Make it easy to create 3D molecules / materials

One million downloads

1600+ academic citations

25+ foreign language translations

Avogadro History

- Origins - 2006/2007 “Manifesto”
- Google Summer of Code 2007
- Pitt Chem- Hutchison, Hanwell, Curtis (+ many)

Releases:

0.1 = 2007-05-17

…

1.0 = 2009-10-23

1.1 = 2012-09-12

1.2 = 2016-06-15

Avogadro 2

0.5 = 2013-04-13

…

1.90 = 2016-12-3

Volunteer Contributions

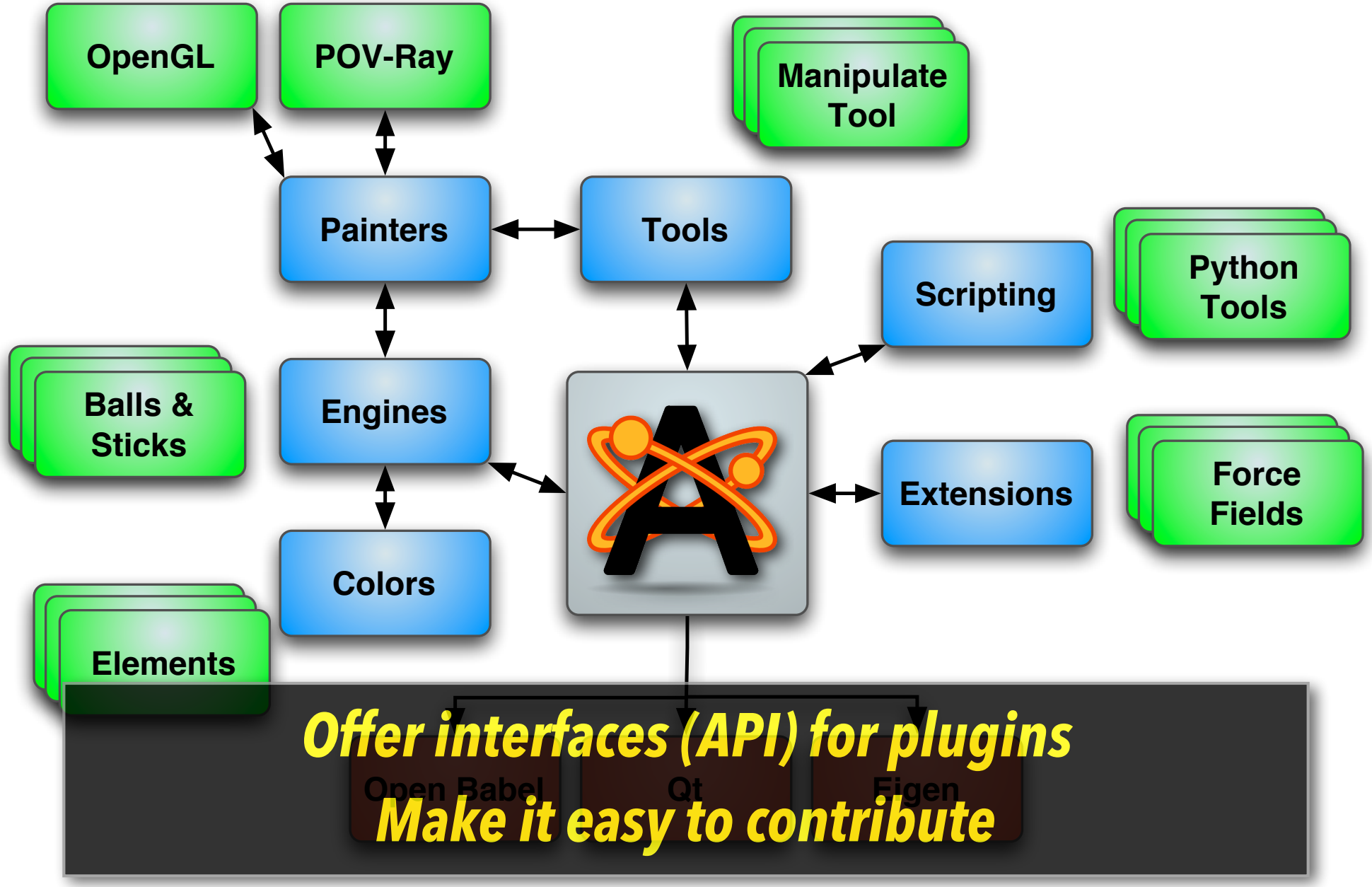
- Google Summer of Code:
  2007, 2008, 2011, 2016, 2017, 2018
- Translations through Launchpad - over 25!
- Tools, rendering, plugins
  - 33 contributors to Avogadro v1
  - 24 contributors (and counting) to v2

