

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 a popular symbolic library for the scientific Python ecosystem. This paper presents the architecture of SymPy, a description of its features, and a discussion of select submodules. The supplementary material provide additional examples and further outline details of the architecture and features of SymPy.

1 INTRODUCTION

SymPy is a full featured computer algebra system (CAS) written in the Python [32] programming language. It is free and open source software, licensed under the 3-clause BSD license [49]. 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 [43]. 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.¹ Due in part to this focus, it has become a popular language for scientific computing and data science, with a broad ecosystem of libraries [37]. SymPy is itself used as a dependency by many libraries and tools to support research within a variety of domains, such as SageMath [58] (pure and applied mathematics), yt [64] (astronomy and astrophysics), PyDy [19] (multibody dynamics), and SfePy [10] (finite elements).

Unlike many CAS's, SymPy does not invent its own programming language. Python itself is used both for the internal implementation and end user interaction. By using the operator overloading functionality of Python, SymPy follows the embedded domain specific language paradigm proposed by Hudak [24]. 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 officially supports Python 2.6, 2.7 and 3.2–3.5.

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.

Being a library, SymPy does not have a built-in graphical user interface (GUI). However, SymPy exposes a rich interactive display system, and supports registering display formatters with Jupyter [29] frontends, including the Notebook and Qt Console, which will render SymPy expressions using MathJax [9] or L^AT_EX.

The remainder of this paper discusses key components of the SymPy library. Section 2 enumerates the features of SymPy and takes a closer look at some of the important ones. The section 3 looks at the numerical features of SymPy and its dependency library, mpmath. Section 4 looks at the domain specific physics submodules for performing symbolic and numerical calculations in classical mechanics and quantum mechanics. Section 5 discusses the architecture of SymPy. Section 6 looks at a selection of packages that depend on SymPy. Conclusions and future directions for SymPy are given in section 7. All examples in this paper use SymPy version 1.0 and mpmath version 0.19.

Additionally, the supplementary material takes a deeper look at a few SymPy topics. Supplement section 1 discusses the Gruntz algorithm, which SymPy uses to calculate symbolic limits. Sections 2–9 of the supplement discuss the series, logic, Diophantine equations, sets, statistics, category theory, tensor, and numerical simplification submodules of SymPy, respectively. Supplement section 10 provides additional examples for topics discussed in the main paper. Supplement section 11 discusses the SymPy Gamma project. Finally, section 12 of the supplement contains a

¹This paper assumes a moderate familiarity with the Python programming language.

97 brief comparison of SymPy with Wolfram Mathematica.
 98 The following statement imports all SymPy functions into the global Python namespace.²
 99 From here on, all examples in this paper assume that this statement has been executed.³

100 `>>> from sympy import *`

101 All the examples in this paper can be tested on [SymPy Live](https://live.sympy.org/), an online Python shell that
 102 uses the Google App Engine [11] to execute SymPy code. SymPy Live is also integrated into the
 103 SymPy documentation at <http://docs.sympy.org>.

104 2 OVERVIEW OF CAPABILITIES

105 This section gives a basic introduction of SymPy, and lists its features. A few features—
 106 assumptions, simplification, calculus, polynomials, printers, solvers, and matrices—are core
 107 components of SymPy and are discussed in depth. Many other features are discussed in depth in
 108 the supplementary material.

109 2.1 Basic Usage

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

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

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

120 Expressions are created from symbols using Python’s mathematical syntax. For instance, the
 121 following Python code creates the expression $(x^2 - 2x + 3)/y$. Note that the expression remains
 122 unevaluated: it is represented symbolically.

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

124 `(x**2 - 2*x + 3)/y`

125 2.2 List of Features

126 Although SymPy’s extensive feature set cannot be covered in depth in this paper, bedrock areas,
 127 that is, those areas that are used throughout the library, are discussed in their own subsections
 128 below. Additionally, Table 1 gives a compact listing of all major capabilities present in the
 129 SymPy codebase. This grants a sampling from the breadth of topics and application domains
 130 that SymPy services. Unless stated otherwise, all features noted in Table 1 are symbolic in
 131 nature. Numeric features are discussed in Section 3.

Table 1. SymPy Features and Descriptions.

Feature (submodules)	Description
Calculus (<code>sympy.core</code> , <code>sympy.calculus</code> , <code>sympy.integrals</code> , <code>sympy.series</code>)	Algorithms for computing derivatives, integrals, and limits.

