3

4

5

6

8

9

11

12

13

14 15

16

AARON MEURER\*, MATEUSZ PAPROCKI<sup>†</sup>, ONDŘEJ ČERTÍK<sup>‡</sup>, MATTHEW ROCKLIN<sup>§</sup>, AMIT KUMAR<sup>¶</sup>, SERGIU IVANOV<sup>||</sup>, JASON K. MOORE<sup>#</sup>, SARTAJ SINGH<sup>†</sup>, THILINA RATHNAYAKE<sup>‡</sup>, SEAN VIG<sup>§</sup>, BRIAN E. GRANGER<sup>¶</sup>, RICHARD P. MULLER<sup>||</sup>, FRANCESCO BONAZZI<sup>#</sup>, HARSH GUPTA<sup>1</sup>, SHIVAM VATS<sup>2</sup>, FREDRIK JOHANSSON<sup>3</sup>, FABIAN PEDREGOSA<sup>4</sup>, ASHUTOSH SABOO<sup>5</sup>, ISURU FERNANDO<sup>6</sup>, SUMITH<sup>7</sup>, ROBERT CIMRMAN<sup>8</sup>, AND ANTHONY SCOPATZ<sup>9</sup>

1. Introduction. SymPy is a full featured computer algebra system (CAS) written in the Python programming language [33]. It is free and open source software, being licensed under the 3-clause BSD license [46]. The SymPy project was started by Ondřej Čertík in 2005, and it has since grown to over 500 contributors. Currently, SymPy is developed on GitHub using a bazaar community model [44]. The accessibility of the codebase and the open community model allow SymPy to rapidly respond to the needs of the community of users and developers.

Python is a dynamically typed programming language that has a focus on ease of use and readability. Due in part to this focus, it has become a popular language for scientific computing and data science, with a broad ecosystem of libraries [39]. SymPy is itself used by many libraries and tools to support research within a variety

<sup>\*</sup>University of South Carolina, Columbia, SC 29201 (asmeurer@gmail.com).

<sup>&</sup>lt;sup>†</sup>Continuum Analytics, Inc., Austin, TX 78701 (mattpap@gmail.com).

<sup>&</sup>lt;sup>‡</sup>Los Alamos National Laboratory, Los Alamos, NM 87545 (certik@lanl.gov).

<sup>§</sup>Continuum Analytics, Inc., Austin, TX 78701 (mrocklin@gmail.com).

<sup>&</sup>lt;sup>¶</sup>Delhi Technological University, Shahbad Daulatpur, Bawana Road, New Delhi 110042, India (dtu.amit@gmail.com).

Université Paris Est Créteil, 61 av. Général de Gaulle, 94010 Créteil, France (sergiu.ivanov@upec.fr).

<sup>#</sup>University of California, Davis, Davis, CA 95616 (jkm@ucdavis.edu).

<sup>††</sup>Indian Institute of Technology (BHU), Varanasi, Uttar Pradesh 221005, India (singhsartaj94@gmail.com).

<sup>&</sup>lt;sup>‡‡</sup>University of Moratuwa, Bandaranayake Mawatha, Katubedda, Moratuwa 10400, Sri Lanka (thilinarmtb.10@cse.mrt.ac.lk).

<sup>§§</sup>University of Illinois at Urbana-Champaign, Urbana, IL 61801 (sean.v.775@gmail.com).

<sup>¶</sup>California Polytechnic State University, San Luis Obispo, CA 93407 (ellisonbg@gmail.com).

<sup>|| ||</sup> Center for Computing Research, Sandia National Laboratories, Albuquerque, NM 87185 (rmuller@sandia.gov).

<sup>##</sup>Max Planck Institute of Colloids and Interfaces, Am Mühlenberg 1, 14476 Potsdam, Germany (francesco.bonazzi@mpikg.mpg.de).

<sup>&</sup>lt;sup>1</sup>Indian Institute of Technology Kharagpur, Kharagpur, West Bengal 721302, India (hargup@protonmail.com).

 $<sup>^2</sup>$  Indian Institute of Technology Kharagpur, Kharagpur, West Bengal 721302, India (shivam-vats.iitkgp@gmail.com).

<sup>&</sup>lt;sup>3</sup>INRIA Bordeaux-Sud-Ouest - LFANT project-team, 200 Avenue de la Vieille Tour, 33405 Talence, France (fredrik.johansson@gmail.com).

<sup>&</sup>lt;sup>4</sup>INRIA - SIERRA project-team, 2 Rue Simone IFF, 75012 Paris, France (f@bianp.net).

<sup>&</sup>lt;sup>5</sup>Birla Institute of Technology and Science, Pilani, K.K. Birla Goa Campus, NH 17B Bypass Road, Zuarinagar, Sancoale, Goa 403726, India (ashutosh.saboo@gmail.com).

 $<sup>^6\</sup>mathrm{University}$  of Moratuwa, Bandaranayake Mawatha, Katubedda, Moratuwa 10400, Sri Lanka (isuru.11@cse.mrt.ac.lk).

<sup>&</sup>lt;sup>7</sup>Indian Institute of Technology Bombay, Powai, Mumbai, Maharashtra 400076, India (sumith@cse.iitb.ac.in).

<sup>&</sup>lt;sup>8</sup>New Technologies - Research Centre, University of West Bohemia, Univerzitní 8, 306 14 Plzeň, Czech Republic (cimrman3@ntc.zcu.cz).

<sup>&</sup>lt;sup>9</sup>University of South Carolina, Columbia, SC 29201 (scopatz@cec.sc.edu).

domains, such as Sage [51] (pure mathematics), yt [55] (astronomy and astrophysics), PyDy [25] (multibody dynamics), and SfePy [19] (finite elements).

Unlike many CASs, SymPy does not invent its own programming language. Python itself is used both for the internal implementation and the end user interaction. The exclusive usage of a single programming language makes it easier for people already familiar with that language to use or develop SymPy. Simultaneously, it enables developers to focus on mathematics, rather than language design.

SymPy is designed with a strong focus on usability as a library. Extensibility is important in its application program interface (API) design. Thus, SymPy makes no attempt to extend the Python language itself. The goal is for users of SymPy to be able to include SymPy alongside other Python libraries in their workflow, whether that is in an interactive environment or programmatic use as part of a larger system.

As a library, SymPy does not have a built-in graphical user interface (GUI). However, SymPy exposes a rich interactive display system, including registering printers with Jupyter [41] frontends, including the Notebook and Qt Console, which will render SymPy expressions using MathJax [18] or LATEX.

The remainder of this paper discusses key components of the SymPy software. Section 2 discusses the architecture of SymPy. Section 3 enumerates the features of SymPy and takes a closer look at some of the important ones. Following that, section 4 looks at the numerical features of SymPy and its dependency library, mpmath. Section 5 looks at the domain specific physics submodules for performing symbolic and numerical calculations in classical mechanics and quantum mechanics. Finally, section 6 concludes the paper and discusses future work.

- 2. Architecture. Software architecture is of central importance in any large software project because it establishes predictable patterns of usage and development [48]. This section describes the essential structural components of SymPy, provides justifications for the design decisions that have heretofore been made, and the provides example user-facing code as appropriate
- **2.1.** Basic Usage. SymPy requires that all variable names be defined prior to use because it is built on Python. The following statement imports all SymPy functions into the global Python namespace. From here on, all examples in this paper assume that this statement has been executed.

```
>>> from sympy import *
```

Symbolic variables, called symbols, must be defined and assigned to Python variables before they can be used. This is typically done through the <code>symbols</code> function, which may create multiple symbols in a single function call. For instance,

```
>>> x, y, z = symbols('x y z')
```

creates three symbols representing variables named x, y, and z. In this particular instance, these symbols are all assigned to Python variables of the same name. However, the user is free to assign them to different Python variables, while representing the same symbol, such as a, b, c = symbols('x y z'). In order to minimize potential confusion, though, all examples in this paper will assume that the symbols x, y, and z have been assigned to Python variables identical to their symbolic names.

Expressions are created from symbols using Python mathematical syntax. Note that in Python, exponentiation is represented by the \*\* binary infix operator. For instance, the following Python code creates the expression  $(x^2 - 2x + 3)/y$ .

```
65 >>> (x**2 - 2*x + 3)/y
66 (x**2 - 2*x + 3)/y
```

Importantly, SymPy expressions are immutable. This simplifies the design of SymPy by allowing expression interning. It also enables expressions to be hashed and stored in Python dictionaries, thereby permitting features such as caching.

**2.2.** The Core. A computer algebra system (CAS) represents mathematical expressions as data structures. For example, the mathematical expression x + y is represented as a tree with three nodes, +, x, and y, where x and y are ordered children of +. As users manipulate mathematical expressions with traditional mathematical syntax, the CAS manipulates the underlying data structures. Automated optimizations and computations such as integration, simplification, etc. are all functions that consume and produce expression trees.

In SymPy every symbolic expression is an instance of a Python Basic class, a superclass of all SymPy types providing common methods to all SymPy tree-elements, such as traversals. The children of a node in the tree are held in the args attribute. A terminal or leaf node in the expression tree has empty args.

For example, consider the expression xy + 2:

```
82 >>> expr = x*y + 2
```

By order of operations, the parent of the expression tree for expr is an addition, so it is of type Add. The child nodes of expr are 2 and x\*y.

```
85 >>> type(expr)
86 <class 'sympy.core.add.Add'>
87 >>> expr.args
```

88 (2, x\*y)

67 68

69

70

71 72

73

74

75 76

77

78

79

80

81

89

90

91

98

99

100 101

103

105

107

113

Traversing further into the expression tree grants the full expression. For example, the first child node, given by expr.args[0], is 2. Its class is Integer, and it has empty an args tuple, indicating that it is a leaf node.

```
92 >>> expr.args[0]
93 2
94 >>> type(expr.args[0])
95 <class 'sympy.core.numbers.Integer'>
96 >>> expr.args[0].args
97 ()
```

A useful way to view an expression tree is with the srepr function. This returns a string representation of an expression as valid Python code with all the nested class constructor calls to create the given expression.

```
>>> srepr(expr)
```

```
102 \quad \text{"Add(Mul(Symbol('x'), Symbol('y')), Integer(2))"}
```

Every SymPy expression satisfies a key identity invariant:

```
104 expr.func(*expr.args) == expr
```

This means that expressions are rebuildable from their  $args.^1$  Note that in SymPy the == operator represents exact structural equality, not mathematical equality. This allows testing if any two expressions are equal to one another as expression trees. For example, even though  $(x+1)^2$  and  $x^2+2x+1$  are equal mathematically, SymPy gives

 $109 \implies (x + 1)**2 == x**2 + 2*x + 1$ 

110 False

because they are different as expression trees (the former is a Pow object and the latter is an Add object).

Python allows classes to override mathematical operators. The Python interpreter

<sup>&</sup>lt;sup>1</sup>expr.func is used instead of type(expr) to allow the function of an expression to be distinct from its actual Python class. In most cases the two are the same.

translates the above x\*y + 2 to, roughly, (x.\_\_mul\_\_(y)).\_\_add\_\_(2). Both x and y, returned from the symbols function, are Symbol instances. The 2 in the expression is processed by Python as a literal, and is stored as Python's built in int type. When 2 is passed to the \_\_add\_\_ method of Symbol, it is converted to the SymPy type Integer(2) before being stored in the resulting expression tree. In this way, SymPy expressions can be built in the natural way using Python operators and numeric literals.

**2.3. Assumptions.** SymPy performs logical inference through its assumptions system. The assumptions system allows users to specify that symbols have certain common mathematical properties, such as being positive, imaginary, or integral. SymPy is careful to never perform simplifications on an expression unless the assumptions allow them. For instance, the identity  $\sqrt{t^2} = t$  holds if t is nonnegative  $(t \ge 0)$ . If t is real, the identity  $\sqrt{t^2} = |t|$  holds. However, for general complex t, no such identity holds.

