SYMPY: SYMBOLIC COMPUTING IN PYTHON

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Abstract. SymPy is an open source computer algebra system written in pure Python. It is built with a focus on extensibility and ease of use, through both interactive and programmatic applications. These characteristics have led SymPy to become the standard symbolic library for the scientific Python ecosystem. This paper presents the architecture of SymPy, a description of its features, and a discussion of select domain specific submodules.

1. Introduction. SymPy is a full featured computer algebra system (CAS) written in the Python programming language [24]. It is free and open source software, being licensed under the 3-clause BSD license [36]. The SymPy project was started

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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 [32]. The accessibility of the codebase and the open community model allow SymPy to rapidly respond to the needs 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 [27]. SymPy is itself used by many libraries and tools to support research within a variety of domains, such as Sage [39] (pure mathematics), yt [44] (astronomy and astrophysics), PyDy [15] (multibody dynamics), and SfePy [10] (finite elements).

Unlike many CASs, SymPy does not invent its own programming language. Python itself is used both for the internal implementation and 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 be in an interactive environment or as a programmatic part in 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 [29] frontends, including the Notebook and Qt Console, which will render SymPy expressions using MathJax [9] 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. The 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. Conclusions and future directions for SymPy are given in section 6.

- 2. Architecture. Software architecture is of central importance in any large software project because it establishes predictable patterns of usage and development [38]. This section describes the essential structural components of SymPy, provides justifications for the design decisions that have been made, and gives example user-facing code as appropriate.
- **2.1.** Basic Usage. 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 symbols 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's mathematical syntax. Note that in Python, exponentiation is represented by the ** binary infix operator. For instance, the following Python code creates the expression $(x^2 - 2x + 3)/y$.

```
70 >>> (x**2 - 2*x + 3)/y
71 (x**2 - 2*x + 3)/y
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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:

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

88 By order of operations, the parent of the expression tree for expr is an addition, so it 89 is of type Add. The child nodes of expr are 2 and x*y.

```
90 >>> type(expr)
```

```
91 <class 'sympy.core.add.Add'>
92 >>> expr.args
```

93 (2, x*y)

Descending further down into the expression tree yields the full expression. For example, the next child node (given by expr.args[0]) is 2. Its class is Integer, and it has an empty args tuple, indicating that it is a leaf node.

```
97 >>> expr.args[0]
98 2
99 >>> type(expr.args[0])
100 <class 'sympy.core.numbers.Integer'>
101 >>> expr.args[0].args
102 ()
```

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

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

```
"Add(Mul(Symbol('x'), Symbol('y')), Integer(2))"
```

Every SymPy expression satisfies a key identity invariant:

```
109 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

¹expr.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.

```
example, even though (x+1)^2 and x^2+2x+1 are equal mathematically, SymPy gives >>> (x+1)^**2 == x^**2 + 2^*x + 1
115 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 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.

```
135 >>> t = Symbol('t')
136 >>> sqrt(t**2)
137 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.

```
144 >>> t = Symbol('t', positive=True)
145 >>> sqrt(t**2)
146 t
```

Some of the common assumptions that SymPy allows are positive, negative, real, nonpositive, nonnegative, real, integer, and commutative.² 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 given assumptions do not unambiguously specify the truth of an attribute. For instance, Symbol('x', real=True).is_positive will give None because a real symbol might be positive or negative. The None could also mean that not enough is known or implemented to compute

 $^{^2 \}text{If } A \text{ and } B \text{ are Symbols created with commutative=False then SymPy will keep } A \cdot B \text{ and } B \cdot A \text{ distinct.}$

the given fact. For instance, (pi + E).is_irrational gives None, because determining whether $\pi + e$ is rational or irrational is an open problem in mathematics [23].

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, expressions 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 whereas $(x - y).is_positive$ will be True whereas True whereas True is True whereas True whereas True is True whereas True whereas True is True whereas True where True whereas True where True whereas True where True where True where True where True whe

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 trees³ 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 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 gamma explicitly so that potential subclasses of gamma can reuse the methods.

Listing 1: A minimal implementation of sympy.gamma.

