The RDKit: History and Status

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Basel

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  - Gianluca Sforna (Fedora)
  - Michael Banck (Debian)

Overview

- **History**
- Where are we today?
- What next?

An amusing bit of email…

```
On 13/09/2007, Greg Landrum <greg.landrum@gmail.com> wrote:
> On 9/13/07, Noel O'Boyle <baoilleach@gmail.com> wrote:
> (4) Why haven't you publicised RDKit, if you don't mind me asking? For
> example, there is an excellent (if I do say so myself) website called
> Linux4Chemistry which lists the excellent (if you do say so yourself)
> YaEHMOP. Also there's the CCL mailing list. I only found RDKit because
> of trawling through the SF software map. Is this, um, shyness,
> intentional?

There are many components to the answer to this question. Some are:
 1) Promotion isn't something I enjoy or am particularly good at.
 2) I'm kind of afraid of having more users. I do a lot of this as a
free-time project and I'm afraid of spending all my time answering
questions. This is, of course, a bit stupid because if the whole open
source thing works then other people will pitch in and help with those
questions. For that to happen I need those other people as users,
which requires that I find them, which... it's a Catch 22
```

History and milestones

- 2000-2006: initial development work at Rational Discovery
- 2006: code open sourced and released on sourceforge.net
- 2007: First NIBR contribution (chemical reaction handling); Noel discovers the RDKit (=first rdkit-discuss post?)
- 2008: first POC of Java wrapper; Mac support added; SLN and Mol2 parsers;
- 2009: Morgan fingerprints; switch to cmake; switch to VF2 for SSS
- 2010: PostgreSQL cartridge; First iteration of the KNIME nodes; $RDBASE/Contrib appears; SaltRemover and FunctionalGroups code
- 2011: New Java wrappers; more functionality moved to C++; InChI support; Avalontools integration
- 2012: Speed improvements; MCS implementation; ???