By default, SymPy performs all calculations assuming that symbols are complex valued. This assumption makes it easier to treat mathematical problems in full generality.

```
130 >>> t = Symbol('t')
131 >>> sqrt(t**2)
132 sqrt(t**2)
```

 By assuming the most general case, that symbols are complex by default, SymPy avoids performing mathematically invalid operations. However, in many cases users will wish to simplify expressions containing terms like  $\sqrt{t^2}$ .

Assumptions are set on Symbol objects when they are created. For instance Symbol('t', positive=True) will create a symbol named t that is assumed to be positive.

```
139 >>> t = Symbol('t', positive=True)
140 >>> sqrt(t**2)
141 t
```

Some of the common assumptions that SymPy allows are positive, negative, real, nonpositive, nonnegative, real, integer, and commutative.<sup>2</sup> Assumptions on any object can be checked with the is assumption attributes, like t.is positive.

Assumptions are only needed to restrict a domain so that certain simplifications can be performed. They are not required to make the domain match the input of a function. For instance, one can create the object  $\sum_{n=0}^{m} f(n)$  as Sum(f(n), (n, 0, m)) without setting integer=True when creating the Symbol object n.

The assumptions system additionally has deductive capabilities. The assumptions use a three-valued logic using the Python built in objects True, False, and None. None represents the "unknown" case. This could mean that the given assumption could be either true or false under the given information, for instance, Symbol('x', real=True).is\_positive will give None because a real symbol might be positive or it might not. It could also mean not enough is implemented to compute the given fact. For instance, (pi + E).is\_irrational gives None, because SymPy does not know how to determine if  $\pi + e$  is rational or irrational. Indeed, this case is an open problem in mathematics.

Basic implications between the facts are used to deduce assumptions. For instance, the assumptions system knows that being an integer implies being rational, so Symbol('x', integer=True).is rational returns True. Furthermore, expres-

sions compute the assumptions on themselves based on the assumptions of their arguments. For instance, if x and y are both created with positive=True, then  $(x + y).is_positive$  will be True.

**2.4. Extensibility.** While the core of SymPy is relatively small, it has been extended to a wide variety of domains by a broad range of contributors. This is due in part because the same language, Python, is used both for the internal implementation and the external usage by users. All of the extensibility capabilities available to users are also utilized by SymPy itself. This eases the transition pathway from SymPy user to SymPy developer.

The typical way to create a custom SymPy object is to subclass an existing SymPy class, usually Basic, Expr, or Function. All SymPy classes used for expression trees<sup>3</sup> should be subclasses of the base class Basic, which defines some basic methods for symbolic expression trees. Expr is the subclass for mathematical expressions that can be added and multiplied together. Instances of Expr typically represent complex numbers, but may also include other "rings" like matrix expressions. Not all SymPy classes are subclasses of Expr. For instance, logic expressions such as And(x, y) are subclasses of Basic but not of Expr.

The Function class is a subclass of Expr which makes it easier to define mathematical functions called with arguments. This includes named functions like  $\sin(x)$  and  $\log(x)$  as well as undefined functions like f(x). Subclasses of Function should define a class method eval, which returns values for which the function should be automatically evaluated, and None for arguments that should not be automatically evaluated.

Many SymPy functions perform various evaluations down the expression tree. Classes define their behavior in such functions by defining a relevant <code>\_eval\_\*</code> method. For instance, an object can indicate to the <code>diff</code> function how to take the derivative of itself by defining the <code>\_eval\_derivative(self, x)</code> method, which may in turn call <code>diff</code> on its <code>args</code>. The most common <code>\_eval\_\*</code> methods relate to the assumptions. <code>\_eval\_is\_assumption</code> defines the assumptions for <code>assumption</code>.

As an example of the notions presented in this section, Listing 1 presents a minimal version of the gamma function  $\Gamma(x)$  from SymPy, which evaluates itself on positive integer arguments, has the positive and real assumptions defined, can be rewritten in terms of factorial with  $\operatorname{gamma}(x)$ .rewrite(factorial), and can be differentiated. fdiff is a convenience method for subclasses of Function. fdiff returns the derivative of the function without considering the chain rule. self.func is used throughout instead of referencing  $\operatorname{gamma}$  explicitly so that potential subclasses of  $\operatorname{gamma}$  can reuse the methods.

Listing 1: A stripped down version of sympy.gamma.

```
from sympy import Integer, Function, floor, factorial, polygamma
from sympy import Integer, floor, floor, factorial, polygamma
from sympy import Integer, floor, floor
```

 $<sup>^{3}</sup>$ Some internal classes, such as those used in the polynomial module, do not follow this rule for efficiency reasons.

```
206
         def eval is positive(self):
207
             x = self.args[0]
208
             if x.is_positive:
                 return True
209
210
             elif x.is_noninteger:
                 return floor(x).is even
211
212
         def eval is real(self):
213
             x = self.args[0]
214
215
             # noninteger means real and not integer
             if x.is positive or x.is noninteger:
216
217
                 return True
218
         def eval rewrite as factorial(self, z):
219
             return factorial(z - 1)
220
221
         def fdiff(self, argindex=1):
222
223
             from sympy.core.function import ArgumentIndexError
             if argindex == 1:
224
                 return self.func(self.args[0])*polygamma(0, self.args[0])
225
226
             else:
                 raise ArgumentIndexError(self, argindex)
227
```

228

229

230

231

232

233234

235

236

The gamma function implemented in SymPy has many more capabilities than the above listing, such as evaluation at rational points and series expansion.

**3. Features.** SymPy has an extensive feature set that is too encompassing for complete, in-depth coverage in this paper. However, calculus and other bedrock areas receive their own subsections here. Additionally, Table 1 gives a compact listing of all major capabilities present in the SymPy codebase. This grants a sampling from the breadth of topics and application domains that SymPy services. Unless stated otherwise, all features noted in Table 1 are symbolic in nature. Numeric features are discussed in Section 4.

Table 1: SymPy Features and Descriptions

Feature	Description
Calculus	Algorithms for computing derivatives, integrals, and limits.
Category Theory	Representation of objects, morphisms, and diagrams. Tools
	for drawing diagrams with Xy-pic.
Code Generation	Enables generation of compilable and executable code in a va-
	riety of different programming languages directly from expres-
	sions. Target languages include C, Fortran, Julia, JavaScript,
	Mathematica, MATLAB and Octave, Python, and Theano.
Combinatorics &	Implements permutations, combinations, partitions, subsets,
Group Theory	various permutation groups (such as polyhedral, Rubik, sym-
	metric, and others), Gray codes [38], and Prufer sequences [13].

Concrete Math Summation, products, tools for determining whether summa-

tion and product expressions are convergent, absolutely convergent, hypergeometric, and other properties. May also compute Gosper's normal form [43] for two univariate polynomials.

Cryptography Represents block and stream ciphers, including shift, Affine,

substitution, Vigenere's, Hill's, bifid, RSA, Kid RSA, linear-

feedback shift registers, and Elgamal encryption

Differential Ge- Classes to represent manifolds, metrics, tensor products, and ometry coordinate systems in Riemannian and pseudo-Riemannian ge-

ometries [52].

Geometry Allows the creation of 2D geometrical entities, such as lines

and circles. Enables queries on these entities, such as asking the area of an ellipse, checking for collinearity of a set of points,

or finding the intersection between two lines.

Lie Algebras Represents Lie algebras and root systems.

Logic Boolean expression, equivalence testing, satisfiability, and nor-

mal forms.

Matrices Tools for creating matrices of symbols and expressions. This is

capable of both sparse and dense representations and performing symbolic linear algebraic operations (e.g., inversion and

factorization).

Matrix Expres- Matrices with symbolic dimensions (unspecified entries). Block

sions matrices.

Number Theory Prime number generation, primality testing, integer factoriza-

tion, continued fractions, Egyptian fractions, modular arithmetic, quadratic residues, partitions, binomial and multinomial coefficients, prime number tools, and integer factoriza-

tion.

Plotting Hooks for visualizing expressions via matplotlib [30] or as text

drawings when lacking a graphical back-end. 2D function plotting, 3D function plotting, and 2D implicit function plotting

are supported.

Polynomials Computes polynomial algebras over various coefficient do-

mains. Functionality ranges from the simple (e.g., polynomial division) to the advanced (e.g., Gröbner bases [10] and multi-

variate factorization over algebraic number domains).

Printing Functions for printing SymPy expressions in the terminal with

ASCII or Unicode characters and converting SymPy expres-

sions to LATEX and MathML.

Quantum Mechanics Quantum states, bra-ket notation, operators, basis sets, representations, tensor products, inner products, outer products, commutators, anticommutators, and specific quantum system

implementations.

Series Implements series expansion, sequences, and limit of sequences.

This includes Taylor, Laurent, and Puiseux series as well as

special series, such as Fourier and formal power series.

Sets Representations of empty, finite, and infinite sets. This in-

cludes special sets such as for all natural, integer, and complex numbers. Operations on sets such as union, intersection,

Cartesian product, and building sets from other sets.

Simplification	Functions for manipulating and simplifying expressions. Includes algorithms for simplifying hypergeometric functions, trigonometric expressions, rational functions, combinatorial functions, square root denesting, and common subexpression elimination.
Solvers	Functions for symbolically solving equations algebraically, systems of equations, both linear and non-linear, inequalities, ordinary differential equations, partial differential equations, Diophantine equations, and recurrence relations.
Special Functions	Implements a number of well known special functions, including Dirac delta, Gamma, Beta, Gauss error functions, Fresnel integrals, Exponential integrals, Logarithmic integrals, Trigonometric integrals, Bessel, Hankel, Airy, B-spline, Riemann Zeta, Dirichlet eta, polylogarithm, Lerch transcendent, hypergeometric, elliptic integrals, Mathieu, Jacobi polynomials, Gegenbauer polynomial, Chebyshev polynomial, Legendre polynomial, Hermite polynomial, Laguerre polynomial, and spherical harmonic functions.
Statistics	Support for a random variable type as well as the ability to declare this variable from prebuilt distribution functions such as Normal, Exponential, Coin, Die, and other custom distributions [45].
Tensors Vectors	Symbolic manipulation of indexed objects. Provides basic vector math and differential calculus with respect to 3D Cartesian coordinate systems.

**3.1. Simplification.** The generic way to simplify an expression is by calling the simplify function. It must be emphasized that simplification is not an unambiguously defined mathematical operation [17]. The simplify function applies several simplification routines along with heuristics to make the output expression as "simple" as possible.

It is often preferable to apply more directed simplification functions. These apply very specific rules to the input expression and are typically able to make guarantees about the output. Take for instance the factor function, which given a polynomial with rational coefficients in several variables, is guaranteed to produce a factorization into irreducible factors. Table 2 lists common simplification functions.

Table 2: Some SymPy Simplification Functions

expand	expand the expression
factor	factor a polynomial into irreducibles
collect	collect polynomial coefficients
cancel	rewrite a rational function as $p/q$ with common factors canceled
apart	compute the partial fraction decomposition of a rational function
trigsimp	simplify trigonometric expressions [23]

Substitutions are performed through the .subs method.

237

238

239

241

242

243244

$$249 \quad (y + 1)**2 + \sin(y + 1) + 1$$

**3.2. Calculus.** Integrals are calculated with the integrate function. SymPy implements a combination of the Risch algorithm [16], table lookups, a reimplementation of Manuel Bronstein's "Poor Man's Integrator" [15], and an algorithm for computing integrals based on Meijer G-functions. These allow SymPy to compute a wide variety of indefinite and definite integrals. The Meijer G-function algorithm and the Risch algorithm are respectively demonstrated below by the computation of

$$\int_{0}^{\infty} e^{-st} \log(t) dt = -\frac{\log(s) + \gamma}{s}$$

and

$$\int \frac{-2x^2 (\log (x) + 1) e^{x^2} + (e^{x^2} + 1)^2}{x (e^{x^2} + 1)^2 (\log (x) + 1)} dx = \log (\log (x) + 1) + \frac{1}{e^{x^2} + 1}.$$

```
250 >>> s, t = symbols('s t', positive=True)
251 >>> integrate(exp(-s*t)*log(t), (t, θ, oo)).simplify()
252 -(log(s) + EulerGamma)/s
253 >>> integrate((-2*x**2*(log(x) + 1)*exp(x**2) +
254 ... (exp(x**2) + 1)**2)/(x*(exp(x**2) + 1)**2*(log(x) + 1)), x)
255 log(log(x) + 1) + 1/(exp(x**2) + 1)
```

Derivatives are computed with the diff function. Derivatives are computed recursively using the various differentiation rules.