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

204 class gamma(Function)

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

```
205
        @classmethod
206
         def eval(cls, arg):
             if isinstance(arg, Integer) and arg.is_positive:
207
                 return factorial(arg - 1)
208
209
210
         def eval is positive(self):
             x = self.args[0]
211
             if x.is positive:
212
                 return True
213
214
             elif x.is noninteger:
                 return floor(x).is even
215
216
         def eval is real(self):
217
             x = self.args[0]
218
             # noninteger means real and not integer
219
             if x.is positive or x.is noninteger:
220
221
                 return True
222
         def _eval_rewrite_as_factorial(self, z):
223
             return factorial(z - 1)
224
225
         def fdiff(self, argindex=1):
226
227
             from sympy.core.function import ArgumentIndexError
228
             if argindex == 1:
                 return self.func(self.args[0])*polygamma(0, self.args[0])
229
             else:
230
                 raise ArgumentIndexError(self, argindex)
231
```

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

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3. Features. Although SymPy's extensive feature set cannot be covered indepth in this paper, calculus and other bedrock areas are discussed in their own subsections. 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	Generation of compilable and executable code in a variety
	of different programming languages from expressions directly.
	Target languages include C, Fortran, Julia, JavaScript, Math-
	ematica, MATLAB and Octave, Python, and Theano.

Combinatorics & Group Theory

Permutations, combinations, partitions, subsets, various permutation groups (such as polyhedral, Rubik, symmetric, and

others), Gray codes [26], and Prufer sequences [4].

Concrete Math

Summation, products, tools for determining whether summation and product expressions are convergent, absolutely convergent, hypergeometric, and for determining other properties; computation of Gosper's normal form [31] for two univariate

polynomials.

Cryptography

Block and stream ciphers, including shift, Affine, substitution, Vigenère's, Hill's, bifid, RSA, Kid RSA, linear-feedback shift registers, and Elgamal encryption.

Differential Geometry

Representations of manifolds, metrics, tensor products, and coordinate systems in Riemannian and pseudo-Riemannian geometries [40].

Geometry

Representations 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 objects.

Lie Algebras

Representations of Lie algebras and root systems.

Logic

Boolean expressions, equivalence testing, satisfiability, and

normal forms.

Matrices

Tools for creating matrices of symbols and expressions. Both sparse and dense representations, as well as symbolic linear algebraic operations (e.g., inversion and factorization), are supported.

Matrix Expres-

sions

Matrices with symbolic dimensions (unspecified entries). Block matrices.

Number Theory

Prime number generation, primality testing, integer factorization, continued fractions, Egyptian fractions, modular arithmetic, quadratic residues, partitions, binomial and multinomial coefficients, prime number tools, hexidecimal digits of pi, and integer factorization.

Plotting

Hooks for visualizing expressions via matplotlib [20] or as text drawings when lacking a graphical back-end. 2D function plotting, 3D function plotting, and 2D implicit function plotting are supported.

Polynomials

Polynomial algebras over various coefficient domains. Functionality ranges from simple operations (e.g., polynomial division) to advanced computations (e.g., Gröbner bases [1] and multivariate factorization over algebraic number domains).

Printing

Functions for printing SymPy expressions in the terminal with ASCII or Unicode characters and converting SymPy expressions 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

Series expansion, sequences, and limits 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 com-
	plex numbers. Operations on sets such as union, intersection,
	Cartesian product, and building sets from other sets are sup-
	ported.
Simplification	Functions for manipulating and simplifying expressions. In-
	cludes algorithms for simplifying hypergeometric functions,
	trigonometric expressions, rational functions, combinatorial
	functions, square root denesting, and common subexpression
	elimination.
Solvers	Functions for symbolically solving equations, systems of equa-
	tions, both linear and non-linear, inequalities, ordinary dif-
	ferential equations, partial differential equations, Diophantine
	equations, and recurrence relations.
Special Func-	Implementations of a number of well known special functions,
tions	including Dirac delta, Gamma, Beta, Gauss error functions,
	Fresnel integrals, Exponential integrals, Logarithmic integrals,
	Trigonometric integrals, Bessel, Hankel, Airy, B-spline, Rie-
	mann Zeta, Dirichlet eta, polylogarithm, Lerch transcendent,
	hypergeometric, elliptic integrals, Mathieu, Jacobi polynomi-
	als, 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 distri-
	butions [35].
Tensors	Symbolic manipulation of indexed objects.
Vectors	Basic operations on vectors and differential calculus with re-
	spect 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 [8]. 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. For instance, the factor function, 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

Substitutions are performed using the .subs method.