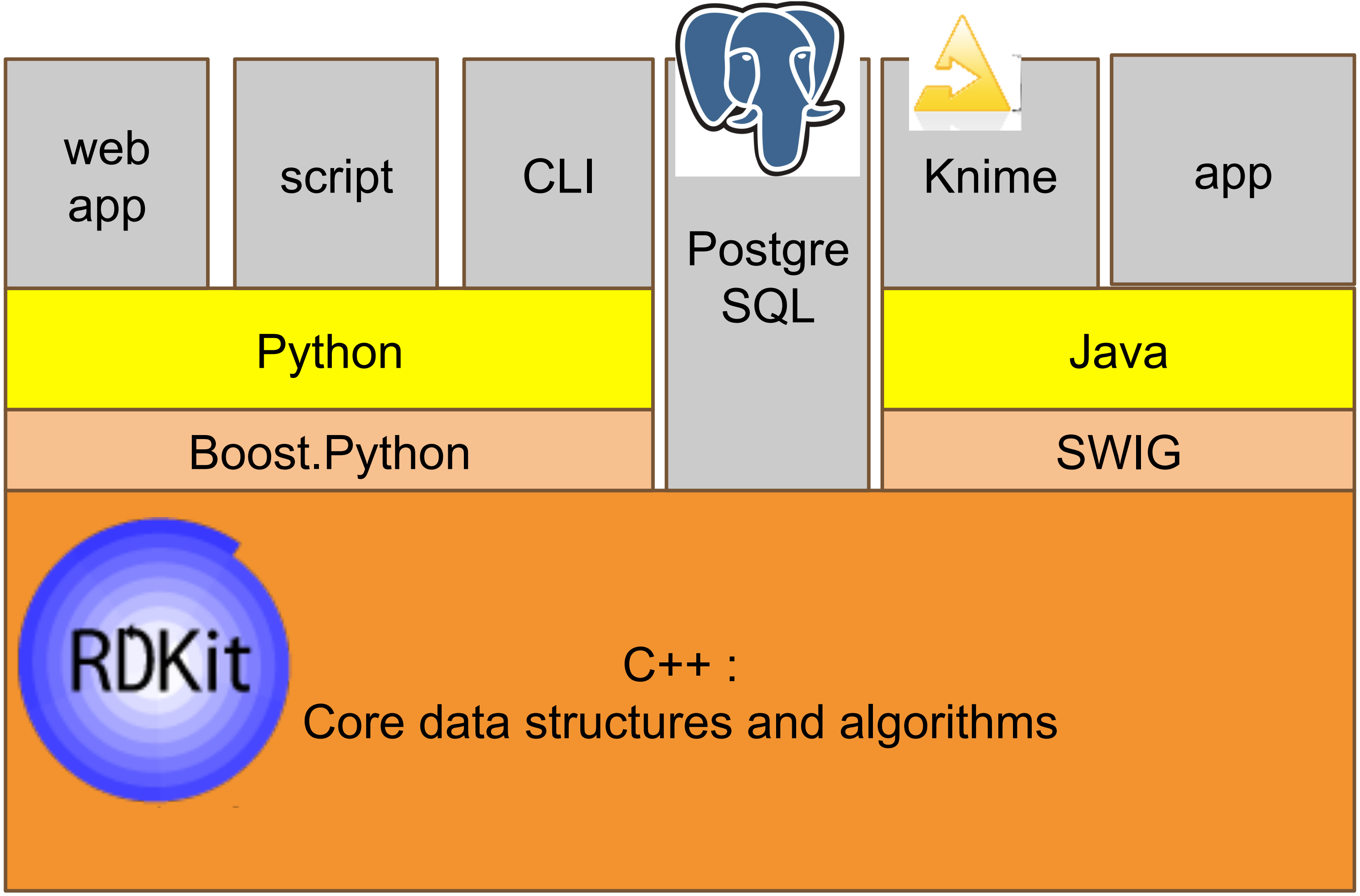
Overview

- History
- **Where are we today?**
- What next?

RDKit: What is it?

- Python (2.x), Java, and C++ toolkit for cheminformatics
  - Core data structures and algorithms in C++
  - Python wrapper generated using Boost.Python
  - Java wrapper generated with SWIG
- Functionality:
  - 2D and 3D molecular operations
  - Descriptor generation for machine learning
  - Molecular database cartridge
  - Supports Mac/Windows/Linux
- History:
  - 2000-2006: Developed and used at Rational Discovery for building predictive models for ADME, Tox, biological activity
  - June 2006: Open-source (BSD license) release of software, Rational Discovery shuts down
  - to present: Open-source development continues, use within Novartis, contributions from Novartis back to open-source version

The RDKit "ecosystem"



Exact same algorithms/implementations accessible from many different endpoints

NOVARTIS

What can you do with it?

A laundry list

- Input/Output: SMILES/SMARTS, SDF, TDT, SLN[1], Corina mol2[1]
- “Cheminformatics”:
  - Substructure searching
  - Canonical SMILES
  - Chirality support (i.e. R/S or E/Z labeling)
  - Chemical transformations (e.g. remove matching substructures)
  - Chemical reactions
  - Molecular serialization (e.g. mol <-> text)
- 2D depiction, including constrained depiction
- 2D->3D conversion/conformational analysis via distance geometry
- UFF implementation for cleaning up structures
- Fingerprinting:

  Daylight-like, atom pairs, topological torsions, Morgan algorithm, “MACCS keys”, etc.
- Similarity/diversity picking (including fuzzy similarity)
- 2D pharmacophores[1]
- Gasteiger-Marsili charges
- Hierarchical subgraph/fragment analysis
- RECAP and BRICS implementations
- Multi-molecule maximum common substructure[2]

[1] *functional, but not great implementations*

[2] *Contribution from A. Dalke*

What can you do with it?

A laundry list, cntd

- Feature maps
- Shape-based similarity
- Molecule-molecule alignment
- Shape-based alignment (subshape alignment) [1]
- Integration with PyMOL for 3D visualization
- Database integration
- Molecular descriptor library:
  - Topological (κ3, Balaban J, etc.)
  - Electrotopological state (Estate)
  - clogP, MR (Wildman and Crippen approach)
  - “MOE like” VSA descriptors
  - Feature-map vectors
- Machine Learning:
  - Clustering (hierarchical)
  - Information theory (Shannon entropy, information gain, etc.)
  - Decision trees, *naïve Bayes*[1]*, kNN*[1]
  - Bagging, random forests
  - Infrastructure (data splitting, shuffling, enrichment plots, serializable models, etc.)