258  $\Rightarrow$  diff(sin(x)\*exp(x), x)

exp(x)\*sin(x) + exp(x)\*cos(x)

Summations and products are computed with summation and product, respectively. Summations are computed using a combination of Gosper's algorithm, an algorithm that uses Meijer G-functions, and heuristics. Products are computed via a suite of heuristics.

Limits are computed with the limit function. The limit module implements the Gruntz algorithm [27] for computing symbolic limits (a description of the Gruntz algorithm can be found in the supplement). For example, the following computes  $\lim x \sin(\frac{1}{x}) = 1$  (note that  $\infty$  is **oo** in SymPy).

 $268 \Rightarrow \lim_{x\to\infty} \lim_{x\to\infty} (1/x), x, oo)$ 

269

 $256 \\ 257$ 

259260

261

263

264

265

266

267

As a more complex example, SymPy computes

$$\lim_{x \to 0} \left(2e^{\frac{1-\cos{(x)}}{\sin{(x)}}}-1\right)^{\frac{\sinh{(x)}}{\tan^2{(x)}}} = e.$$

- 270 >>> limit((2\*E\*\*((1-cos(x))/sin(x))-1)\*\*(sinh(x)/atan(x)\*\*2), x, 0)
- 271 **E**

276

Integrals, derivatives, summations, products, and limits that cannot be computed return unevaluated objects. These can also be created directly if the user chooses.

- $274 \gg integrate(x**x, x)$
- 275 Integral(x\*\*x, x)
  - **3.3. Polynomials.** SymPy implements a suite of algorithms for polynomial manipulation, which ranges from relatively simple algorithms for doing arithmetic of

polynomials, to advanced methods for factoring multivariate polynomials into irreducibles, symbolically determining real and complex root isolation intervals, or computing Gröbner bases.

Polynomial manipulation is useful on its own. Within SymPy, though, it is mostly used indirectly as a tool in other areas of the library. In fact, many mathematical problems in symbolic computing are first expressed using entities from the symbolic core, preprocessed, and then transformed into a problem in the polynomial algebra, where generic and efficient algorithms are used to solve the problem and solutions to the original problem are recovered. This is a common scheme in symbolic integration or summation algorithms.

SymPy implements dense and sparse polynomial representations.<sup>4</sup> Both are used in the univariate and multivariate cases. The dense representation is the default for univariate polynomials. For multivariate polynomials, the choice of representation is based on the application. The most common case for the sparse representation is algorithms for computing Gröbner bases (Buchberger, F4, and F5). This is because different monomial orderings can be expressed easily in this representation. However, algorithms for computing multivariate GCDs or factorizations, at least those currently implemented in SymPy, are better expressed when the representation is dense. The dense multivariate representation is specifically a recursively dense representation, where polynomials in  $K[x_0, x_1, \ldots, x_n]$  are viewed as a polynomials in  $K[x_0][x_1] \ldots [x_n]$ . Note that despite this, the coefficient domain K, can be a multivariate polynomial domain as well. The dense recursive representation in Python becomes inefficient when the number of variables gets high.

Some examples for the sympy.polys module can be found in the supplement.

**3.4. Printers.** SymPy has a rich collection of expression printers for displaying expressions to the user. By default, an interactive Python session will render the str form of an expression, which has been used in all the examples in this paper so far. The str form of an expression is valid Python and roughly matches what a user would type to enter the expression.

```
>>> phi0 = Symbol('phi0')
>>> str(Integral(sqrt(phi0), phi0))
'Integral(sqrt(phi0), phi0)'
```

Expressions can be printed with 2D, monospace fonts via pprint. This uses Unicode characters to render mathematical symbols such as integral signs, square roots, and parentheses. Greek letters and subscripts in symbol names that have Unicode code points associated with them are also rendered automatically.

Alternately, the use\_unicode=False flag can be set, which causes the expression to be printed using only ASCII characters.

```
317 >>> pprint(Integral(sqrt(phi0 + 1), phi0), use_unicode=False)
318  /
319  |
320  |
```

<sup>&</sup>lt;sup>4</sup>In a dense representation, the coefficients for all terms up to the degree of each variable are stored in memory. In a sparse representation, only the nonzero coefficients are stored.

Users are encouraged to run the init\_printing function at the beginning of interactive sessions, which automatically enables the best pretty printing supported by their environment. In the Jupyter Notebook or Qt Console [41], the LATEX printer is used to render expressions using MathJax or LATEX, if it is installed on the system. The 2D text representation is used otherwise.

Other printers such as MathML are also available. SymPy uses an extensible printer subsystem for customizing the printing for any given printer, and for custom objects to define their printing behavior for any printer. The code generation capabilities of SymPy use this subsystem to convert expressions into code in various target programming languages.

**3.5.** Solvers. SymPy has a module of equation solvers for symbolic equations. There are two functions for solving algebraic equations in SymPy: solve and solveset. solveset has several design changes with respect to the older solve function. This distinction is present in order to resolve the usability issues with the previous solve function API while maintaining backward compatibility with earlier versions of SymPy. solveset only requires the necessary input information from the user. The function signatures of solve and solveset are

```
344 solve(f, *symbols, **flags)
345 solveset(f, symbol, domain=S.Complexes)
```

 The domain parameter is typically either S.Complexes (the default) or S.Reals, which causes it to only return real solutions.

Additionally, solve has an inconsistent output API for various types of inputs. For instance, depending on the input, sometimes it returns a Python list and sometimes it returns a Python dictionary. On the other hand, the solveset has a canonical output API. solveset always returns a SymPy set object.

Both functions implicitly assume that expressions are equal to 0. For instance, solveset (x - 1, x) solves x - 1 = 0 for x.

solveset is under active development as a planned replacement for solve. There are certain features which are implemented in solve that are not yet implemented in solveset. Notably, these include nonlinear multivariate system and transcendental equations.

More examples of solveset and solve can be found in the supplement.

3.6. Matrices. Computations on matrices with symbolic entries are important for many algorithms within SymPy, as well as being an important feature in its own right.

```
362 >>> A = Matrix(2, 2, [x, x + y, y, x])
363 >>> A
364 Matrix([
365 [x, x + y],
366 [y, x]])
```

SymPy matrices support common symbolic linear algebra manipulations, including matrix addition, multiplication, exponentiation, computing determinants, solving linear systems, and computing inverses using LU decomposition, LDL decomposi-

tion, Gauss-Jordan elimination, Cholesky decomposition, Moore-Penrose pseudoinverse, and adjugate matrix.

All operations are computed symbolically. For instance, eigenvalues are computed by generating the characteristic polynomial using the Berkowitz algorithm and then solving it using polynomial routines.

```
5 >>> A.eigenvals()
```

370 371

372

373

374

377

378

379

380 381

382

383

384

385 386

387

388

389

390

391

392

393

394

395

396

397 398

402

```
376 \{x - sqrt(y*(x + y)): 1, x + sqrt(y*(x + y)): 1\}
```

Internally these matrices store the elements as a list of lists (LIL), making it a dense representation.<sup>5</sup> For storing sparse matrices, the SparseMatrix class can be used. Sparse matrices store the elements in a dictionary of keys (DOK) format.

SymPy also supports matrices with symbolic dimension values. MatrixSymbol represents a matrix with dimensions  $m \times n$ , where m and n can be symbolic. Matrix addition and multiplication, scalar operations, matrix inverse, and transpose are stored symbolically as matrix expressions.

Block matrices are also implemented in SymPy. BlockMatrix elements can be any matrix expression, including explicit matrices, matrix symbols, and other block matrices. All functionalities of matrix expressions are also present in BlockMatrix.

When symbolic matrices are combined with the assumptions module for logical inference, they provide powerful reasoning over invertibility, semi-definiteness, orthogonality, etc., which are valuable in the construction of numerical linear algebra systems.

More examples for Matrix and BlockMatrix may be found in the supplement.

4. Numerics. Floating point numbers in SymPy are represented by the Float class, which represents an arbitrary-precision binary floating-point number by storing its value and precision (in bits). This representation is distinct from the Python built in float type, which is a wrapper around machine double types and uses a fixed precision (53-bit).

Because Python float literals are limited in precision, strings should be used to input precise decimal values:

```
399 >>> Float(1.1)
```

400 1.10000000000000

```
401 >>> Float(1.1, 30) # precision equivalent to 30 digits
```

1.10000000000000008881784197001

```
403 >>> Float("1.1", 30)
```

The evalf method converts a constant symbolic expression to a Float with the spec-

406 ified precision, here 25 digits:

407 >>> (pi + 1).evalf(25)

408 4.141592653589793238462643

Float numbers do not track their *accuracy*, and should be used with caution within symbolic expressions since familiar dangers of floating-point arithmetic apply [26]. A

1 notorious case is that of catastrophic cancellation:

```
412 >>> cos(exp(-100)).evalf(25) - 1
```

413

414 Applying the evalf method to the whole expression solves this problem. Internally,

evalf estimates the number of accurate bits of the floating-point approximation for

6 each sub-expression, and adaptively increases the working precision until the esti-

<sup>&</sup>lt;sup>5</sup>Similar to the polynomials module, dense here means that all entries are stored in memory, contrasted with a sparse representation where only nonzero entries are stored.

```
mated accuracy of the final result matches the sought number of decimal digits:
417
418
     >>> (cos(exp(-100)) - 1).evalf(25)
     -6.919482633683687653243407e-88
419
     The evalf method works with complex numbers and supports more complicated ex-
420
     pressions, such as special functions, infinite series, and integrals. The internal error
421
     tracking does not provide rigorous error bounds (in the sense of interval arithmetic)
422
     and cannot be used to accurately track uncertainty in measurement data; the sole pur-
423
     pose is to mitigate loss of accuracy that typically occurs when converting symbolic
424
     expressions to numerical values.
```

**4.1.** The mpmath library. The implementation of arbitrary-precision floatingpoint arithmetic is supplied by the mpmath library, which originally was developed as a SymPy module but subsequently has been moved to a standalone pure Python package. The basic datatypes in mpmath are mpf and mpc, which respectively act as multiprecision substitutes for Python's float and complex. The floating-point precision is controlled by a global context:

```
432
    >>> import mpmath
433
    >>> mpmath.mp.dps = 30
                               # 30 digits of precision
    >>> mpmath.mpf("0.1") + mpmath.exp(-50)
434
    mpf('0.10000000000000000000192874984794')
435
    >>> print( )
                    # pretty-printed
436
    0.10000000000000000000192874985
437
```

425

426

427

428

429

430

431

438

439

440

441

442

443 444

445

446

447

448

449

450

451

452

453

454

456

457

458 459

460 461

462

463

464 465

For pure numerical computing, it is convenient to use mpmath directly with from mpmath import \* (it is best to avoid such an import statement when using SymPy simultaneously, since numerical functions such as exp will collide names with the symbolic counterparts in SymPy).

Like SymPy, mpmath is a pure Python library. Internally, mpmath represents a floating-point number  $(-1)^s x \cdot 2^y$  by a tuple (s, x, y, b) where x and y are arbitrary-size Python integers and the redundant integer b stores the bit length of x for quick access. If GMPY [29] is installed, mpmath automatically uses the gmpy.mpz type for x, and GMPY methods for rounding-related operations, improving performance.

The mpmath library supports special functions, root-finding, linear algebra, polynomial approximation, and numerical computation of limits, derivatives, integrals, infinite series, and ODE solutions. All features work in arbitrary precision and use algorithms that allow computing hundreds of digits rapidly, except in degenerate cases.

The double exponential (tanh-sinh) quadrature is used for numerical integration by default. For smooth integrands, this algorithm usually converges extremely rapidly, even when the integration interval is infinite or singularities are present at the endpoints [53, 11]. However, for good performance, singularities in the middle of the interval must be specified by the user. To evaluate slowly converging limits and infinite series, mpmath automatically tries Richardson extrapolation and the Shanks transformation (Euler-Maclaurin summation can also be used) [12]. A function to evaluate oscillatory integrals by means of convergence acceleration is also available.