Problem Domains

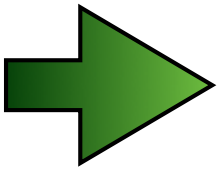
- Small molecules
  - Organic vs. Inorganic
- Biomolecules
  - Peptides, DNA, RNA, Sugars…
- Polymers
- Crystals
- Nanotubes, Nanoparticles, NanoXYZ

Avogadro aims to be the best "builder" for chemistry simulation and visualization

Avogadro Architecture



Current Status



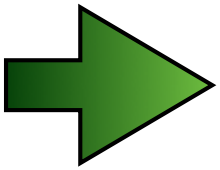
1.2.0
2016-06-15

github.com/cryos/avogadro

1.90
2016-12-3

github.com/openchemistry/avogadrolibs

Current Status



1.2.0
2016-06-15

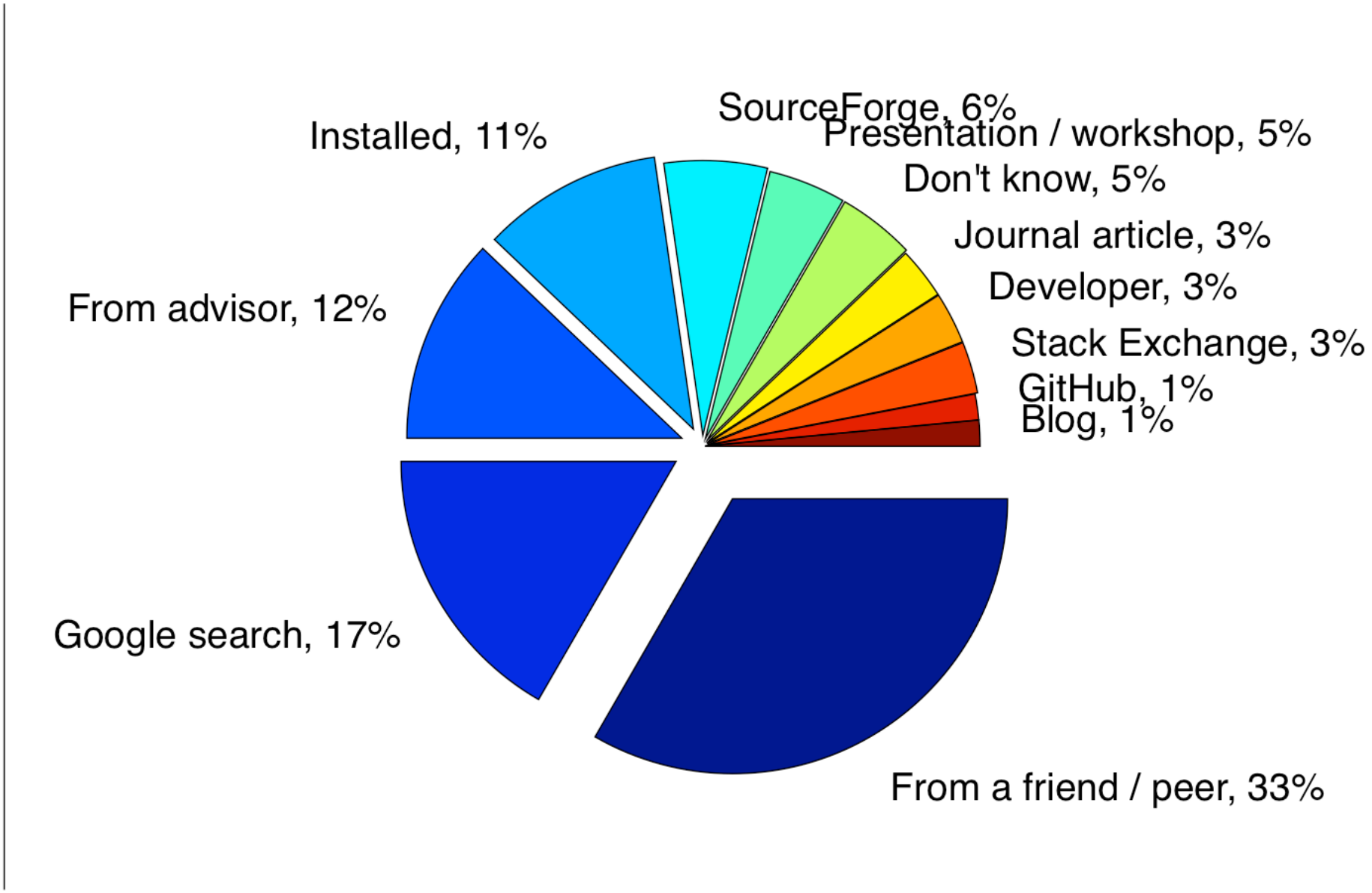
1.90
2016-12-3

1.91
2018-8-22

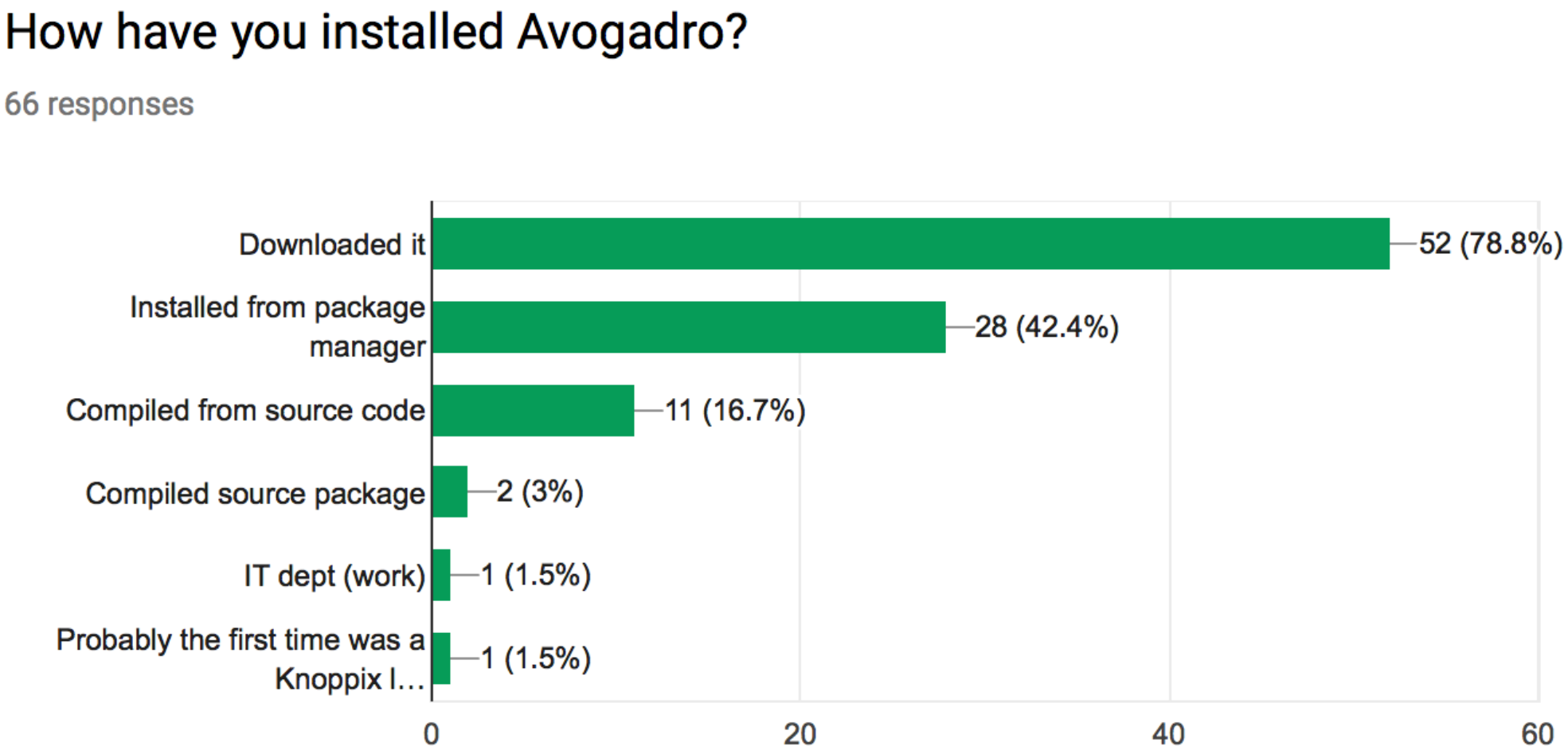
github.com/cryos/avogadro

github.com/openchemistry/avogadrolibs

Community Survey - Spread the Word