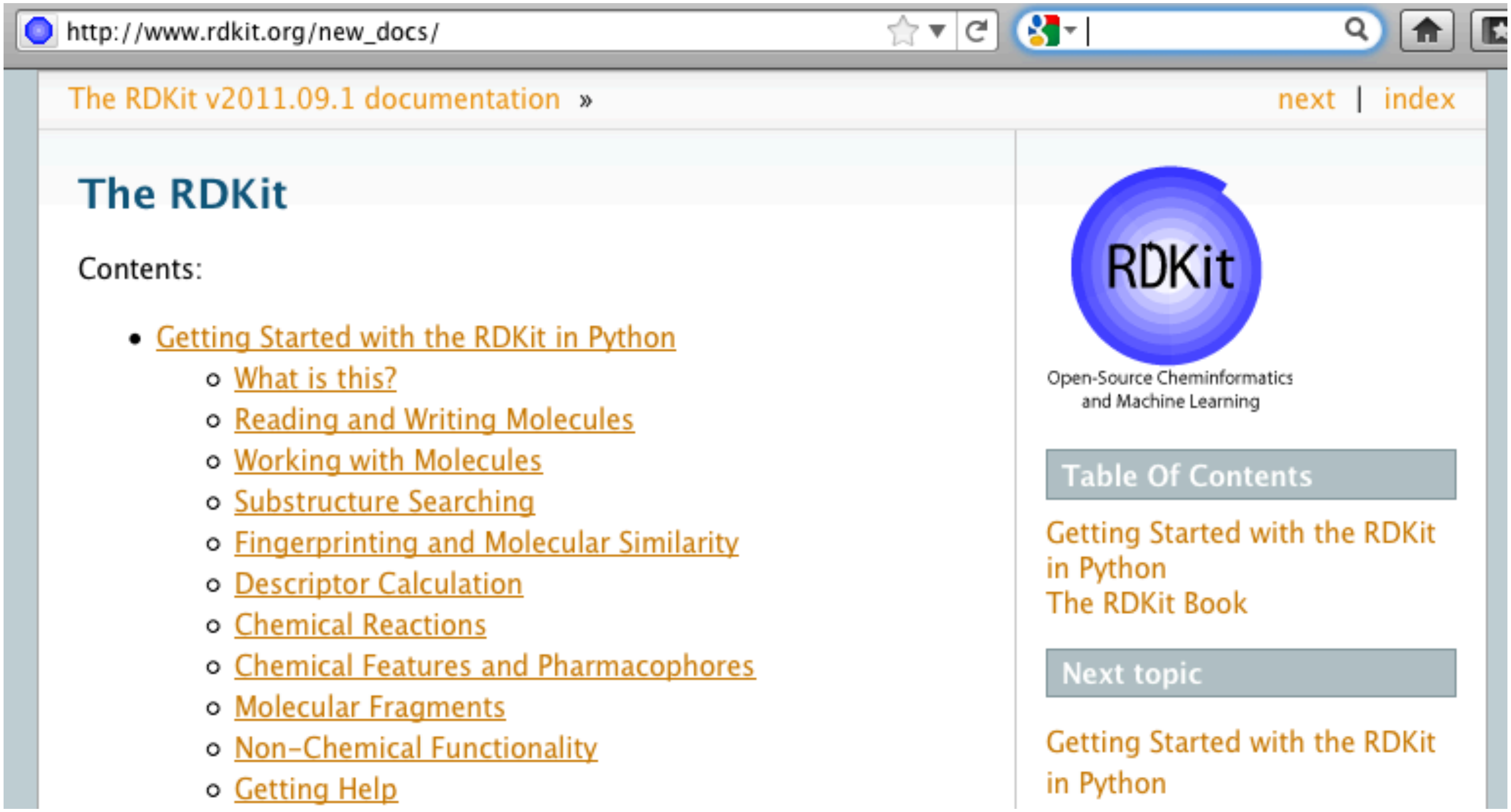
[1] *functional, but not great implementations*

RDKit: Where is it?