A wide array of higher mathematical functions are implemented with full support for complex values of all parameters and arguments, including complete and incomplete gamma functions, Bessel functions, orthogonal polynomials, elliptic functions and integrals, zeta and polylogarithm functions, the generalized hypergeometric function, and the Meijer G-function. The Meijer G-function instance  $G_{1,3}^{3,0}(0;\frac{1}{2},-1,-\frac{3}{2}|x)$ is a good test case [54]; past versions of both Maple and Mathematica produced incorrect numerical values for large x > 0. Here, mpmath automatically removes an

```
internal singularity and compensates for cancellations (amounting to 656 bits of precision when x = 10000), giving correct values:

>>> mpmath.mp.dps = 15

>>> mpmath.meijerg([[],[0]],[[-0.5,-1,-1.5],[]],10000)

mpf('2.4392576907199564e-94')

Equivalently, with SymPy's interface this function can be evaluated as:

>>> meijerg([[],[0]],[[-S(1)/2,-1,-S(3)/2],[]],10000).evalf()

2.43925769071996e-94
```

Symbolic integration and summation often produces hypergeometric and Meijer G-function closed forms (see section 3.2); numerical evaluation of such special functions is a useful complement to direct numerical integration and summation.

- 5. Domain Specific Submodules. SymPy includes several packages that allow users to solve domain specific problems. For example, a comprehensive physics package is included that is useful for solving problems in mechanics, optics, and quantum mechanics along with support for manipulating physical quantities with units.
- **5.1. Classical Mechanics.** One of the core domains that SymPy suports is the physics of classical mechanics. This is in turn separated into two distinct components: vector algebra symbolics and mechanics.
- **5.1.1.** Vector Algebra. The sympy.physics.vector package provides reference frame, time, and space aware vector and dyadic objects that allow for three-dimensional operations such as addition, subtraction, scalar multiplication, inner and outer products, and cross products. Both of these objects can be written in very compact notation that make it easy to express the vectors and dyadics in terms of multiple reference frames with arbitrarily defined relative orientations. The vectors are used to specify the positions, velocities, and accelerations of points, orientations, angular velocities, and angular accelerations of reference frames, and force and torques. The dyadics are essentially reference frame aware  $3 \times 3$  tensors. The vector and dyadic objects can be used for any one-, two-, or three-dimensional vector algebra and they provide a strong framework for building physics and engineering tools.

The following Python code demonstrates how a vector is created using the orthogonal unit vectors of three reference frames that are oriented with respect to each other and the result of expressing the vector in the A frame. The B frame is oriented with respect to the A frame using Z-X-Z Euler Angles of magnitude  $\pi$ ,  $\frac{\pi}{2}$ , and  $\frac{\pi}{3}$  rad, respectively, whereas the C frame is oriented with respect to the B frame through a simple rotation about the B frame's X unit vector through  $\frac{\pi}{2}$  rad.

```
>>> from sympy.physics.vector import ReferenceFrame
501
    >>> A = ReferenceFrame('A')
502
    >>> B = ReferenceFrame('B')
503
504
    >>> C = ReferenceFrame('C')
    >>> B.orient(A, 'body', (pi, pi / 3, pi / 4), 'zxz')
505
    >>> C.orient(B, 'axis', (pi / 2, B.x))
506
    >>> v = 1 * A.x + 2 * B.z + 3 * C.y
507
    >>> V
508
    A.x + 2*B.z + 3*C.y
509
510
    >>> v.express(A)
    A.x + 5*sqrt(3)/2*A.y + 5/2*A.z
```

**5.1.2. Mechanics.** The sympy.physics.mechanics package utilizes the sympy. physics.vector package to populate time aware particle and rigid body objects to

fully describe the kinematics and kinetics of a rigid multi-body system. These objects store all of the information needed to derive the ordinary differential or differential algebraic equations that govern the motion of the system, i.e., the equations of motion. These equations of motion abide by Newton's laws of motion and can handle arbitrary kinematic constraints or complex loads. The package offers two automated methods for formulating the equations of motion based on Lagrangian Dynamics [32] and Kane's Method [31]. Lastly, there are automated linearization routines for constrained dynamical systems [42].

**5.2. Quantum Mechanics.** The sympy.physics.quantum package has extensive capabilities for performing symbolic quantum mechanics, using Python objects to represent the different mathematical objects relevant in quantum theory [47]: states (bras and kets), operators (unitary, Hermitian, etc.), and basis sets, as well as operations on these objects such as representations, tensor products, inner products, outer products, commutators, and anticommutators. The base objects are designed in the most general way possible to enable any particular quantum system to be implemented by subclassing the base operators and defining the relevant class methods to provide system specific logic.

Symbolic quantum operators and states may be defined, and one can perform a full range of operations with them:

```
>>> from sympy.physics.quantum import Commutator, Dagger, Operator
    >>> from sympy.physics.quantum import Ket, qapply
534
    >>> A = Operator('A')
536
    >>> B = Operator('B')
    >>> C = Operator('C')
537
    >>> D = Operator('D')
538
    >>> a = Ket('a')
540
    >>> comm = Commutator(A, B)
541
    >>> comm
    [A,B]
542
    >>> qapply(Dagger(comm*a)).doit()
543
     -<a|*(Dagger(A)*Dagger(B) - Dagger(B)*Dagger(A))</pre>
544
    Commutators can be expanded using common commutator identities:
545
    >>> Commutator(C+B, A*D).expand(commutator=True)
546
     -[A,B]*D - [A,C]*D + A*[B,D] + A*[C,D]
547
```

522

523 524

526

527

528

529 530

531

532

548

549

550 551

552

553

554

558

559

560

561562

On top of this set of base objects, a number of specific quantum systems have been implemented in a fully symbolic framework. These include:

- Many of the exactly solvable quantum systems, including simple harmonic oscillator states and raising/lowering operators, infinite square well states, and 3D position and momentum operators and states.
- Second quantized formalism of non-relativistic many-body quantum mechanics [22].
- Quantum angular momentum [56]. Spin operators and their eigenstates can be represented in any basis and for any quantum numbers. A rotation operator representing the Wigner-D matrix, which may be defined symbolically or numerically, is also implemented to rotate spin eigenstates. Functionality for coupling and uncoupling of arbitrary spin eigenstates is provided, including symbolic representations of Clebsch-Gordon coefficients and Wigner symbols.
- Quantum information and computing [37]. Multidimensional qubit states, and a full set of one- and two-qubit gates are provided and can be represented

```
563
             symbolically or as matrices/vectors. With these building blocks, it is possible
564
             to implement a number of basic quantum algorithms including the quantum
             Fourier transform, quantum error correction, quantum teleportation, Grover's
565
             algorithm, dense coding, etc. In addition, any quantum circuit may be plotted
566
             using the circuit plot function (Figure 1).
567
         Here are a few short examples of the quantum information and computing capa-
568
     bilities in sympy.physics.quantum. Start with a simple four-qubit state and flip the
569
     second qubit from the right using a Pauli-X gate:
570
    >>> from sympy.physics.quantum.qubit import Qubit
571
    >>> from sympy.physics.quantum.qate import XGate
    >>> q = Qubit('0101')
573
574
    >>> q
    |0101>
575
    >>> X = XGate(1)
576
    >>> qapply(X*q)
577
    |0111>
578
579
    Qubit states can also be used in adjoint operations, tensor products, inner/outer
580
    products:
    >>> Dagger(q)
581
    <0101
582
    >>> ip = Dagger(q)*q
583
584
    >>> ip
585
    <0101|0101>
    >>> ip.doit()
586
587
    Quantum gates (unitary operators) can be applied to transform these states and then
588
    classical measurements can be performed on the results:
    >>> from sympy.physics.quantum.qubit import measure all
591
    >>> from sympy.physics.quantum.gate import H, X, Y, Z
    >>> c = H(0)*H(1)*Qubit('00')
592
593
    >>> C
    H(0)*H(1)*|00>
594
595
    >>> q = qapply(c)
    >>> measure all(q)
    [(|00>, 1/4), (|01>, 1/4), (|10>, 1/4), (|11>, 1/4)]
597
    Lastly, the following example demonstrates creating a three-qubit quantum Fourier
     transform, decomposing it into one- and two-qubit gates, and then generating a circuit
599
     plot for the sequence of gates (see Figure 1).
600
601
    >>> from sympy.physics.quantum.qft import QFT
602
    >>> from sympy.physics.quantum.circuitplot import circuit plot
603
    >>> fourier = QFT(0,3).decompose()
    >>> fourier
    SWAP(0,2)*H(0)*C((0),S(1))*H(1)*C((0),T(2))*C((1),S(2))*H(2)
605
    >>> c = circuit plot(fourier, ngubits=3)
```

6. Conclusion and future work. SymPy is a robust computer algebra system that provides a wide spectrum of features both in traditional computer algebra and 608 in a plethora of scientific disciplines. This allows SymPy to be used in a first-class 609 way with other Python projects, including the scientific Python stack. Unlike many 610 other CASs, SymPy is designed to be used in an extensible way: both as an end-user



Fig. 1: The circuit diagram for a three-qubit quantum Fourier transform generated by SymPy.

application and as a library.

SymPy expressions are immutable trees of Python objects. SymPy uses Python both as the internal language and the user language. This permits users to access to the same methods that the library implements in order to extend it for their needs. Additionally, SymPy has a powerful assumptions system for declaring and deducing mathematical properties on expressions.

SymPy has submodules for many areas of mathematics. This includes functions for simplifying expressions, performing common calculus operations, pretty printing expressions, solving equations, and representing symbolic matrices. Other included areas are discrete math, concrete math, plotting, geometry, statistics, polynomials, sets, series, vectors, combinatorics, group theory, code generation, tensors, Lie algebras, cryptography, and special functions. Additionally, SymPy contains submodules targeting certain specific domains, such as classical mechanics and quantum mechanics. This breadth of domains has been engendered by a strong and vibrant user community. Anecdotally, these users likely chose SymPy because of its ease of access.

Some of the planned future work for SymPy includes work on improving code generation, improvements to the speed of SymPy, improving the assumptions system, and improving the solvers module.

Work is being done on an assumptions subsystem, distinct from the one discussed in section 2.3. The new system stores assumption predicates separate from objects, and uses a SAT solver to perform inference calculations.

7. Acknowledgements. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

Google Summer of Code is an international annual program where Google awards stipends to all students who successfully complete a requested free and open-source software coding project during the summer.

## 8. References.

REFERENCES

- 642 [1] https://github.com/sympy/sympy/blob/master/doc/src/modules/polys/ringseries.rst.
- 643 [2] https://github.com/scolobb/sympy/tree/ct4-commutativity.
- 644 [3] https://scolobb.wordpress.com/.