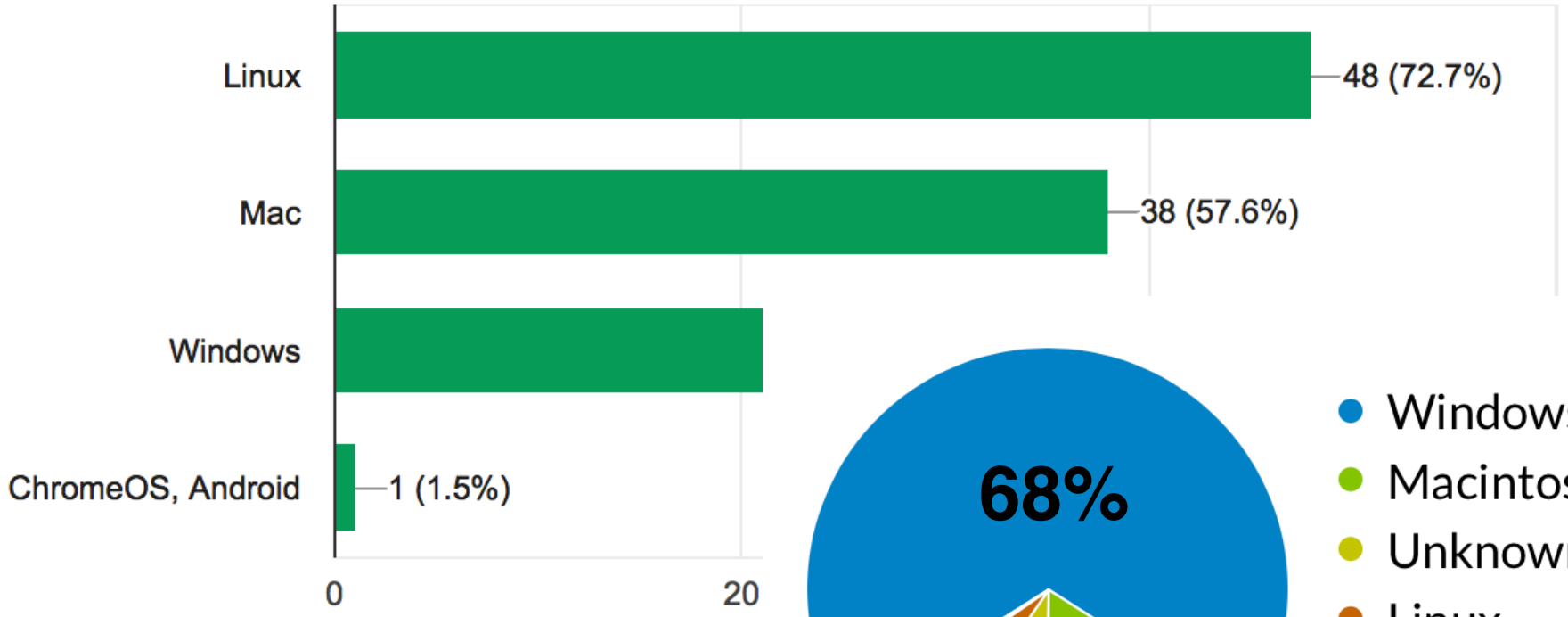
Community Survey - Installs



Community Survey - Operating Systems

What operating system(s) do you use?

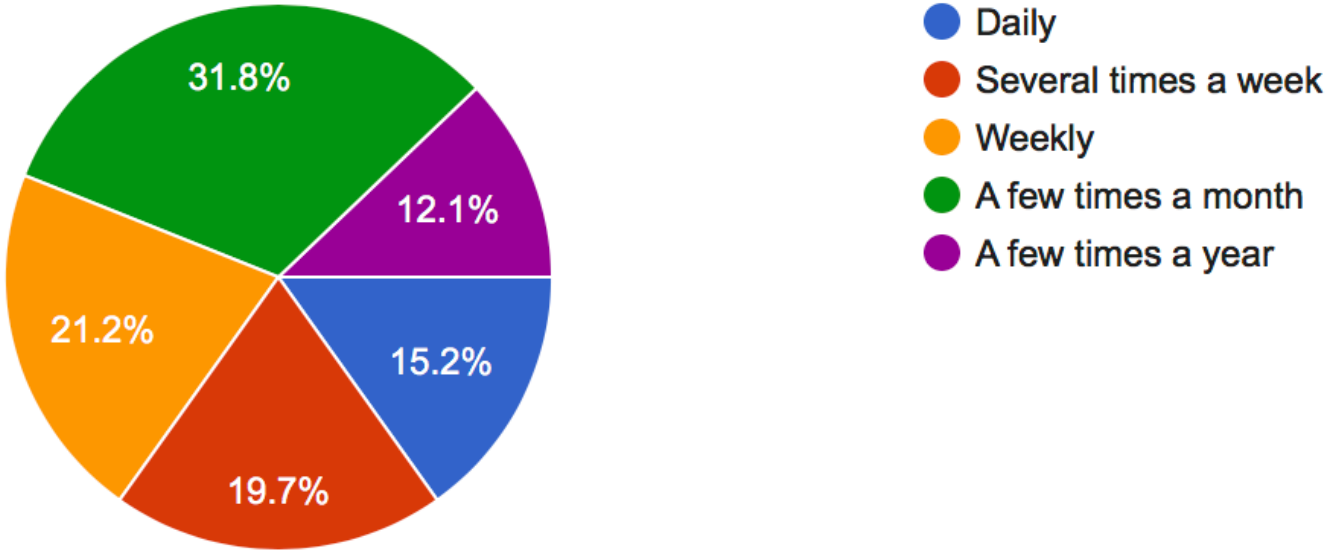
66 responses



Community Survey - Usage

How frequently do you use Avogadro?

66 responses



56% Use at least weekly!

Complaints / Concerns from Survey

- Stability / scalability

  "it needs to crash less often"

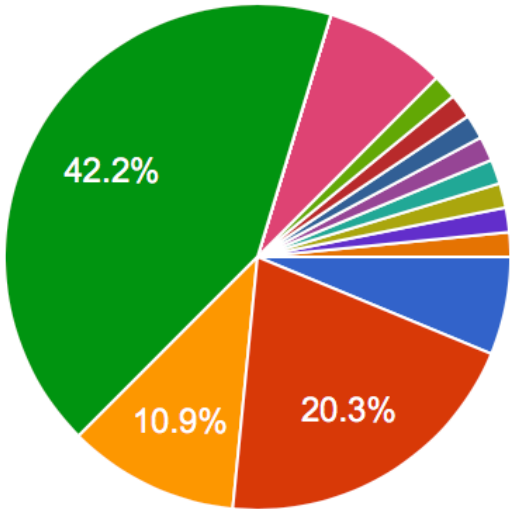
  "The size of the system […] until the ram collapse"

  "Stability. […] plenty of program crashes on macOS."
- Performance / Rendering
- Feature parity between v1 and v2
- Automation / Scripting

Community Survey - Programming

Can you code? If so, what languages?