251 >>>
$$(\sin(x) + x**2 + 1). \operatorname{subs}(x, y + 1)$$

252 $(y + 1)**2 + \sin(y + 1) + 1$

3.2. Calculus. Integrals are calculated with the integrate function. SymPy implements a combination of the Risch algorithm [6], table lookups, a reimplementation of Manuel Bronstein's "Poor Man's Integrator" [5], and an algorithm for computing integrals based on Meijer G-functions [33, 34]. 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

$$\int_0^\infty e^{-st} \log(t) dt = -\frac{\log(s) + \gamma}{s}$$

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

- 262 >>> s, t = symbols('s t', positive=True)
- 263 >>> integrate(exp(-s*t)*log(t), (t, 0, oo)).simplify()
- 264 -(log(s) + EulerGamma)/s
- 265 >>> integrate($(-2*x**2*(\log(x) + 1)*\exp(x**2) +$
- 266 ... $(\exp(x^{**2}) + 1)^{**2}/(x^{*}(\exp(x^{**2}) + 1)^{**2}(\log(x) + 1)), x)$
- $267 \log(\log(x) + 1) + 1/(\exp(x^{**}2) + 1)$

Derivatives are computed with the diff function, which recursively uses the various differentiation rules.

- 270 >>> diff(sin(x)*exp(x), x)
- $271 \exp(x) \cdot \sin(x) + \exp(x) \cdot \cos(x)$

Summations and products are computed with summation and product, respectively. Summations are computed using a combination of Gosper's algorithm [17], an algorithm that uses Meijer G-functions [33, 34], and heuristics. Products are computed via a suite of heuristics.

- 276 >>> i, n = symbols('i n')
- 277 >>> summation(2**i, (i, 0, n 1))
- 278 **2**n 1**

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- 279 >>> summation(i*factorial(i), (i, 1, n))
- 280 n*factorial(n) + factorial(n) 1

Limits are computed with the limit function. The limit module implements the Gruntz algorithm [18] for computing symbolic limits (a description of the Gruntz algorithm may be found in the supplement). For example, the following computes $\lim_{x \to \infty} x \sin(\frac{1}{x}) = 1$. Note that SymPy denotes ∞ as ∞ .

- 285 >>> limit(x*sin(1/x), x, oo)
- 286 **1**
- 287 As a more complex example, SymPy computes

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

```
289 >>> limit((2*E**((1-cos(x))/sin(x))-1)**(sinh(x)/atan(x)**2), x, 0)
290 E
291 Integrals, derivatives, summations, products, and limits that cannot be computed
292 return unevaluated objects. These can also be created directly if the user chooses.
293 >>> integrate(x**x, x)
294 Integral(x**x, x)
295 >>> Sum(2**i, (i, 0, n - 1))
296 Sum(2**i, (i, 0, n - 1))
```

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 in its own right. 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. The solutions to the original problem are subsequently recovered from the results. This is a common scheme in symbolic integration or summation algorithms.

SymPy implements dense and sparse polynomial representations.⁴ 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) [7, 11, 12]. 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 [28], 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 gets inefficient as the number of variables increases.

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

3.4. Printers. SymPy has a rich collection of expression printers. 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)'
```

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

⁴In 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.

```
>>> pprint(Integral(sqrt(phi0 + 1), phi0))
      \sqrt{\phi_0 + 1} d(\phi_0)
334
    Alternately, the use unicode=False flag can be set, which causes the expression to be
335
    printed using only ASCII characters.
336
337
    >>> pprint(Integral(sqrt(phi0 + 1), phi0), use unicode=False)
338
339
340
       341
342
343
         The function latex returns a LATEX representation of an expression.
344
    >>> print(latex(Integral(sqrt(phi0 + 1), phi0)))
345
```

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 [29], the LATEX printer is used to render expressions using MathJax or IAT_FX, 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 any given printer, and allows custom objects to define their printing behavior for any printer. The code generation functionality of SymPy relies on this subsystem to convert expressions into code in various target programming languages.

3.5. Solvers. SymPy has a module of equation solvers that can handle ordinary differential equations, recurrence relationships, Diophantine equations, and algebraic equations. There is also rudimentary support for simple partial differential 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 essential input information from the user. The function signatures of solve and solveset are

```
solve(f, *symbols, **flags)
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```

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378 379 solveset(f, symbol, domain=S.Complexes)

 $\int \int \int d\pi \{0\} + 1\}\$

The domain parameter is typically either S.Complexes (the default) or S.Reals; the latter causes solveset to only return real solutions.

An important difference between the two functions is that the output API of solve varies with input (sometimes returning a Python list and sometimes a Python dictionary) whereas 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.

It should be noted that solve has an inconsistent output API for different types of inputs. For instance, depending on the input, it may return a Python list or a Python dictionary. On the other hand, solveset has a canonical output API: it always returns a SymPy set object.