648

651

652

653

654

655

665

666

667

 $668 \\ 669$ 

670

671

672

673

 $674 \\ 675$ 

678

679

684

685 686

687

688

- 645 [4] https://reference.wolfram.com/language/ref/Flat.html.
- [5] https://reference.wolfram.com/language/ref/Orderless.html.
- 647 [6] https://reference.wolfram.com/language/ref/OneIdentity.html.
  - [7] https://reference.wolfram.com/language/tutorial/FlatAndOrderlessFunctions.html.
- [8] The software engineering of the wolfram system, 2016, https://reference.wolfram.com/ language/tutorial/TheSoftwareEngineeringOfTheWolframSystem.html.
  - [9] M. ABRAMOWITZ AND I. A. STEGUN, Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables, Dover Publications, New York, NY, USA, ninth printing ed., 1964, http://www.math.ucla.edu/~cbm/aands/.
  - [10] W. W. ADAMS AND P. LOUSTAUNAU, An introduction to Gröbner bases, no. 3, American Mathematical Soc., 1994.
- [11] D. H. BAILEY, K. JEYABALAN, AND X. S. LI, A comparison of three high-precision quadrature
   schemes, Experimental Mathematics, 14 (2005), pp. 317–329.
- [658 [12] C. M. BENDER AND S. A. ORSZAG, Advanced Mathematical Methods for Scientists and Engineers, Springer, 1st ed., October 1999.
- [660 [13] N. BIGGS, E. K. LLOYD, AND R. J. WILSON, *Graph Theory*, 1736-1936, Oxford University
   Press, 1976.
- [662 [14] R. P. Brent and P. Zimmermann, Modern Computer Arithmetic, Cambridge University Press,
   wersion 0.5.1 ed.
- 664 [15] M. Bronstein, Poor Man's Integrator, http://www-sop.inria.fr/cafe/Manuel.Bronstein/pmint.
  - [16] M. BRONSTEIN, Symbolic Integration I: Transcendental Functions, Springer-Verlag, New York, NY, USA, 2005.
  - [17] J. CARETTE, Understanding Expression Simplification, in ISSAC '04: Proceedings of the 2004 International Symposium on Symbolic and Algebraic Computation, New York, NY, USA, 2004, ACM Press, pp. 72–79, http://dx.doi.org/http://doi.acm.org/10.1145/ 1005285.1005298.
  - [18] D. CERVONE, Mathjax: a platform for mathematics on the web, Notices of the AMS, 59 (2012), pp. 312–316.
  - [19] R. CIMRMAN, SfePy write your own FE application, in Proceedings of the 6th European Conference on Python in Science (EuroSciPy 2013), P. de Buyl and N. Varoquaux, eds., 2014, pp. 65–70. http://arxiv.org/abs/1404.6391.
- [676 [20] R. J. FATEMAN, A review of Mathematica, Journal of Symbolic Computation, 13 (1992),
   pp. 545-579, http://dx.doi.org/DOI:10.1016/S0747-7171(10)80011-2.
  - [21] H. R. P. FERGUSON, D. H. BAILEY, AND S. ARNO, Analysis of PSLQ, an integer relation finding algorithm, Mathematics of Computation, 68 (1999), pp. 351–369.
- [680 [22] A. FETTER AND J. WALECKA, Quantum Theory of Many-Particle Systems, Dover Publications, 681 2003.
- [682 [23] H. Fu, X. Zhong, and Z. Zeng, Automated and Readable Simplification of Trigonometric
   Expressions, Mathematical and Computer Modelling, 55 (2006), pp. 1169-1177.
  - [24] Y. C. Fung, A first course in continuum mechanics, Pearson, third edition ed., 1993.
    - [25] G. Gede, D. L. Peterson, A. S. Nanjangud, J. K. Moore, and M. Hubbard, Constrained multibody dynamics with python: From symbolic equation generation to publication, in ASME 2013 International Design Engineering Technical Conferences and Computers and Information in Engineering Conference, American Society of Mechanical Engineers, 2013, pp. V07BT10A051-V07BT10A051.
- [690 [26] D. GOLDBERG, What every computer scientist should know about floating-point arithmetic,
   691 ACM Computing Surveys (CSUR), 23 (1991), pp. 5-48.
- [692 [27] D. GRUNTZ, On Computing Limits in a Symbolic Manipulation System, PhD thesis, Swiss
   [693 Federal Institute of Technology, Zürich, Switzerland, 1996.
- 694 [28] D. Gruntz and W. Koepf, Formal power series, (1993).
- 695 [29] C. V. Horsen, GMPY. https://pypi.python.org/pypi/gmpy2, 2015.
- [30] J. D. Hunter, Matplotlib: A 2d graphics environment, Computing In Science & Engineering,
   9 (2007), pp. 90–95.
- 698 [31] T. R. KANE AND D. A. LEVINSON, Dynamics, Theory and Applications, McGraw Hill, 1985.
- 699 [32] J. LAGRANGE, Mécanique analytique, no. v. 1 in Mécanique analytique, Ve Courcier, 1811.
- 700 [33] M. Lutz, Learning python, "O'Reilly Media, Inc.", 2013.
- 701 [34] L. R. U. Manssur, R. Portugal, and B. F. Svaiter, Group-theoretic approach for symbolic tensor manipulation, Int. J. Mod. Phys. C, 13 (2002), http://dx.doi.org/http://dx.doi.org/ 10.1142/S0129183102004571.

- 704 [35] J. Martín-García, xact, efficient tensor computer algebra, 2002-2016, http://metric.iem.csic. 705 es/Martin-Garcia/xAct/.
- 706 [36] M. Moskewicz, C. Madigan, and S. Malik, Method and system for efficient implementation 707of boolean satisfiability, Aug. 26 2008, http://www.google.co.in/patents/US7418369. US 708 Patent 7,418,369.
- 709 [37] M. NIELSEN AND I. CHUANG, Quantum Computation and Quantum Information, Cambridge 710 University Press, 2011.
- [38] A. Nijenhuis and H. S. Wilf, Combinatorial Algorithms: For Computers and Calculators, 711 712 Academic Press, New York, NY, USA, second ed., 1978.
  - [39] T. E. OLIPHANT, Python for scientific computing, Computing in Science & Engineering, 9 (2007), pp. 10-20.
- 715 [40] K. Peeters, Cadabra: a field-theory motivated symbolic computer algebra system, Computer 716 Physics Communications, (2007). 717
  - [41] F. PÉREZ AND B. E. GRANGER, Ipython: a system for interactive scientific computing, Computing in Science & Engineering, 9 (2007), pp. 21-29.
  - [42] D. L. Peterson, G. Gede, and M. Hubbard, Symbolic linearization of equations of motion of constrained multibody systems, Multibody System Dynamics, 33 (2014), pp. 143–161, http://dx.doi.org/10.1007/s11044-014-9436-5.
  - [43] M. Petkovšek, H. S. Wilf, and D. Zeilberger, A = bak peters, Wellesley, MA, (1996).
- 723 [44] E. RAYMOND, The cathedral and the bazaar, Knowledge, Technology & Policy, 12 (1999), pp. 23-724
- [45] M. ROCKLIN AND A. R. TERREL, Symbolic statistics with sympy, Computing in Science and 726 Engineering, 14 (2012), http://dx.doi.org/10.1109/MCSE.2012.56.
  - [46] L. Rosen, Open source licensing, vol. 692, Prentice Hall, 2005.
- 728 [47] J. SAKURAI AND J. NAPOLITANO, Modern Quantum Mechanics, Addison-Wesley, 2010.
- 729 [48] M. Shaw and D. Garlan, Software Architecture: Perspectives on an Emerging Discipline, 730Prentice Hall, 1996. Prentice Hall Ordering Information.
- 731 [49] M. Sofroniou and G. Spaletta, Precise numerical computation, Journal of Logic and Alge-732 braic Programming, 64 (2005), pp. 113–134.
  - [50] P. Solin, K. Segeth, and I. Dolezel, Higher-Order Finite Element Methods, Chapman & Hall / CRC Press, 2003.
  - [51] W. Stein and D. Joyner, SAGE: System for Algebra and Geometry Experimentation, Communications in Computer Algebra, 39 (2005).
- 737 [52] G. J. Sussman and J. Wisdom, Functional Differential Geometry, Massachusetts Institute of 738 Technology Press, 2013.
  - [53] H. TAKAHASI AND M. MORI, Double exponential formulas for numerical integration, Publications of the Research Institute for Mathematical Sciences, 9 (1974), pp. 721-741.
- 741 [54] V. T. TOTH, Maple and Meijer's G-function: a numerical instability and a cure. http://www. 742 vttoth.com/CMS/index.php/technical-notes/67, 2007.
  - [55] M. J. Turk, B. D. Smith, J. S. Oishi, S. Skory, S. W. Skillman, T. Abel, and M. L. NORMAN, yt: A Multi-code Analysis Toolkit for Astrophysical Simulation Data, The Astrophysical Journal Supplement Series, 192 (2011), pp. 9-+, http://dx.doi.org/10.1088/ 0067-0049/192/1/9, arXiv:1011.3514.
  - [56] R. Zare, Angular Momentum: Understanding Spatial Aspects in Chemistry and Physics, Wiley, 1991.
- [57] O. ZIENKIEWICZ, R. TAYLOR, AND J. ZHU, The Finite Element Method: Its Basis and Fun-749 750 damentals, Butterworth-Heinemann, seventh edition ed., 2013, http://dx.doi.org/http: 751 //dx.doi.org/10.1016/B978-1-85617-633-0.00019-8.

## 9. Supplement.

713

714

718

719

720

721

722

725

727

733

734

735736

739

740

743 744

745 746

747 748

752

753

754

755

756 757

758

759

760

9.1. Limits: The Gruntz Algorithm. SymPy calculates limits using the Gruntz algorithm, as described in [27]. The basic idea is as follows: any limit can be converted to a limit  $\lim_{x\to\infty} f(x)$  by substitutions like  $x\to \frac{1}{x}$ . Then the most varying subexpression  $\omega$  (that converges to zero as  $x \to \infty$  the fastest from all subexpressions) is identified in f(x), and f(x) is expanded into a series with respect to  $\omega$ . Any positive powers of  $\omega$  converge to zero. If there are negative powers of  $\omega$ , then the limit is infinite. The constant term (independent of  $\omega$ , but could depend on x) then determines the limit (one might need to recursively apply the Gruntz algorithm on this term to determine the limit).

To determine the most varying subexpression, the comparability classes must first be defined, by calculating L:

764 (1) 
$$L \equiv \lim_{x \to \infty} \frac{\log |f(x)|}{\log |g(x)|}$$

And then operations <, >, and  $\sim$  are defined as follows: f > g when  $L = \pm \infty$  (it is said that if f is more rapidly varying than g, i.e., f goes to  $\infty$  or 0 faster than g, f is greater than any power of g), f < g when L = 0 (f is less rapidly varying than g) and  $f \sim g$  when  $L \neq 0, \pm \infty$  (both f and g are bounded from above and below by suitable integral powers of the other). Here are some examples of comparability classes:

$$2 < x < e^x < e^{x^2} < e^{e^x}$$

$$2 \sim 3 \sim -5$$

$$x \sim x^2 \sim x^3 \sim \frac{1}{x} \sim x^m \sim -x$$

$$e^x \sim e^{-x} \sim e^{2x} \sim e^{x+e^{-x}}$$

$$f(x) \sim \frac{1}{f(x)}$$

The Gruntz algorithm is now illustrated on the following example:

766 (2) 
$$f(x) = e^{x+2e^{-x}} - e^x + \frac{1}{x}.$$

- The goal is to calculate  $\lim_{x\to\infty} f(x)$ . First, the set of most rapidly varying subexpres-
- sions is determined—the so called *mrv set*. For (2), the following mrv set  $\{e^x, e^{-x}, e^{x+2e^{-x}}\}$
- 769 is obtained. These are all subexpressions of (2) and they all belong to the same com-
- parability class. This calculation can be done using SymPy as follows:
- 771 >>> from sympy.series.gruntz import mrv
  - 72 >>> mrv(exp(x+2\*exp(-x))-exp(x) + 1/x, x)[0].keys()
- 773 dict keys([exp(x + 2\*exp(-x)), exp(x), exp(-x)])
- Next any item  $\omega$  is taken from mrv that converges to zero for  $x \to \infty$ . The item  $\omega = e^{-x}$  is obtained. If such a term is not present in the mrv set (i.e., all terms converge to infinity instead of zero), the relation  $f(x) \sim \frac{1}{f(x)}$  can be used.
- Next step is to rewrite the mrv in terms of  $\omega$ :  $\{\frac{1}{\omega}, \omega, \frac{1}{\omega}e^{2\omega}\}$ . Then the original subexpressions are substituted back into f(x) and expanded with respect to  $\omega$ :

779 (3) 
$$f(x) = \frac{1}{x} - \frac{1}{\omega} + \frac{1}{\omega}e^{2\omega} = 2 + \frac{1}{x} + 2\omega + O(\omega^2)$$

Since  $\omega$  is from the mrv set, then in the limit  $x \to \infty$  it is  $\omega \to 0$  and so  $2\omega + O(\omega^2) \to 0$  in (3):

782 (4) 
$$f(x) = \frac{1}{x} - \frac{1}{\omega} + \frac{1}{\omega}e^{2\omega} = 2 + \frac{1}{x} + 2\omega + O(\omega^2) \to 2 + \frac{1}{x}$$

Since the result  $(2 + \frac{1}{x})$  still depends on x, the above procedure is iterated on the result until just a number (independent of x) is obtained, which is the final limit. In the above case the limit is 2, as can be verified by SymPy:

786 >>>  $\lim_{x \to \infty} (\exp(x+2*\exp(-x)) - \exp(x) + 1/x, x, oo)$ 787 2

In general, when f(x) is expanded in terms of  $\omega$ , it is obtained:

789 (5) 
$$f(x) = \underbrace{O\left(\frac{1}{\omega^3}\right)}_{\infty} + \underbrace{\frac{C_{-2}(x)}{\omega^2}}_{\infty} + \underbrace{\frac{C_{-1}(x)}{\omega}}_{\infty} + C_0(x) + \underbrace{C_1(x)\omega}_{0} + \underbrace{O(\omega^2)}_{0}$$

well as further details are given in Gruntz's PhD thesis [27].