64 responses



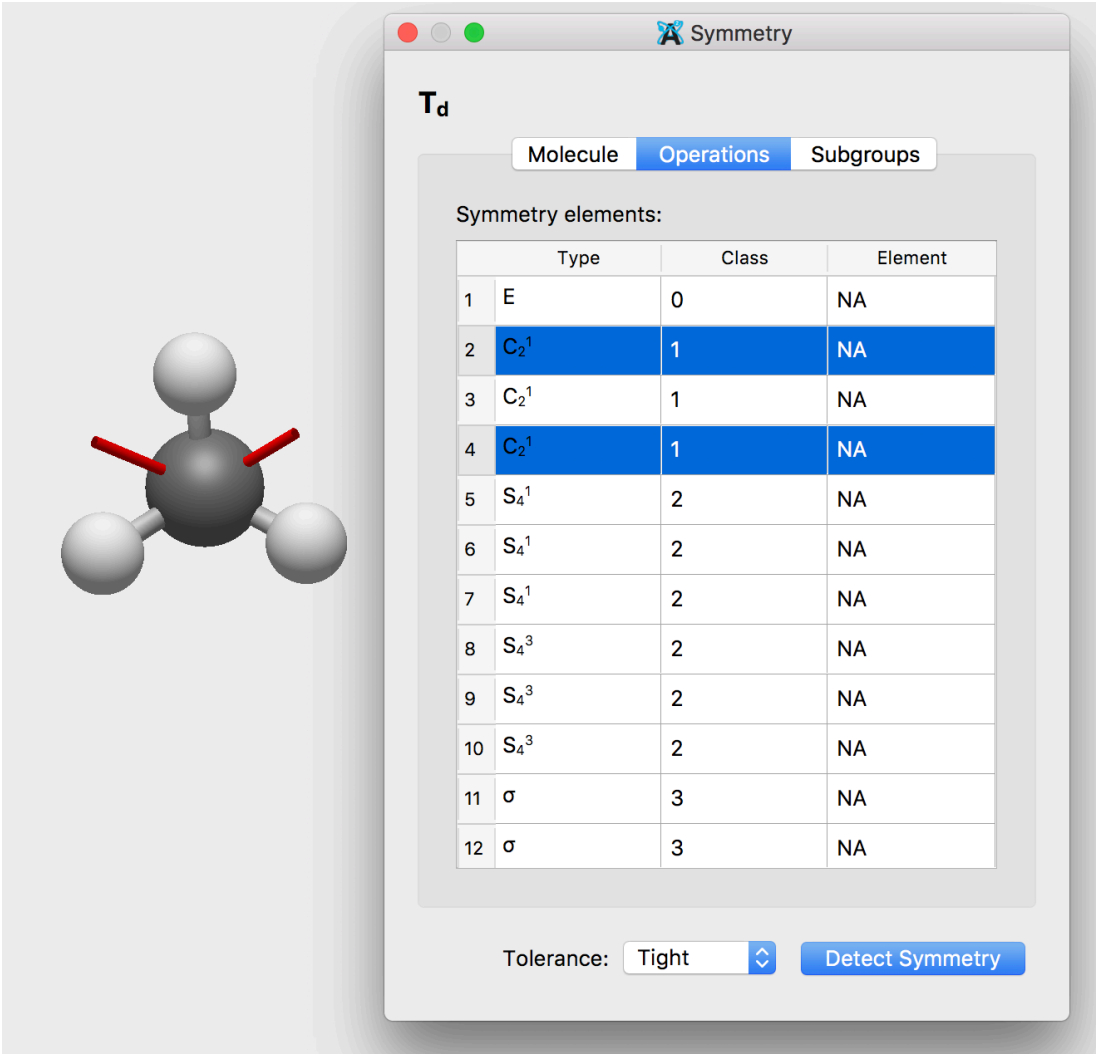
>40% know python

Progress in Avogadro v2

- Modular design - run as separate processes
- Stability & scalability - handle $>10^6$ atoms
- Downloadable plugin scripts, data, translations
- Code more with Python
  - Input generators
  - Workflows
  - Force field calculators
  - Electrostatics

