SymEngine: A Fast Symbolic Manipulation Library

Ondřej Čertík, Isuru Fernando, Thilina Rathnayake, Abhinav Agarwal, Sumith Kulal, Abinash Meher, Rajith Vidanaarachchi, Shikhar Jaiswal, Ranjith Kumar

July 17, 2017

Outline

SymEngine

- Introduction
- Features
- Demo (Python, Ruby, Julia)
- ▶ Why C++, how to write safe code
- Internals of SymEngine
- SymEngine and SymEngine.py
- Roadmap for using SymEngine in SymPy
- Roadmap for using SymEngine in Sage
- Roadmap for using SymEngine in PyDy
- Benchmarks

Introduction

About SymEngine

- ► Symbolic manipulation library written in C++
- ► Thin wrappers to Python, Ruby, Julia, C and Haskell
- MIT licensed
- ► Started in 2012
- 46 contributors
- Runs on Linux (GCC, Clang, Intel), OS X (GCC, Clang), Windows (MSVC, MinGW, MinGW-w64)
- ▶ Part of the SymPy organization, but the C++ library is Python independent

Introduction

Goals

- Be the fastest symbolic manipulation library (open-source or commercial)
- Serve as the core for SymPy and Sage, optionally supporting PyDy
- Serve as the default symbolic manipulation library in other languages thanks to thin wrappers (Python, Ruby, Julia, C and Haskell)

Choice of Language

Problem

SymPy speed is sometimes insufficient

- Handling of very large expressions
- Large calculations using small/medium size expressions

Let's Fix That

- We tried: pure Python/PyPy, Cython, C, ...
- Investigated Julia, Rust, Scala, Javascript, ...
- ► Chose C++

Current Features

- Core (Symbols, +, -, *, /, **)
- Elementary Functions (sin, cos, gamma, erf)
- Number Theory
- Differentiation, Substitution
- Matrices and Sets
- Polynomials (Piranha, Flint)
- Series Expansion
- Solvers (Polynomial and Trigonometric)
- Printing, Parsing and Code Generation
- Numeric Evaluation (Double and Arbitrary Precision)

Demo

Demo Time

Why Pure C++

- Fast in Release mode, but safe in Debug mode
- Compiler helps (not as good as Scala or Haskell, but much better than Python)
- ▶ Just one language to learn, thus easy to maintain (as opposed to several intertwined layers such as C + Cython + Python)
- ► Thin wrappers (that core developers do not need to maintain), all functionality in C++
- Easier to create bindings to other languages like Python, Julia, Ruby and Haskell

Why Pure C++: Fast in Release Mode

- Allows direct memory handling (allocation, deallocation, access)
- ► Allows to tweak how and when things are done
- ▶ It is possible to go to bare metal
- Allows reasonably high level abstractions (simple, maintainable code)

Why Pure C++: Safe in Debug Mode

- Reference counted pointers Teuchos::RCP (from Trilinos)
- Checks for dangling and null pointers (exception is raised)
- ► No raw pointers/references (use Ptr and RCP)
- ▶ Use a safe subset of C++
- ▶ Few other rules, e.g. how to use Ptr and RCP properly
- Possible to visually verify in a PR (pull request) review
- ► Hopefully eventually there are plugins to Clang to check automatically (since the rules are simple and static)
- As fast as raw pointers in Release mode (but it could segfault)

Conclusion: the code cannot segfault or have undefined behavior in Debug mode — always get an exception at runtime, or a compile error.

How Add Class Works

- ► Add stores the various algebraic terms in a dictionary as variable-coefficient pairs, while separately storing the constant term of the expression
- Add uses std::unordered_map (hashtable) for the dictionary
 - $2xy^2 + 3x^2y + 5 \rightarrow \{xy^2 : 2, x^2y : 3\}$; coeff = 5
- ► Each object is reference counted (RCP), hence very fast implementation in Release mode

How Mul Class Works

- ► Mul stores the various algebraic terms in a dictionary as base-exponent pairs, while separately storing the constant coefficient of the expression
- ► Mul uses std::map (red-black tree)
 - $2xy^2 \rightarrow \{x: 1, y: 2\}$; coeff = 2
- Pow just stores the base and exponent
- Each object is, like in the case of Add class, reference counted (RCP)

How Pow Class Works

- Pow just stores the base and exponent as individual RCP objects, no dictionaries are used for storage
 - \rightarrow $x^5 \rightarrow base = x$; coeff = 5

Extensibility using Visitor Pattern

- ▶ All algorithms implemented using visitor pattern
- Algorithm is implemented in its own file, separate from the core
- Two virtual function calls (can be implemented in third party code or user code)
- Special version with just one virtual function call (faster, but must be compiled as part of the SymEngine source code)
- The speed difference between the two is minor

SymPy, SymEngine and the Interface

Using SymPy in SymEngine

 SymEngine will convert any SymPy object to a corresponding SymEngine object before doing any operation

```
>>> from symengine import symbols, Add
>>> import sympy
>>> x = symbols("x")
>>> y = sympy.symbols("y")
>>> x + y
x + y
>>> type(x+y)
<type 'symengine.lib.symengine_wrapper.Add'>
```

▶ What if there is no corresponding SymEngine object?