- Web page: http://www.rdkit.org
- Sourceforge: svn repository, bug tracker, mailing lists, downloads
  - http://sourceforge.net/projects/rdkit
- Google code: wiki, downloads
  - http://code.google.com/p/rdkit/
- Releases: quarterly
- Licensing: new BSD
- Documentation:
  - HTML/PDF “Getting Started” documentation
  - in-code docs extracted by either doxygen (C++) or epydoc (python)
- Getting help:
  - Check the wiki and “Getting Started” document
  - The rdkit-discuss mailing list

RDKit: Documentation?

The documentation:



http://www.rdkit.org/new_docs/

The RDKit v2011.09.1 documentation » next | index

The RDKit

Contents:

- Getting Started with the RDKit in Python
  - What is this?
  - Reading and Writing Molecules
  - Working with Molecules
  - Substructure Searching
  - Fingerprinting and Molecular Similarity
  - Descriptor Calculation
  - Chemical Reactions
  - Chemical Features and Pharmacophores
  - Molecular Fragments
  - Non-Chemical Functionality
  - Getting Help

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Getting Started with the RDKit in Python
The RDKit Book

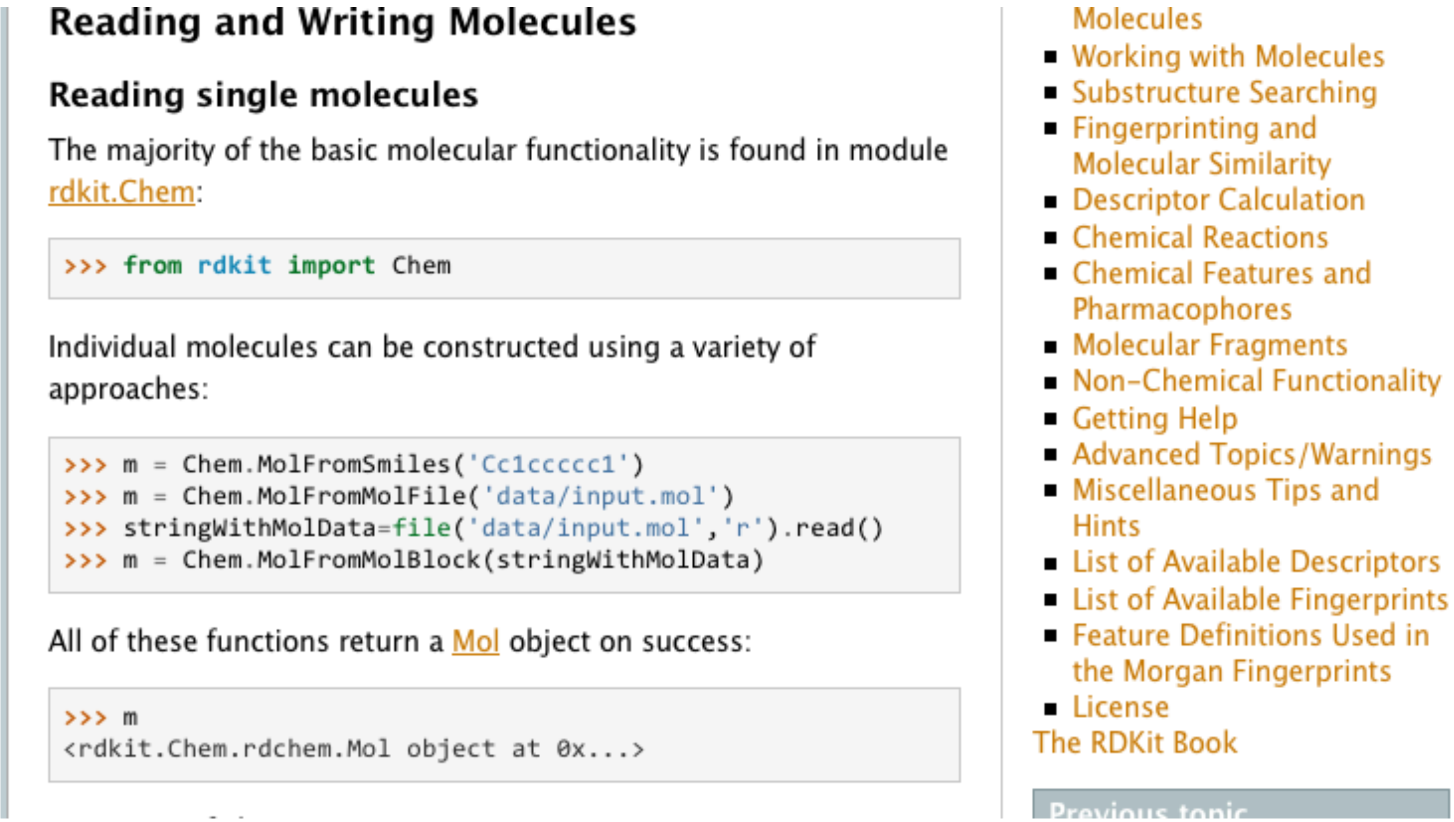
Next topic

Getting Started with the RDKit in Python

Built using Python’s standard docs tool: Sphinx

RDKit: Documentation?

Sample section from introductory docs:



Reading and Writing Molecules

Reading single molecules

The majority of the basic molecular functionality is found in module rdkit.Chem:

```
>>> from rdkit import Chem
```

Individual molecules can be constructed using a variety of approaches:

```
>>> m = Chem.MolFromSmiles('Cc1ccccc1')
>>> m = Chem.MolFromMolFile('data/input.mol')
>>> stringWithMolData=file('data/input.mol','r').read()
>>> m = Chem.MolFromMolBlock(stringWithMolData)
```

All of these functions return a Mol object on success:

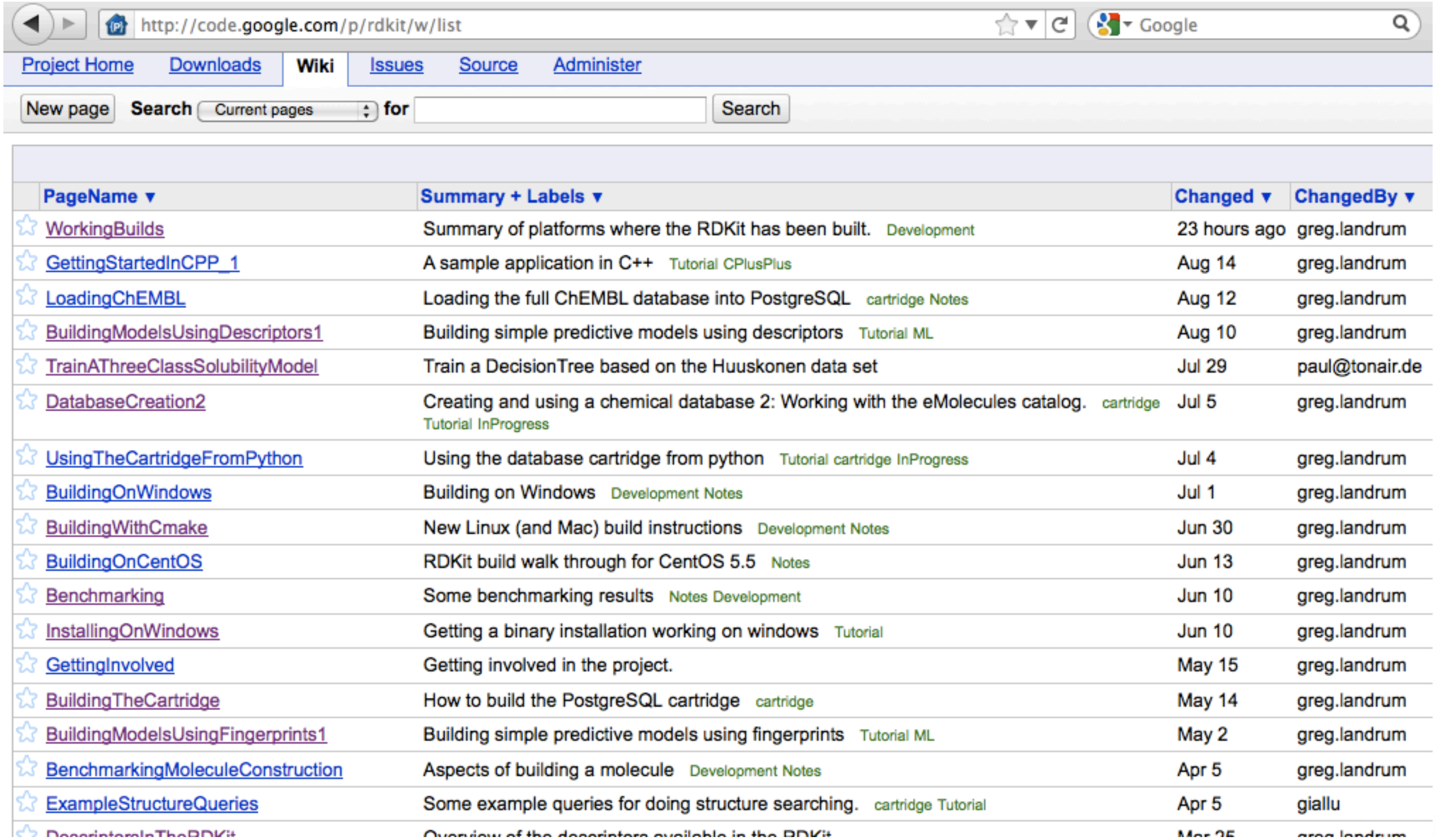
```
>>> m
<rdkit.Chem.rdchem.Mol object at 0x...>
```