The positive powers of  $\omega$  are zero. If there are any negative powers of  $\omega$ , then the result of the limit is infinity, otherwise the limit is equal to  $\lim_{x\to\infty} C_0(x)$ . The expression  $C_0(x)$  is simpler than f(x) and so the algorithm always converges. A proof of this, as

## 9.2. Series.

**9.2.1.** Series Expansion. SymPy is able to calculate the symbolic series expansion of an arbitrary series or expression involving elementary and special functions and multiple variables. For this it has two different implementations: the series method and Ring Series.

The first approach stores a series as an object of the Basic class. Each function has its specific implementation of its expansion which is able to evaluate the Puiseux series expansion about a specified point. For example, consider a Taylor expansion about 0:

```
803 >>> from sympy import symbols, series
804 >>> x, y = symbols('x, y')
805 >>> series(sin(x+y) + cos(x*y), x, 0, 2)
806 1 + sin(y) + x*cos(y) + 0(x**2)
```

The newer and much faster[1] approach called Ring Series makes use of the observation that a truncated Taylor series, is in fact a polynomial. Ring Series uses the efficient representation and operations of sparse polynomials. The choice of sparse polynomials is deliberate as it performs well in a wider range of cases than a dense representation. Ring Series gives the user the freedom to choose the type of coefficients he wants to have in his series, allowing the use of faster operations on certain types.

For this, several low level methods for expansion of trigonometric, hyperbolic and other elementary functions like inverse of a series, calculating nth root, etc, are implemented using variants of the Newton Method [14]. All these support Puiseux series expansion. The following example demonstrates the use of an elementary function that calculates the Taylor expansion of the sine of a series.

```
819 >>> from sympy import ring
820 >>> from sympy.polys.ring_series import rs_sin
821 >>> R, t = ring('t', QQ)
822 >>> rs_sin(t**2 + t, t, 5)
823 -1/2*t**4 - 1/6*t**3 + t**2 + t
```

The function <code>sympy.polys.rs\_series</code> makes use of these elementary functions to expand an arbitrary SymPy expression. It does so by following a recursive strategy of expanding the lower most functions first and then composing them recursively to calculate the desired expansion. Currently, it only supports expansion about 0 and is under active development. Ring Series is several times faster than the default implementation with the speed difference increasing with the size of the series. The <code>sympy.polys.rs series</code> takes as input any SymPy expression and hence there is no

```
need to explicitly create a polynomial ring. An example demonstrating its use:
831
832
    >>> from sympy.polys.ring_series import rs_series
    >>> from sympy.abc import a, b
833
    >>> from sympy import sin, cos
    >>> rs series(sin(a + b), a, 4)
835
     -1/2*(\sin(b))*a**2 + (\sin(b)) - 1/6*a**3*(\cos(b)) + a*(\cos(b))
836
         9.2.2. Formal Power Series. SymPy can be used for computing the Formal
837
     Power Series of a function. The implementation is based on the algorithm described
838
     in the paper on Formal Power Series [28]. The advantage of this approach is that an
839
     explicit formula for the coefficients of the series expansion is generated rather than
840
     just computing a few terms.
841
         The following example shows how to use fps:
842
    >> f = fps(sin(x), x, x0=0)
843
     >>> f.truncate(6)
    x - x^{**}3/6 + x^{**}5/120 + 0(x^{**}6)
845
     >>> f[15]
846
     -x**15/1307674368000
847
848
         9.2.3. Fourier Series. SymPy provides functionality to compute Fourier se-
     ries of a function using the fourier series function. Under the hood, this function
849
     computes a0, an, bn coefficients using standard integration formulas.
850
         Here's an example on how to compute Fourier series in SymPy:
851
     >>> L = symbols('L')
852
     >>> expr = 2 * (Heaviside(x/L) - Heaviside(x/L - 1)) - 1
853
     >>> f = fourier series(expr, (x, 0, 2*L))
    >>> f.truncate(3)
855
     4*sin(pi*x/L)/pi + 4*sin(3*pi*x/L)/(3*pi) + 4*sin(5*pi*x/L)/(5*pi)
856
         9.3. Logic. SymPy supports construction and manipulation of boolean expres-
857
     sions through the logic module. SymPy symbols can be used as propositional vari-
858
     ables and also be substituted as True or False. A good number of manipulation
859
860
     features for boolean expressions have been implemented in the logic module.
         9.3.1. Constructing boolean expressions. A boolean variable can be de-
861
     clared as a SymPy symbol. Python operators &, | and ~ are overridden when using
862
     SymPy objects to use the SymPy functionality for logical And, Or, and negate. Other
863
     logic functions are also integrated into SymPy, including Xor and Implies, which are
864
     constructed with ^ and >>, respectively. The above are just a shorthand, expressions
865
     can also be constructed by directly creating the relevant objects: And(), Or(), Not(),
866
     Xor(), Nand(), Nor(), etc.
867
    >>> from sympy import *
868
    >>> x, y, z = symbols('x y z')
869
870
    >>> e = (x \& y) | z
871
    >>> e.subs({x: True, y: True, z: False})
872
    True
873
         9.3.2. CNF and DNF. Any boolean expression can be converted to conjunctive
    normal form, disjunctive normal form, and negation normal form. The API also
874
     exposes methods to check if a boolean expression is in any of the above mentioned
875
876
    forms.
    >>> from sympy.logic.boolalg import is_dnf, is_cnf
```

```
878
    >>> x, y, z = symbols('x y z')
879
    >>> to_cnf((x & y) | z)
    And (0r(x, z), 0r(y, z))
880
    >>> to dnf(x & (y | z))
    Or(And(x, y), And(x, z))
882
    >> is cnf((x | y) \& z)
883
    True
884
    >> is dnf((x \& y) | z)
885
    True
886
```

**9.3.3.** Simplification and Equivalence. The module supports simplification 887 of given boolean expression by making deductions from the expression. Equivalence 888 889 of two logical expressions can also be checked. In the case of equivalence, it is possible to return the mapping of variables in two expressions so as to represent the same 890 logical behavior. 891

```
>>> from sympy import *
892
    >>> a, b, c, x, y, z = symbols('a b c x y z')
893
894
    >>> e = a \& (~a | ~b) \& (a | c)
    >>> simplify(e)
895
    And(Not(b), a)
897
    >>> e1 = a & (b | c)
    >>> e2 = (x \& y) | (x \& z)
    >>> bool map(e1, e2)
899
    (And(Or(b, c), a), {a: x, b: y, c: z})
900
```

901 **9.3.4.** SAT solving. The module also supports satisfiability (SAT) checking of a given boolean expression. If satisfiable, it is possible to return a model for which the 902 expression is satisfiable. The API also supports returning all possible models. The 903 904 SAT solver has a clause learning DPLL algorithm implemented with a watch literal scheme and VSIDS heuristic[36]. 905

```
>>> from sympy import *
906
    >>> a, b, c = symbols('a b c')
907
    >>> satisfiable(a & (~a | b) & (~b | c) & ~c)
908
909
    False
    >>> satisfiable(a & (~a | b) & (~b | c) & c)
910
    {a: True, b: True, c: True}
911
```

912

913 914

915

916

917

918

919

921

923

924

9.4. Diophantine Equations. Diophantine equations play a central and an important role in number theory. A Diophantine equation has the form,  $f(x_1, x_2, \dots, x_n) =$ 0 where  $n \geq 2$  and  $x_1, x_2, \ldots, x_n$  are integer variables. If we can find n integers  $a_1, a_2, \ldots, a_n$  such that  $x_1 = a_1, x_2 = a_2, \ldots, x_n = a_n$  satisfies the above equation, we say that the equation is solvable.

Currently, the following five types of Diophantine equations can be solved using SymPy's Diophantine module.

- Linear Diophantine equations:  $a_1x_1 + a_2x_2 + \cdots + a_nx_n = b$
- General binary quadratic equation:  $ax^2 + bxy + cy^2 + dx + ey + f = 0$
- Homogeneous ternary quadratic equation:  $ax^2+by^2+cz^2+dxy+eyz+fzx=0$
- Extended Pythagorean equation:  $a_1x_1^2 + a_2x_2^2 + \cdots + a_nx_n^2 = a_{n+1}x_{n+1}^2$  General sum of squares:  $x_1^2 + x_2^2 + \cdots + x_n^2 = k$ 922

When an equation is fed into Diophantine module, it factors the equation (if 925 possible) and solves each factor separately. Then, all the results are combined to 926 create the final solution set. The following examples illustrate some of the basic 927 functionalities of the Diophantine module.

```
>>> from sympy.solvers.diophantine import *
928
    >> diophantine(2*x + 3*y - 5)
     set([(3*t 0 - 5, -2*t 0 + 5)])
930
931
    >>> diophantine(2*x + 4*y - 3)
932
933
934
     \Rightarrow diophantine(x**2 - 4*x*y + 8*y**2 - 3*x + 7*y - 5)
935
     set([(2, 1), (5, 1)])
936
937
    >>> diophantine(x**2 - 4*x*y + 4*y**2 - 3*x + 7*y - 5)
938
     set([(-2*t**2 - 7*t + 10, -t**2 - 3*t + 5)])
939
940
    \Rightarrow diophantine(3*x**2 + 4*y**2 - 5*z**2 + 4*x*y - 7*y*z + 7*z*x)
941
     set([(-16*p**2 + 28*p*q + 20*q**2,
942
     3*p**2 + 38*p*q - 25*q**2,
943
     4*p**2 - 24*p*q + 68*q**2)])
944
945
946
    >>> from sympy.abc import a, b, c, d, e, f
    \Rightarrow diophantine(9*a**2 + 16*b**2 + c**2 + 49*d**2 + 4*e**2 - 25*f**2)
947
     set([(70*t1**2 + 70*t2**2 + 70*t3**2 + 70*t4**2 - 70*t5**2, 105*t1*t5,
    420*t2*t5, 60*t3*t5, 210*t4*t5,
949
     42*t1**2 + 42*t2**2 + 42*t3**2 + 42*t4**2 + 42*t5**2)])
950
951
     >>> diophantine(a^{**2} + b^{**2} + c^{**2} + d^{**2} + e^{**2} + f^{**2} - 112)
952
     set([(8, 4, 4, 4, 0, 0)])
953
```

**9.5.** Sets. SymPy supports representation of a wide variety of mathematical sets. This is achieved by first defining abstract representations of atomic set classes and then combining and transforming them using various set operations.

Each of the set classes inherits from the base class Set and defines methods to check membership and calculate unions, intersections, and set differences. When these methods are not able to evaluate to atomic set classes, they are represented as abstract unevaluated objects.

SymPy has the following atomic set classes:

• EmptySet represents the empty set  $\emptyset$ .