SymPy, SymEngine and the Interface

Using SymPy in SymEngine

 SymEngine will keep a reference to a SymPy object if there is no corresponding SymEngine object using Python/C API.
 SymEngine will use Python callbacks to evaluate the SymPy object

```
>>> e = x + sympy.Mod(x, 2)
>>> assert str(e) == "x + Mod(x, 2)"
>>> assert isinstance(e, Add)

>>> f = e.subs({x : 10})
>>> assert f == 10

>>> f = e.subs({x : 2})
>>> assert f == 2
```

SymPy, SymEngine and the Interface Using SymEngine in SymPy

- ▶ >>> from sympy.core.backend import symbols, sin, diff
- Most things can be used unmodified
- Few things are fundamentally different (e.g. SymPy stores I as ImaginaryUnit, SymEngine has a Complex class)
- ► We will have a compatibility layer, probably similar to Python 2 and 3 support using the same source base.

Benchmark setup

Benchmarks were run in a Intel(R) Core(TM) i5-5200U CPU @ 2.20GHz running Ubuntu 16.04 with gcc 5.4.0

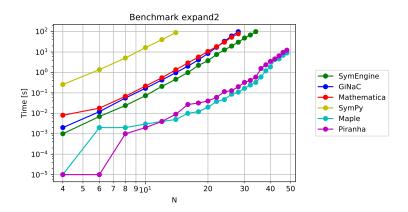
- SymEngine master (with GMP and FLINT)
- ► GiNaC 1.6.6
- ▶ SymPy 1.0
- Mathematica 10.2.0.0
- ► Maple 2015.2

Expand Benchmark

- $e = (x + y + z + w)^n$
- f = e * (e + w)
- Measure time taken for expanding f
- using SymEngine
 using TimeIt

```
@vars x y z w
n = 30
e = (x + y + z + w)^n
f = e * (e + w)
@timeit expand(f)
```

Expand Benchmark



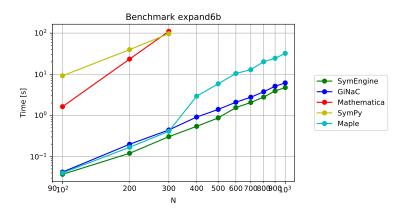
Modified GiNaC Benchmark

- Let e be the expanded sum of 2 symbols $\{a_0, a_1\}$ and n-2 trigonometric functions $\{sin(a_2), sin(a_3)...sin(a_{n-1})\}$ squared: $e \leftarrow (a_0 + a_1 + \sum_{i=2}^{n-1} sin(a_i))^2$
- ▶ Substitute $a_0 \leftarrow -\sum_{i=2}^{n-1} \sin(a_i)$
- ▶ Expand e again so it collapses to a_1^2

Modified GiNaC Benchmark

```
from symengine import symbols, sin
from time import clock
n = 100
a0, a1 = symbols("a0, a1")
t = sum([sin(symbols("a%s" % i)) for i in range(2, n)])
e = a0 + a1 + t
f = -t
t1 = clock()
e = (e**2).expand()
e = e.xreplace({a0: f})
e = e.expand()
t2 = clock()
```

Modified GiNaC Benchmark

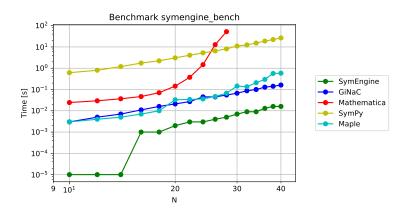


SymEngine Benchmark

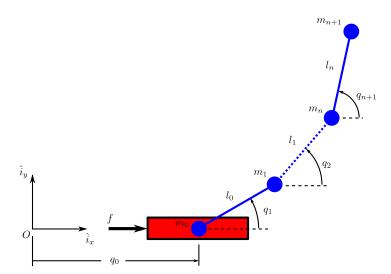
▶ Series expansion of sin(cos(x+1)) around x=0

```
RCP<const Symbol> x = symbol("x");
int n = 15;
RCP<const Basic> ex = sin(cos(add(integer(1), x)));
auto t1 = std::chrono::high_resolution_clock::now();
RCP<const Basic> res = series(ex, x, n);
auto t2 = std::chrono::high_resolution_clock::now();
```

SymEngine Benchmark



PyDy Benchmark

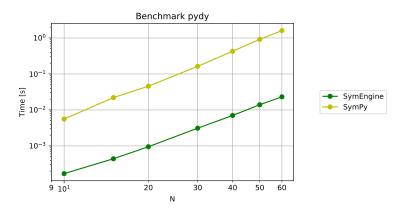


PyDy Benchmark

| n | ${\sf SymEngine} + {\sf SymPy}$ | SymPy only | Speedup |
|----|---------------------------------|------------|---------|
| 10 | 0.17 s | 5.58 s | 32.8x |
| 15 | 0.44 s | 22.07 s | 50.1x |
| 20 | 0.95 s | 45.59 s | 47.9x |
| 30 | 3.11 s | 162.80 s | 52.3x |
| 40 | 7.02 s | 427.16 s | 60.8x |
| 50 | 13.95 s | 915.83 s | 65.6x |
| 60 | 23.16 s | 1596.37 s | 68.9x |

Table: Results

PyDy Benchmark



Summary

- SymEngine aims to be the fastest C++ symbolic manipulation library
- ► Thin wrappers to other languages (Python, Ruby, Julia, C and Haskell)
- Easily usable as an optional backend in SymPy, Sage and PyDy

Thank You

GitHub:

- https://github.com/symengine/symengine
- https://github.com/symengine/symengine.py
- https://github.com/symengine/symengine.rb
- https://github.com/symengine/symengine.jl
- https://github.com/symengine/symengine.hs

Mailinglist:

http://groups.google.com/group/symengine

Gitter:

https://gitter.im/symengine/symengine