Previous topic

Note: docs that include python code snippets are *tested*.

RDKit: Documentation?

The wiki: http://code.google.com/p/rdkit/w/list



PageName ▼	Summary + Labels ▼	Changed ▼	ChangedBy ▼
WorkingBuilds	Summary of platforms where the RDKit has been built. Development	23 hours ago	greg.landrum
GettingStartedInCPP_1	A sample application in C++ Tutorial CPlusPlus	Aug 14	greg.landrum
LoadingChEMBL	Loading the full ChEMBL database into PostgreSQL cartridge Notes	Aug 12	greg.landrum
BuildingModelsUsingDescriptors1	Building simple predictive models using descriptors Tutorial ML	Aug 10	greg.landrum
TrainAThreeClassSolubilityModel	Train a DecisionTree based on the Huuskonen data set	Jul 29	paul@tonair.de
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InstallingOnWindows	Getting a binary installation working on windows Tutorial	Jun 10	greg.landrum
GettingInvolved	Getting involved in the project.	May 15	greg.landrum
BuildingTheCartridge	How to build the PostgreSQL cartridge cartridge	May 14	greg.landrum
BuildingModelsUsingFingerprints1	Building simple predictive models using fingerprints Tutorial ML	May 2	greg.landrum
BenchmarkingMoleculeConstruction	Aspects of building a molecule Development Notes	Apr 5	greg.landrum
ExampleStructureQueries	Some example queries for doing structure searching. cartridge Tutorial	Apr 5	giallu
DescriptorsInTheRDKit	Overview of the descriptors available in the RDKit	Mar 25	greg.landrum

RDKit: Documentation?

The documents that come out of the tutorials here are going to be another good source of information

RDKit: Who is using it?

- Hard to say with any certainty
- ~500 downloads of each new version
- Active contributors to the mailing list from:
  - Big pharma
  - Small pharma/biotech
  - Software/Services
  - Academia
- Starting to see contributions coming from the community (wiki pages, code patches, changes to the build system, etc.) as well as active use in other systems.
- Community contributions for packaging:
  - rpms/debs for Fedora/Debian linux
  - homebrew recipe for MacOS

Sustainability of the RDKit

… thinking about the bus problem

- This clearly isn't just a hobby project any more
- Used internally in NIBR in multiple production systems
- Starting to get contributions from outside
- I'm no longer the only one answering questions on the mailing list