954

955

956

957

958 959

960

961

962

963

964

965

966

967 968

969 970

971

972

- UniversalSet is an abstract "universal set" for which everything is a member. The union of the universal set with any set gives the universal set and the intersection gives the other set itself.
- FiniteSet is functionally equivalent to Python's built in set object. Its members can be any SymPy object including other sets.
- Integers represents the set of integers  $\mathbb{Z}$ .
- Naturals represents the set of natural numbers N, i.e., the set of positive integers.
- Naturals0 represents the set of whole numbers  $\mathbb{N}^0$ , which are all the non-negative integers.
- Range represents a range of integers. A range is defined by specifying a start value, an end value, and a step size. The enumeration of a Range object

- is functionally equivalent to Python's range except it supports infinite endpoints, allowing the representation of infinite ranges.
- Interval represents an interval of real numbers. It is specified by giving the start and end point and specifying if it is open or closed in the respective ends.

Other than unevaluated classes of Union, Intersection, and Complement operations, we have following set classes.

- ProductSet defines the Cartesian product of two or more sets. The product set is useful when representing higher dimensional spaces. For example, to represent a three-dimensional space, we simply take the Cartesian product of three real sets.
- ImageSet represents the image of a function when applied to a particular set. The image set of a function F with respect to a set S is  $\{F(x)|x\in S\}$ . SymPy uses image sets to represent sets of infinite solutions equations such as  $\sin(x)=0$ .
- ConditionSet represents a subset of a set whose members satisfies a particular condition. The condition set of the set S with respect to the condition H is  $\{x|H(x),x\in S\}$ . SymPy uses condition sets to represent the set of solutions of equations and inequalities, where the equation or the inequality is the condition and the set is the domain being solved over.

A few other classes are implemented as special cases of the classes described above. The set of real numbers, Reals, is implemented as a special case of Interval over the interval  $(-\infty,\infty)$ . ComplexRegion is implemented as a special case of ImageSet. ComplexRegion supports both polar and rectangular representation of regions on the complex plane.

- **9.6.** Category Theory. SymPy includes a basic version of the module for dealing with categories abstract mathematical objects representing classes of structures as classes of objects (points) and morphisms (arrows) between the objects. This version of the module was designed with the following two goals in mind:
  - 1. automatic typesetting of diagrams given by a collection of objects and of morphisms between them, and
  - 2. specification and (semi-)automatic derivation of properties using commutative diagrams.

At of version 1.0, SymPy only implements the first goal, while a (very partially working) draft of implementation of the second goal is available at [2].

In order to achieve the two goals, the module categories defines several classes representing some of the essential concepts: objects, morphisms, categories, and diagrams. In category theory, the inner structure of objects is often discarded in the favor of studying the properties of morphisms, so the class <code>Object</code> is essentially a synonym of the class <code>Symbol</code>. There are several morphism classes which do not have a particular internal structure either, though an exception is <code>CompositeMorphism</code>, which essentially stores a list of morphisms.

To capture the properties of morphisms, the class Diagram is expected to be used. This class stores a family of morphisms, the corresponding source and target objects, and, possibly, some properties of the morphisms. Generally, no restrictions are imposed on what the properties may be — for example, one might use strings of the form "forall", "exists", "unique", etc. Furthermore, the morphisms of a diagram are grouped into premises and conclusions, in order to be able to represent logical implications of the form "for a collection of morphisms P with properties  $p: P \to \Omega$ 

(the premises), there exists a collection of morphisms C with properties  $c: C \to \Omega$  (the conclusions)," where  $\Omega$  is the universal collection of properties. Finally, the class Category includes a collection of diagrams which are deemed commutative and which therefore define the properties of this category.

1051

Automatic typesetting of diagrams takes a Diagram and produces LATEX code using the Xy-pic package. Typesetting is done in two stages: layout and generation of Xy-pic code. The layout stage is taken care of by the class DiagramGrid, which takes a Diagram and lays out the objects in a grid, trying to reduce the average length of the arrows in the final picture. By default, DiagramGrid uses a series of triangle-based heuristics to produce a rectangular grid. A linear layout can also be imposed. Furthermore, groups of objects can be given; in this case, the groups will be treated as atomic cells, and the member objects will be typeset independently of the other objects.

The second phase of diagram typesetting consists of actually drawing the picture and is carried out by the class XypicDiagramDrawer. An example of a diagram automatically typeset by DiagramgGrid and XypicDiagramDrawer in given in Figure 2.

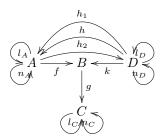


Fig. 2: An automatically typeset commutative diagram

As far as the second main goal of the module is concerned, a (non-working) draft of an implementation is at [2]. The principal idea consists of automatically deciding whether a diagram is commutative or not, given a collection of "axioms" — diagrams known to be commutative. The implementation is based on graph embeddings (injective maps): whenever an embedding of a commutative diagram into a given diagram is found, one concludes that the subdiagram is commutative. Deciding commutativity of the whole diagram is therefore based (theoretically) on finding a "cover" of the target diagram by embeddings of the axioms. The naïve implementation proved to be prohibitively slow; a better optimized version is therefore in order, as well as application of heuristics.

Contributions to automatic inference of commutativity of diagrams are welcome. The source code (both the one in master and in ct4-commutativity) is extensively documented. Even more extensive explanations (including some literary chatter) are given at [3].

**9.7.** SymPy Gamma. SymPy Gamma is a simple web application that runs on Google App Engine. It executes and displays the results of SymPy expressions as well as additional related computations, in a fashion similar to that of Wolfram Alpha. For instance, entering an integer will display its prime factors, digits in the base-10 expansion, and a factorization diagram. Entering a function will display its docstring; in general, entering an arbitrary expression will display its derivative, integral, series

expansion, plot, and roots.

1071

1075

 SymPy Gamma also has several additional features than just computing the results using SymPy.

• SymPy Gamma displays integration and differentiation steps in detail, which can be viewed in Figure 3:

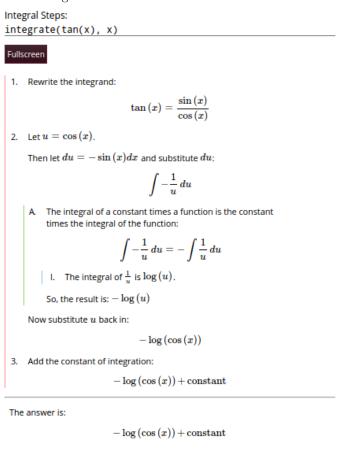


Fig. 3: Integral steps of tan(x)

- SymPy Gamma displays the factor tree diagrams for different numbers.
- SymPy Gamma saves user search queries, and offers many such similar features for free, which Wolfram Alpha only offers to its paid users.

Every input query from the user on SymPy Gamma is first parsed by its own parser, which handles several different forms of function names, which SymPy as a library does not support. For instance, SymPy Gamma supports queries like sin x, whereas SymPy does not support this, and supports only sin(x).

This parser converts the input query to the equivalent SymPy readable code, which is then eventually processed by SymPy, and the result is finally printed with the built-in LaTeX output and rendered on the SymPy Gamma web-application.

**9.8.** SymPy Live. SymPy Live is an online Python shell, which runs on Google App Engine, that executes SymPy code. It is integrated in the SymPy documentation examples, located at this link.

This is accomplished by providing a HTML/JavaScript GUI for entering source code and visualization of output, and a server that evaluates the requested source code. It is an interactive AJAX shell that runs SymPy code using Python on the server.

Certain Features of SymPy Live:

- It supports the exact same syntax as SymPy, hence it can be used easily to test for outputs from various SymPy expressions.
- It can be run as a standalone app or in an existing app as an admin-only handler, and can also be used for system administration tasks, as an interactive way to try out APIs, or as a debugging aid during development.
- It can also be used to plot figures (link), and execute all kinds of expressions that SymPy can evaluate.
- SymPy Live also renders the output in LaTeX for pretty-printing the output.

**9.9.** Comparison with Mathematica. Wolfram Mathematica is a popular proprietary CAS. It features highly advanced algorithms. Mathematica has a core implemented in C++ [8] which interprets its own programming language (know as Wolfram language).

Analogous to Lisp's S-expressions, Mathematica uses its own style of M-expressions, which are arrays of either atoms or other M-expression. The first element of the expression identifies the type of the expression and is indexed by zero, whereas the first argument is indexed by one. Notice that SymPy expression arguments are stored in a Python tuple (that is, an immutable array), while the expression type is identified by the type of the object storing the expression.

Mathematica can associate attributes to its atoms. Attributes may define mathematical properties and behavior of the nodes associated to the atom. In SymPy, the usage of static class fields is roughly similar to Mathematica's attributes, though other programming patterns may also be used the achieve an equivalent behavior, such as class inheritance.

Unlike SymPy, Mathematica's expressions are mutable, that is one can change parts of the expression tree without the need of creating a new object. The mutability of Mathematica allows for a lazy updating of any references to that data structure.

Products in Mathematica are determined by some built in node types, such as Times, Dot, and others. Times is a representation of the \* operator, and is always meant to represent a commutative product operator. The other notable product is Dot, which represents the . operator. This product represents matrix multiplication, it is not commutative. In general, SymPy uses the same node for both scalar and matrix multiplication, the only exception being with abstract matrix symbols. Unlike Mathematica, SymPy determines commutativity with respect to multiplication from the factor's expression type. Mathematica puts the Orderless attribute on the expression type.

Regarding associative expressions, SymPy handles associativity by making associative expressions inherit the class AssocOp, while Mathematica specifies the Flat [4] attribute on the expression type.

Mathematica relies heavily on pattern matching — even the so-called equivalent of function declaration is in reality the definition of a pattern matching generating an expression tree transformation on input expressions. Mathematica's pattern matching is sensitive to associative [4], commutative [5], and one-identity [6] properties of its expression tree nodes [7]. SymPy has various ways to perform pattern matching. All of them play a lesser role in the CAS than in Mathematica and are basically

available as a tool to rewrite expressions. The differential equation solver in SymPy somewhat relies on pattern matching to identify the kind of differential equation, but it is envisaged to replace that strategy with analysis of Lie symmetries in the future. Mathematica's real advantage is the ability to add new overloading to the expression builder at runtime, or for specific subnodes. Consider for example:

```
1135    In[1]:= Unprotect[Plus]
1136
1137    Out[1]= {Plus}
1138
1139    In[2]:= Sin[x_]^2 + Cos[y_]^2 := 1
1140
1141    In[3]:= x + Sin[t]^2 + y + Cos[t]^2
1142
```

Out[3] = 1 + x + y

1173

This expression in Mathematica defines a substitution rule that overloads the functionality of the Plus node (the node for additions in Mathematica). The trailing underscore after a symbol means that it is to be considered a wildcard. This example may not be practical, one may wish to keep this identity unevaluated. Nevertheless, it clearly illustrates the potential to define one's own immediate transformation rules. In SymPy, the operations constructing the addition node in the expression tree are Python class constructors and cannot be modified at runtime. The way SymPy deals with extending the missing runtime overloadability functionality is by subclassing the node types. Subclasses may redefine the class constructor to yield the proper extended functionality.

Unlike SymPy, Mathematica does not support type inheritance or polymorphism [20]. SymPy relies heavily on class inheritance, but for the most part, class inheritance is used to make sure that SymPy objects inherit the proper methods and implement the basic hashing system. Associativity of expressions can be achieved by inheriting the class AssocOp, which may appear a more cumbersome operation than Mathematica's attribute setting.

Matrices in SymPy are types on their own. In Mathematica, nested lists are interpreted as matrices whenever the sublists have the same length. The main difference to SymPy is that ordinary operators and functions do not get generalized the same way as used in traditional mathematics. Using the standard multiplication in Mathematica performs an element-wise product, this is compatible with Mathematica's convention of commutativity of Times nodes. Matrix product is expressed by the dot operator, or the Dot node. The same is true for the other operators, and even functions, most notably calling the exponential function Exp on a matrix returns an element-wise exponentiation of its elements. The real matrix exponential is available through the MatrixExp function.

Unevaluated expressions in Mathematica can be achieved in various ways, most commonly with the HoldForm or Hold nodes, that block the evaluation of subnodes by the parser. Note that such a node cannot be expressed in Python, because of greedy evaluation. Whenever needed in SymPy, it is necessary to add the parameter evaluate=False to all subnodes, or put the input expression in a string.

In Mathematica, the operator == returns a boolean whenever it is able to immediately evaluate the truth of the equality, otherwise it returns an Equal expression.