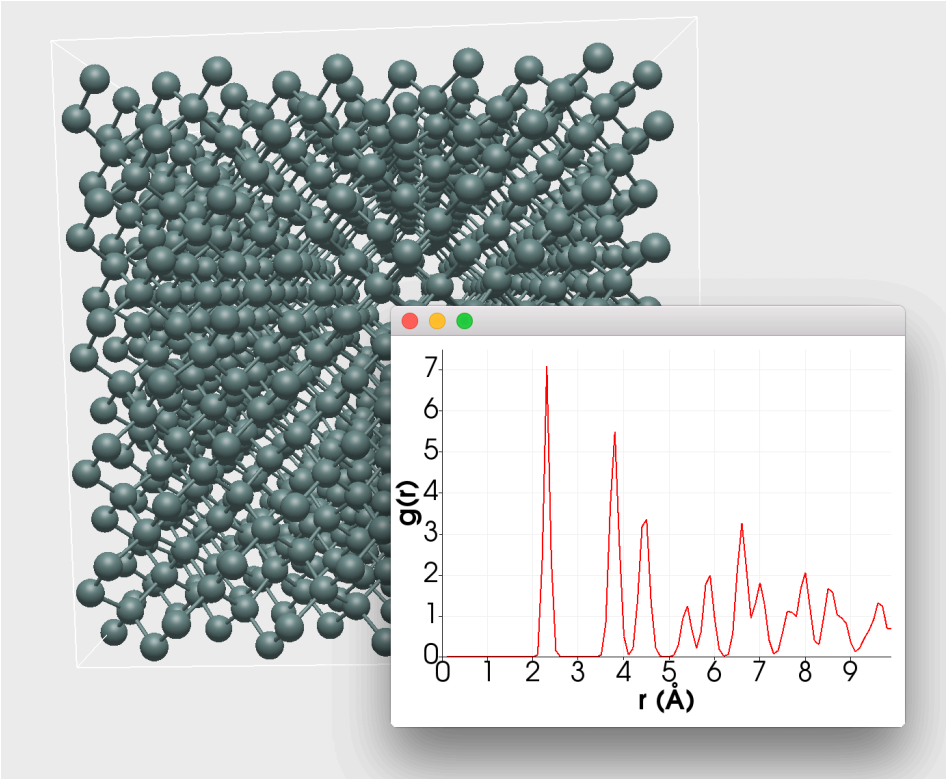
Progress in Avogadro 2

- **Not just parity**
- **New features**
  - Symmetry perception
  - Open shell orbitals
  - Ambient occlusion
  - Volumetric rendering
- **New platform**
  - Build the future



Progress in Avogadro 2 - Dynamics

- **Google Summer of Code 2018 (B. Adarsh)**
- **Read formats**
  LAMMPS, Gromacs trr, DCD
  VASP OUTCAR, Amber mdcrd, pdb
- **Input generators**
  LAMMPS
  OpenMM
- **Movies (GIF, AVI)**
- **Analysis (RMSD, Pair distribution)**