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. Besides being an important feature in its own right, computations on matrices with symbolic entries are important for many algorithms within SymPy. The following code shows some basic usage of the Matrix class.

```
386 SymPy. The following code shows some b
387 >>> A = Matrix(2, 2, [x, x + y, y, x])
388 >>> A
389 Matrix([
390 [x, x + y],
391 [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 decomposition, Gauss-Jordan elimination, Cholesky decomposition, Moore-Penrose pseudoinverse, and adjugate matrix.

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

```
>>> A.eigenvals()
{x - sqrt(y*(x + y)): 1, x + sqrt(y*(x + y)): 1}
```

Internally these matrices store the elements as lists of lists, making it a dense representation.⁵ For storing sparse matrices, the SparseMatrix class can be used. Sparse matrices store their elements as a dictionary of keys.

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 implemented 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:

```
424 >>> Float(1.1)
```

1.10000000000000

 $^{^5}$ 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.

```
1.10000000000000008881784197001
427
    >>> Float("1.1", 30)
428
    429
     The evalf method converts a constant symbolic expression to a Float with the spec-
430
     ified precision, here 25 digits:
431
     >>> (pi + 1).evalf(25)
432
     4.141592653589793238462643
433
     Float numbers do not track their accuracy, and should be used with caution within
434
     symbolic expressions since familiar dangers of floating-point arithmetic apply [16]. A
     notorious case is that of catastrophic cancellation:
436
437
     >>> cos(exp(-100)).evalf(25) - 1
438
     Applying the evalf method to the whole expression solves this problem. Internally,
439
     evalf estimates the number of accurate bits of the floating-point approximation for
440
     each sub-expression, and adaptively increases the working precision until the esti-
441
     mated accuracy of the final result matches the sought number of decimal digits:
442
443
     >>> (cos(exp(-100)) - 1).evalf(25)
     -6.919482633683687653243407e-88
444
     The evalf method works with complex numbers and supports more complicated ex-
445
     pressions, such as special functions, infinite series, and integrals. The internal error
     tracking does not provide rigorous error bounds (in the sense of interval arithmetic)
447
448
     and cannot be used to accurately track uncertainty in measurement data; the sole pur-
     pose is to mitigate loss of accuracy that typically occurs when converting symbolic
449
     expressions to numerical values.
450
```

precision equivalent to 30 digits

4.1. The mpmath library. The implementation of arbitrary-precision floating-point arithmetic is supplied by the mpmath library. Originally, it was developed as a SymPy module but has subsequently 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:

```
457 >>> import mpmath

458 >>> mpmath.mp.dps = 30  # 30 digits of precision

459 >>> mpmath.mpf("0.1") + mpmath.exp(-50)

460 mpf('0.1000000000000000000192874984794')

461 >>> print(_) # pretty-printed

462 0.1000000000000000000192874985
```

>>> Float(1.1, 30)

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For pure numerical computing, it is convenient to use mpmath directly with from mpmath import *. Nevertheless, it is best to avoid such an import statement when using SymPy simultaneously, since the names of numerical functions such as exp will collide 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 [19] is installed, mpmath automatically uses the <code>gmpy.mpz</code> 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 [42, 2]. 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) [3]. 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 $G_{1,3}^{3,0}\left(0;\frac{1}{2},-1,-\frac{3}{2}|x\right)$ is a good test case [43]; 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:

```
494 >>> mpmath.mp.dps = 15

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

496 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

476

Symbolic integration and summation often produces hypergeometric and Meijer G-function closed forms (see Subsection 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 forces and torques. The dyadics are essentially reference frame-aware 3×3 tensors [41]. 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
523
     with respect to the A frame using Z-X-Z Euler Angles of magnitude \pi, \frac{\pi}{2}, and \frac{\pi}{3} rad,
524
     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
     >>> A = ReferenceFrame('A')
528
529
     >>> B = ReferenceFrame('B')
     >>> C = ReferenceFrame('C')
530
    >>> B.orient(A, 'body', (pi, pi/3, pi/4), 'zxz')
531
     >>> C.orient(B, 'axis', (pi/2, B.x))
532
    >>> v = 1*A.x + 2*B.z + 3*C.y
533
534
     A.x + 2*B.z + 3*C.y
     >>> v.express(A)
536
     A.x + 5*sqrt(3)/2*A.y + 5/2*A.z
```

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- **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 [22] and Kane's Method [21]. Lastly, there are automated linearization routines for constrained dynamical systems [30].
- **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 [37]: 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
559
560
    >>> from sympy.physics.quantum import Ket, qapply
561
    >>> A = Operator('A')
    >>> B = Operator('B')
562
    >>> C = Operator('C')
    >>> D = Operator('D')
564
565
    >>> a = Ket('a')
566
    >>> comm = Commutator(A, B)
567
    >>> comm
    [A,B]
568
    >>> gapply(Dagger(comm*a)).doit()
569
    -<a|*(Dagger(A)*Dagger(B) - Dagger(B)*Dagger(A))</pre>
570
```

