

RosettaCon 2011

Monday, August 1, 11

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Build System













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- No automatic subclassing. User can not inherit and re-use arbitrary Rosetta class.
- Can not use newer compilers, have to use GCCXML therefore limiting our options.













Removing PyGCCXML and PyPlusPlus allows us to:

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- PyRosetta classes are first class citizens
- Clang support
- Future: drop GCCXML and move to Clang++ when it is mature.





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- Build PyRosetta.

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Over 90% of Rosetta's 3,000 classes are available in PyRosetta












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32/64 Bit



Mac OS X Snow Leopard



Scientific Linux 64



Mac OS X Lion

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- Each week we getting several posts at RosettaCommons forums as well as personal emails.

Welcoming New Users

- We now can use mini trunk version which allows us to help users much faster.
- PyAsserts
- Help!

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- Support for proper base classes and subclassing in Python: It is now possible to extend Rosetta via Python
- Steadily increasing community of PyRosetta users

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- Extend Library of scripts aka 'Protocol demos'. (Would be great if PyRosetta demo could be added to publishing requirements)
- Build-time test for detecting commits that break PyRosetta (undefined functions, unconventional namespaces, etc.)

Acknowledgments



Evan Baugh



Robert Schleif



Brian Weitzner



Jeffrey Gray

Huge Thanks to **Steven Lewis** who constantly answers questions on RosettaCommons forums and redirects PyRosetta specific questions to me!

Without his help we would be able to provide only a fraction of support available now.

Thank you!

Buckle up your seatbelts, technical slides ahead!

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 - Adapt all these subclasses so they can be used as 'call-back' structure to allow subclassing in Python.

Explain How Subclassing work

 Before in PyRosetta 1.1 to allow subclassing in PyRosetta hand written was needed. For average class it took ~1hr of work plus it would require some effort to keep it in-sync with the main trunk. Now take in to account number of classes in mini and its easy to see how this approach became a problem.

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- Also, due to constraints of build system it was hardimpossible to set correct base which lead to situation when inherited classes in PyRosetta would lack some virtual functions of a base classes.
- Now all this done automatically for all classes in mini. So all classes could be inherited in PyRosetta.