Progress in Avogadro v2

- Input generators: JSON ⇒ GUI ⇒ file / submit

```
userOptions['Calculation Type'] = {}
userOptions['Calculation Type']['type'] = 'stringList'
userOptions['Calculation Type']['default'] = 1
userOptions['Calculation Type']['toolTip'] = 'Type of calculation to perform'
userOptions['Calculation Type']['values'] = \
    ['Single Point', 'Geometry Optimization', 'Frequencies']

userOptions['Theory'] = {}
userOptions['Theory']['type'] = 'stringList'
userOptions['Theory']['default'] = 7
userOptions['Theory']['toolTip'] = 'Hamiltonian or DFT method to use'
userOptions['Theory']['values'] = \
    ['HF', 'MP2', 'CCSD', 'BLYP', 'PBE', 'B3LYP', 'B97', 'wB97X' ]

userOptions['Basis'] = {}
userOptions['Basis']['type'] = 'stringList'
userOptions['Basis']['default'] = 3
userOptions['Basis']['toolTip'] = 'Gaussian basis set'
userOptions['Basis']['values'] = \
    ['6-31G(d)', 'cc-pVDZ', 'aug-cc-pVTZ', 'def2-SVP', 'ma-def2-SVP',
    'def2-SVPD', 'def2-TZVP', 'def2-QZVP', 'pc-2', 'aug-pc-2']
```

github.com/openchemistry/avogenerators

Progress in Avogadro v2

- Workflows - download & run

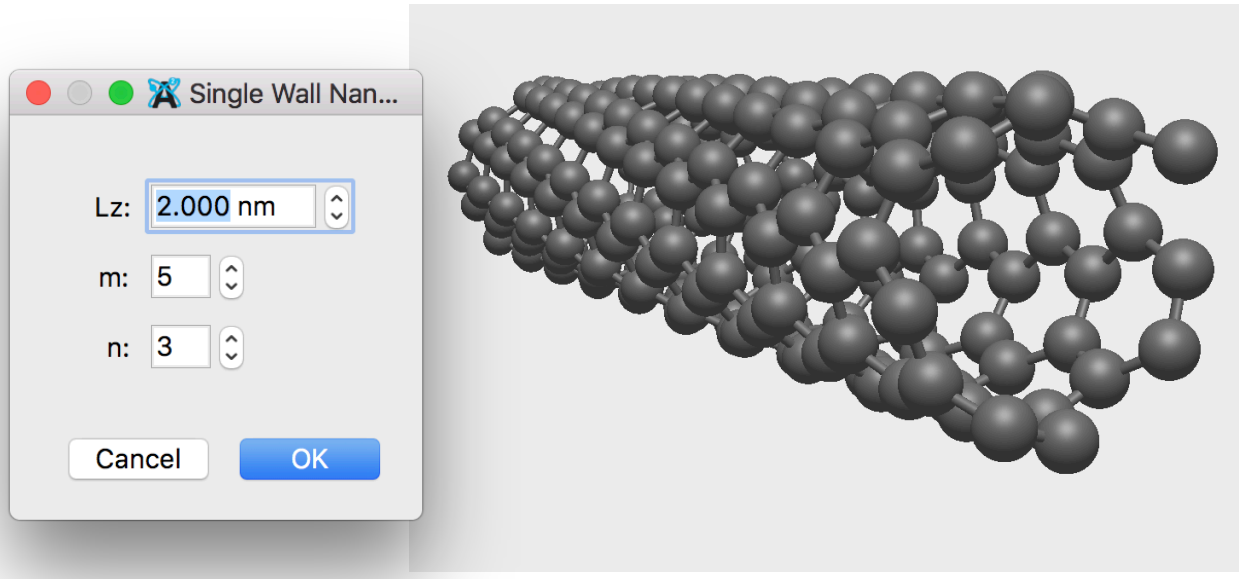
```python
from sknano.generators import SWNTGenerator

def generate(opts):
    l = float(opts['Length'])
    m = int(opts['m'])
    n = int(opts['n'])

    swnt = SWNTGenerator((m, n), Lz=l)
    # need a better random temporary name
    temp = 'temp{}.xyz'.format(randrange(32768))
    swnt.save(fname=temp)

    with open(temp) as f:
        xyzData = f.read()
    os.remove(temp)

    return xyzData
```



2018 User's Group Meeting

- Talks - Science & Development
- Roundtable - What's important, what's needed (how can we make everything easier)
- Hackathon & Tutorials - How to use Avogadro
  Code / edit input generators
  Code / edit workflows
  Contribute bug reports, discussion, **ideas**