Overview

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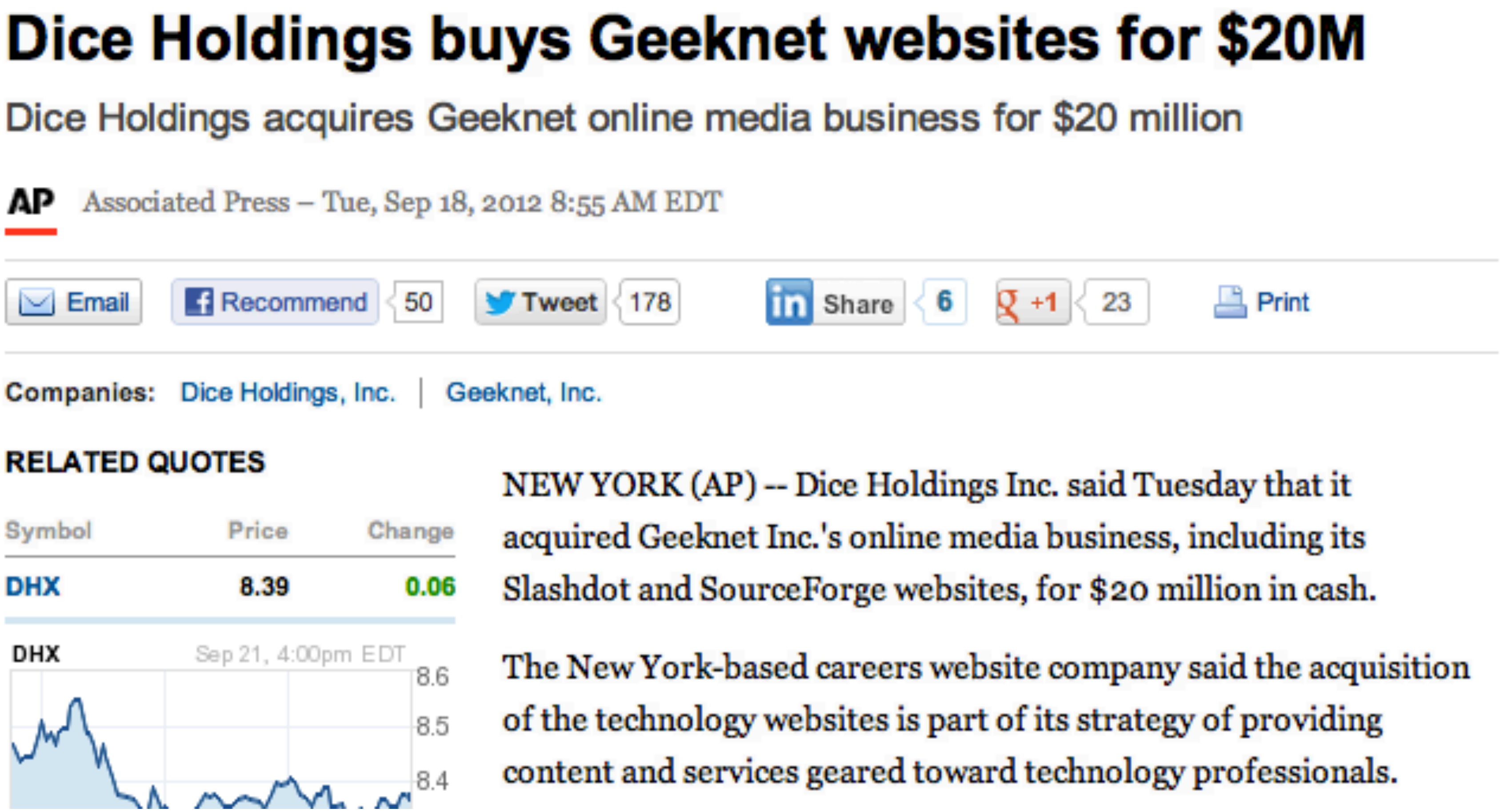
What’s next?

- We’ll decide some of that here in the round-table sessions

- Obvious candidates:
  - Further performance improvements
  - Improved documentation
  - Move more code into C++ (allows access from Knime and the cartridge)

to be aware of…



Dice Holdings buys Geeknet websites for $20M

Dice Holdings acquires Geeknet online media business for $20 million

AP Associated Press – Tue, Sep 18, 2012 8:55 AM EDT

Companies: Dice Holdings, Inc. | Geeknet, Inc.