Commutators can be expanded using common commutator identities:

```
572 >>> Commutator(C+B, A*D).expand(commutator=True)
573 -[A,B]*D - [A,C]*D + A*[B,D] + A*[C,D]
```

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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 [13].
- Quantum angular momentum [45]. 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 [25]. Multidimensional qubit states, and a full set of one- and two-qubit gates are provided and can be represented symbolically or as matrices/vectors. With these building blocks, it is possible to implement a number of basic quantum algorithms including the quantum Fourier transform, quantum error correction, quantum teleportation, Grover's algorithm, dense coding, etc. In addition, any quantum circuit may be plotted using the circuit_plot function (Figure 1).

Here are a few short examples of the quantum information and computing capabilities in sympy.physics.quantum. Start with a simple four-qubit state and flip the second qubit from the right using a Pauli-X gate:

```
596
    >>> from sympy.physics.quantum.qubit import Qubit
597
    >>> from sympy.physics.quantum.gate import XGate
    >>> q = Qubit('0101')
599
600
    >>> q
    |0101>
601
    >>> X = XGate(1)
602
    >>> qapply(X*q)
603
604
    |0111>
    Qubit states can also be used in adjoint operations, tensor products, inner/outer
605
606
    products:
    >>> Dagger(q)
607
608
    <0101|
    >>> ip = Dagger(q)*q
609
   >>> ip
610
611
    <0101 | 0101>
612
    >>> ip.doit()
613
    Quantum gates (unitary operators) can be applied to transform these states and then
614
    classical measurements can be performed on the results:
    >>> from sympy.physics.quantum.qubit import measure all
616
617
    >>> from sympy.physics.quantum.gate import H, X, Y, Z
    >>> c = H(0)*H(1)*Qubit('00')
618
619
620 H(0)*H(1)*|00>
    >>> q = qapply(c)
```

```
622 >>> measure_all(q)
623 [(|00>, 1/4), (|01>, 1/4), (|10>, 1/4), (|11>, 1/4)]
```

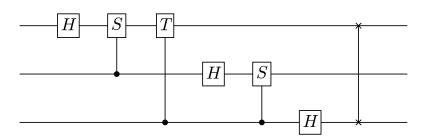


Fig. 1: The circuit diagram for a three-qubit quantum Fourier transform generated by SymPy.

```
Lastly, the following example demonstrates creating a three-qubit quantum Fourier
624
     transform, decomposing it into one- and two-qubit gates, and then generating a circuit
625
     plot for the sequence of gates (see Figure 1).
626
     >>> from sympy.physics.quantum.qft import QFT
627
     >>> from sympy.physics.quantum.circuitplot import circuit plot
628
     >>> fourier = QFT(0,3).decompose()
629
     >>> fourier
630
     SWAP(0,2)*H(0)*C((0),S(1))*H(1)*C((0),T(2))*C((1),S(2))*H(2)
631
     >>> c = circuit plot(fourier, ngubits=3)
632
```

 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 in a plethora of scientific disciplines. This allows SymPy to be used in a first-class way with other Python projects, including the scientific Python stack. Unlike many other CASs, SymPy is designed to be used in an extensible way: both as an end-user 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 of 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 (one area of work in this direction is SymEngine, a C++ symbolic manipulation library that is planned to be usable as 656 a alternative core for SymPy), improving the assumptions system, and improving the solvers module.

7. Acknowledgements. The Los Alamos National Laboratory is operated by Los Alamos National Security, LLC, for the National Nuclear Security Administration of the U.S. Department of Energy under Contract No. DE-AC52-06NA25396.

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 in which Google awards stipends to all students who successfully complete a requested free and opensource software coding project during the summer.

The author of this paper Francesco Bonazzi thanks the Deutsche Forschungsgemeinschaft (DFG) for its financial support via the International Research Training Group 1524 "Self-Assembled Soft Matter Nano-Structures at Interfaces."

8. References.

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