 $<sup>^6\</sup>mathrm{In}$  reality, Python supports monkey patching, nonetheless, it is a discouraged programming pattern.

In SymPy, == means structural equality and is always guaranteed to return a boolean expression. To express an equality in SymPy it is necessary to explicitly construct an object of the Equality class.

SymPy, in accordance with Python and unlike the usual programming convention, uses \*\* to express the power operator, while Mathematica uses the more common ^.

SymPy's use of floating-point numbers is similar to that of most other CASs, including Maple and Maxima. By contrast, Mathematica uses a form of significance arithmetic [49] for approximate numbers. This offers further protection against numerical errors, although it comes with its own set of problems (for a critique of significance arithmetic, see Fateman [20]). Internally, SymPy's evalf method works similarly to Mathematica's significance arithmetic, but the semantics are isolated from the rest of the system.

**9.10.** Other Projects that use SymPy. There are several projects that use SymPy as a library for implementing a part of their project, or even as a part of back-end for their application as well.

Some of them are listed below:

1205

- Cadabra: Cadabra is a symbolic computer algebra system (CAS) designed specifically for the solution of problems encountered in field theory.
- Octave Symbolic: The Octave-Forge Symbolic package adds symbolic calculation features to GNU Octave. These include common Computer Algebra System tools such as algebraic operations, calculus, equation solving, Fourier and Laplace transforms, variable precision arithmetic and other features.
- SymPy.jl: Provides a Julia interface to SymPy using PyCall.
- Mathics: Mathics is a free, general-purpose online CAS featuring Mathematica compatible syntax and functions. It is backed by highly extensible Python code, relying on SymPy for most mathematical tasks.
- Mathpix: An iOS App, that uses Artificial Intelligence to detect handwritten math as input, and uses SymPy Gamma, to evaluate the math input and generate the relevant steps to solve the problem.
- **IKFast**: IKFast is a robot kinematics compiler provided by OpenRAVE. It analytically solves robot inverse kinematics equations and generates optimized C++ files. It uses SymPy for its internal symbolic mathematics.
- Sage: A CAS, visioned to be a viable free open source alternative to Magma, Maple, Mathematica and MATLAB.
- SageMathCloud: SageMathCloud is a web-based cloud computing and course management platform for computational mathematics.
- **PyDy**: Multibody Dynamics with Python.
- galgebra: Geometric algebra (previously sympy.galgebra).
- yt: Python package for analyzing and visualizing volumetric data (yt.units uses SymPy).
- SfePy: Simple finite elements in Python, see section 9.11.1.
- Quameon: Quantum Monte Carlo in Python.
- Lcapy: Experimental Python package for teaching linear circuit analysis.
- Quantum Programming in Python: Quantum 1D Simple Harmonic Oscillator and Quantum Mapping Gate.
- LaTeX Expression project: Easy LaTeX typesetting of algebraic expressions in symbolic form with automatic substitution and result computation.
- Symbolic statistical modeling: Adding statistical operations to complex physical models.

- **9.11. Project Details.** Below we provide particular examples of SymPy use in some of the projects listed above.
- **9.11.1.** SfePy. SfePy (Simple finite elements in Python), cf. [19] is a Python package for solving partial differential equations (PDEs) in 1D, 2D and 3D by the finite element (FE) method [57]. SymPy is used within this package mostly for code generation and testing, namely:
  - generation of the hierarchical FE basis module, involving generation and symbolic differentiation of 1D Legendre and Lobatto polynomials, constructing the FE basis polynomials [50] and generating the C code;
  - generation of symbolic conversion formulas for various groups of elastic constants [24]: provide any two of the Young's modulus, Poisson's ratio, bulk modulus, Lamé's first parameter, shear modulus (Lamé's second parameter) or longitudinal wave modulus and get the other ones;
  - simple physical unit conversions, generation of consistent unit sets;
  - testing FE solutions using method of manufactured (analytical) solutions: the differential operator of a PDE is symbolically applied and a symbolic right-hand side is created, evaluated in quadrature points, and subsequently used to obtain a numerical solution that is then compared to the analytical one;
  - testing accuracy of 1D, 2D and 3D numerical quadrature formulas (cf. [9]) by generating polynomials of suitable orders, integrating them, and comparing the results with those obtained by the numerical quadrature.
- **9.12. Tensors.** Ongoing work to provide the capabilities of tensor computer algebra has so far produced the tensor module. It is composed of three separated submodules, whose purposes are quite different: tensor.indexed and tensor.indexed\_methods support indexed symbols, tensor.array contains facilities to operator on symbolic N-dimensional arrays, and finally tensor.tensor is used to define abstract tensors. The abstract tensors subsection is inspired by xAct [35] and Cadabra [40]. Canonicalization based on the Butler-Portugal [34] algorithm is supported in SymPy. It is currently limited to polynomial tensor expressions.
- 9.13. Numerical simplification. The nsimplify function in SymPy (a wrapper of identify in mpmath) attempts to find a simple symbolic expression that evaluates to the same numerical value as the given input. It works by applying a few simple transformations (including square roots, reciprocals, logarithms and exponentials) to the input and, for each transformed value, using the PSLQ algorithm [21] to search for a matching algebraic number or optionally a linear combination of user-provided base constants (such as  $\pi$ ).

```
1262 >>> t = 1 / (sin(pi/5)+sin(2*pi/5)+sin(3*pi/5)+sin(4*pi/5))**2
1263 >>> nsimplify(t)
1264 -2*sqrt(5)/5 + 1
1265 >>> nsimplify(pi, tolerance=0.01)
1266 22/7
1267 >>> nsimplify(1.783919626661888, [pi], tolerance=1e-12)
1268 pi/(-1/3 + 2*pi/3)
1269 9.14. Examples.
```

9.14.1. Simplification. expand 1271 >>> expand((x + y)\*\*3) 1272 x\*\*3 + 3\*x\*\*2\*y + 3\*x\*y\*\*2 + y\*\*3

1243

```
1273 factor
1274 >>> factor(x**3 + 3*x**2*y + 3*x*y**2 + y**3)
1275 (x + y)**3
1276 collect
1277 >>> collect(y*x**2 + 3*x**2 - x*y + x - 1, x)
1278 \quad x^{**}2^{*}(y + 3) + x^{*}(-y + 1) - 1
1279 cancel
1280 >>> cancel((x**2 + 2*x + 1)/(x**2 - 1))
1281 (x + 1)/(x - 1)
1282 apart
1283 >>> apart((x**3 + 4*x - 1)/(x**2 - 1))
1284 \times + 3/(x + 1) + 2/(x - 1)
1285 trigsimp
1286 \Rightarrow trigsimp(cos(x)**2*tan(x) - sin(2*x))
1287 - \sin(2*x)/2
         9.14.2. Polynomials. Factorization:
1288
1289 >>> t = symbols("t")
1290 >>> f = (2115*x**4*y + 45*x**3*z**3*t**2 - 45*x**3*t**2 - 423*x*y**4 -
               47*x*y**3 + 141*x*y*z**3 + 94*x*y*z*t - 9*y**3*z**3*t**2 +
1291 ...
               9*y**3*t**2 - y**2*z**3*t**2 + y**2*t**2 + 3*z**6*t**2 +
1292 ...
               2*z**4*t**3 - 3*z**3*t**2 - 2*z*t**3
1293
1294 >>> factor(f)
1295 (t^{**}2^{*}z^{**}3 - t^{**}2 + 47^{*}x^{*}y)^{*}(2^{*}t^{*}z + 45^{*}x^{**}3 - 9^{*}y^{**}3 - y^{**}2 + 3^{*}z^{**}3)
1296 Gröbner bases:
1297 >>> x0, x1, x2 = symbols('x:3')
1298 >>> I = [x0 + 2*x1 + 2*x2 - 1,
               x0**2 + 2*x1**2 + 2*x2**2 - x0
1299 ...
               2*x0*x1 + 2*x1*x2 - x1
1300
1301 >>> groebner(I, order='lex')
1302 GroebnerBasis([7*x0 - 420*x2**3 + 158*x2**2 + 8*x2 - 7,
1303 7*x1 + 210*x2**3 - 79*x2**2 + 3*x2,
1304 84*x2**4 - 40*x2**3 + x2**2 + x2], x0, x1, x2, domain='ZZ', order='lex')
1305 Root isolation:
1306 >>> f = 7*z**4 - 19*z**3 + 20*z**2 + 17*z + 20
1307 >>> intervals(f, all=True, eps=0.001)
1308
     ([],
      [((-425/1024 - 625*I/1024, -1485/3584 - 2185*I/3584), 1),
1309
        ((-425/1024 + 2185*I/3584, -1485/3584 + 625*I/1024), 1),
1310
        ((3175/1792 - 2605*I/1792, 1815/1024 - 10415*I/7168), 1),
1311
1312
        ((3175/1792 + 10415*I/7168, 1815/1024 + 2605*I/1792), 1)])
         9.14.3. Solvers. Single solution:
1314 >>> solveset(x - 1, x)
1315 {1}
1316 Finite solution set, quadratic equation:
1317 >>> solveset(x**2 - pi**2, x)
1318 {-pi, pi}
1319 No solution:
1320 >>> solveset(1, x)
1321 EmptySet()
```

```
1322 Interval solution:
1323 \Rightarrow solveset(x**2 - 3 > 0, x, domain=S.Reals)
1324 (-oo, -sqrt(3)) U (sqrt(3), oo)
1325 Infinitely many solutions:
1326 >>> solveset(x - x, x, domain=S.Reals)
     (-00, 00)
1327
1328 >>> solveset(x - x, x, domain=S.Complexes)
1329 S.Complexes
1330 Linear systems (linsolve)
1331 >>> A = Matrix([[1, 2, 3], [4, 5, 6], [7, 8, 10]])
1332 >>> b = Matrix([3, 6, 9])
1333 >>> linsolve((A, b), x, y, z)
1334 {(-1, 2, 0)}
     >>> linsolve(Matrix(([1, 1, 1, 1], [1, 1, 2, 3])), (x, y, z))
1335
     \{(-y - 1, y, 2)\}
1336
         Below are examples of solve applied to problems not yet handled by solveset.
1337
1338
     Nonlinear (multivariate) system of equations (the intersection of a circle and a parabola):
1339
     >>> solve([x**2 + y**2 - 16, 4*x - y**2 + 6], x, y)
     [(-2 + sqrt(14), -sqrt(-2 + 4*sqrt(14))),
      (-2 + sqrt(14), sqrt(-2 + 4*sqrt(14))),
1341
1342
      (-sqrt(14) - 2, -I*sqrt(2 + 4*sqrt(14))),
      (-sqrt(14) - 2, I*sqrt(2 + 4*sqrt(14)))]
1343
1344 Transcendental equations:
1345 >>> solve((x + log(x))**2 - 5*(x + log(x)) + 6, x)
     [LambertW(exp(2)), LambertW(exp(3))]
1346
1347 >>> solve(x**3 + exp(x))
     [-3*LambertW((-1)**(2/3)/3)]
1349
         9.14.4. Matrices. Matrix expressions
     >>> m, n, p = symbols("m, n, p", integer=True)
1350
1351 >>> R = MatrixSymbol("R", m, n)
1352 >>> S = MatrixSymbol("S", n, p)
1353 >>> T = MatrixSymbol("T", m, p)
1354 >>> U = R*S + 2*T
1355 >>> U.shape
1356 (m, p)
1357 >>> U[0, 1]
1358 2*T[0, 1] + Sum(R[0, k]*S[k, 1], (k, 0, n - 1))
1359 Block Matrices
1360 >>> n, m, l = symbols('n m l')
1361 >>> X = MatrixSymbol('X', n, n)
1362 >>> Y = MatrixSymbol('Y', m ,m)
1363 >>> Z = MatrixSymbol('Z', n, m)
1364 >>> B = BlockMatrix([[X, Z], [ZeroMatrix(m, n), Y]])
1365 >>> B
1366 Matrix([
1367 [X, Z],
1368 [0, Y]])
1369 >>> B[0, 0]
1370 X[0, 0]
```

```
1371 >>> B.shape
1372 (m + n, m + n)
```