RELATED QUOTES

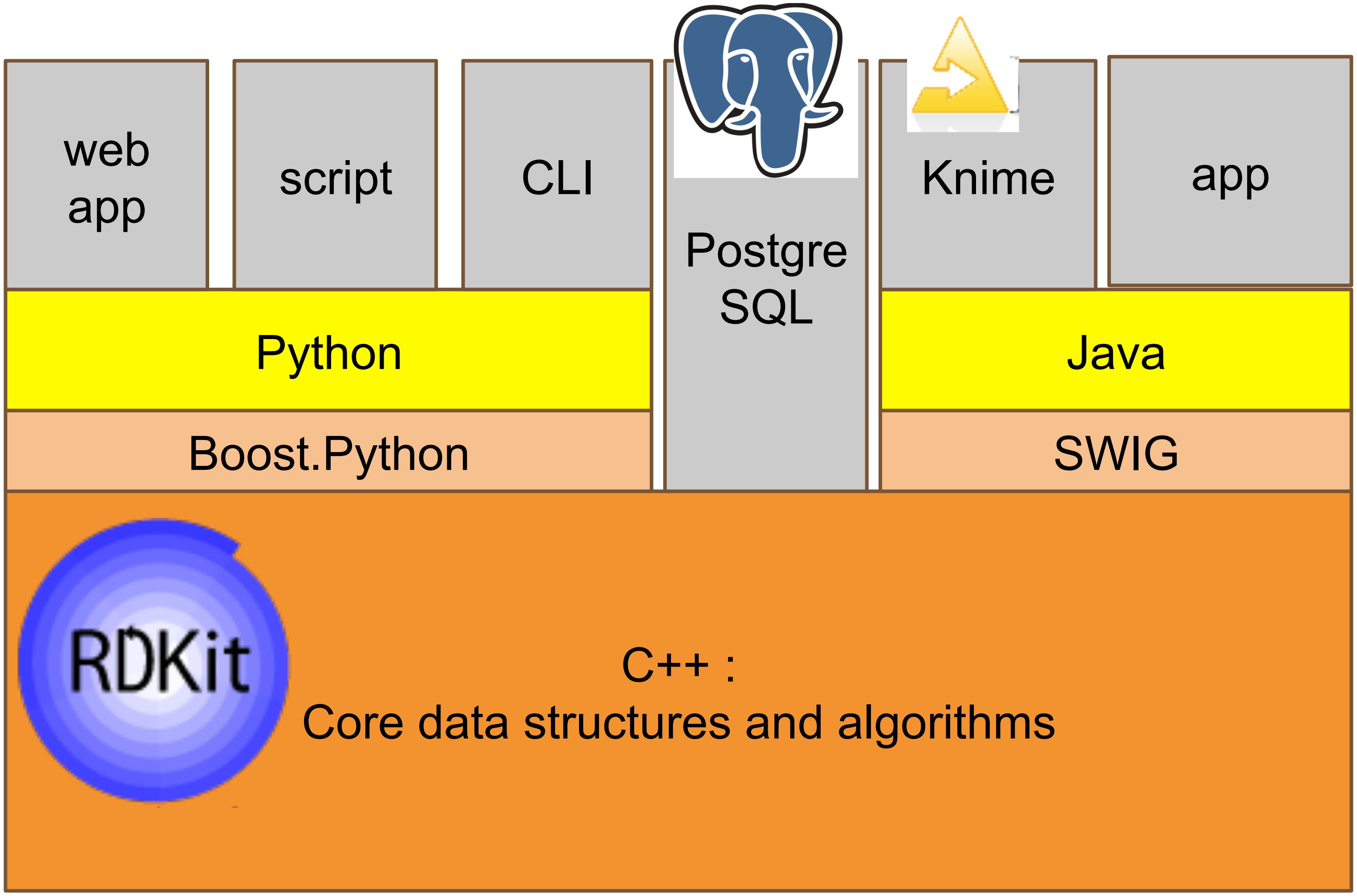
Symbol	Price	Change
DHX	8.39	0.06

NEW YORK (AP) -- Dice Holdings Inc. said Tuesday that it acquired Geeknet Inc.'s online media business, including its Slashdot and SourceForge websites, for $20 million in cash.

The New York-based careers website company said the acquisition of the technology websites is part of its strategy of providing content and services geared toward technology professionals.

It’s not clear what this means for sourceforge

Thanks!



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