²`import *` has been used here to aid the readability of the paper, but is best to avoid such wildcard import statements in production code, as they make it unclear which names are present in the namespace. Furthermore, imported names could clash with already existing imports from another package. For example, SymPy, the standard Python `math` library, and NumPy all define the `exp` function, but only the SymPy one will work with SymPy symbolic expressions.

³ The three greater-than signs denote the user input for the Python interactive session, with the result, if there is one, shown on the next line.

Category Theory (<code>sympy.categories</code>) Code Generation (<code>sympy.printing</code> , <code>sympy.codegen</code>)	Representation of objects, morphisms, and diagrams. Tools for drawing diagrams with Xy-pic [48]. Generation of compilable and executable code in a variety of different programming languages from expressions directly. Target languages include C, Fortran, Julia, JavaScript, Mathematica, MATLAB and Octave, Python, and Theano.
Combinatorics & Group Theory (<code>sympy.combinatorics</code>) Concrete Math (<code>sympy.concrete</code>)	Permutations, combinations, partitions, subsets, various permutation groups (such as polyhedral, Rubik, symmetric, and others), Gray codes [36], and Prufer sequences [4]. 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 [42] for two univariate polynomials.
Cryptography (<code>sympy.crypto</code>)	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 (<code>sympy.diffgeom</code>)	Representations of manifolds, metrics, tensor products, and coordinate systems in Riemannian and pseudo-Riemannian geometries [52].
Geometry (<code>sympy.geometry</code>)	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 (<code>sympy.liealgebras</code>) Logic (<code>sympy.logic</code>)	Representations of Lie algebras and root systems. Boolean expressions, equivalence testing, satisfiability, and normal forms.
Matrices (<code>sympy.matrices</code>)	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 Expressions (<code>sympy.matrices.expressions</code>)	Matrices with symbolic dimensions (unspecified entries). Block matrices.
Number Theory (<code>sympy.ntheory</code>)	Prime number generation, primality testing, integer factorization, continued fractions, Egyptian fractions, modular arithmetic, quadratic residues, partitions, binomial and multinomial coefficients, prime number tools, hexadecimal digits of π , and integer factorization.
Plotting (<code>sympy.plotting</code>)	Hooks for visualizing expressions via matplotlib [25] or as text drawings when lacking a graphical back-end. 2D function plotting, 3D function plotting, and 2D implicit function plotting are supported.
Polynomials (<code>sympy.polys</code>)	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 (<code>sympy.printing</code>)	Functions for printing SymPy expressions in the terminal with ASCII or Unicode characters and converting SymPy expressions to \LaTeX and MathML.
Quantum Mechanics (<code>sympy.physics.quantum</code>)	Quantum states, bra-ket notation, operators, basis sets, representations, tensor products, inner products, outer products, commutators, anticommutators, and specific quantum system implementations.

Series (<code>sympy.series</code>)	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 (<code>sympy.sets</code>)	Representations of empty, finite, and infinite sets (including special sets such as the natural, integer, and complex numbers). Operations on sets such as union, intersection, Cartesian product, and building sets from other sets are supported.
Simplification (<code>sympy.simplify</code>)	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 (<code>sympy.solvers</code>)	Functions for symbolically solving equations, systems of equations, both linear and non-linear, inequalities, ordinary differential equations, partial differential equations, Diophantine equations, and recurrence relations.
Special Functions (<code>sympy.functions</code>)	Implementations of 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 (<code>sympy.stats</code>)	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 [47].
Tensors (<code>sympy.tensor</code>)	Symbolic manipulation of indexed objects.
Vectors (<code>sympy.vector</code>)	Basic operations on vectors and differential calculus with respect to 3D Cartesian coordinate systems.

2.3 Assumptions

The assumptions system allows users to specify that symbols have certain common mathematical properties, such as being positive, imaginary, or integer. SymPy is careful to never perform simplifications on an expression unless the assumptions allow them. For instance, the simplification $\sqrt{t^2} = t$ holds if t is nonnegative ($t \geq 0$), but it does not hold for a general complex t .⁴

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

```
>>> t = Symbol('t')
>>> sqrt(t**2)
sqrt(t**2)
```

By assuming the most general case, that t is 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.

⁴The correct identity that holds for all complex t is $\sqrt{t^2} = (-1)^{\lfloor \frac{\pi - 2 \arg t}{2\pi} \rfloor} t$, where $\arg t$ is the argument function and both sides of the identity assume the usual principal branch with the branch cut along the negative real axis.

```

147 >>> t = Symbol('t', positive=True)
148 >>> sqrt(t**2)
149 t

```

Some of the common assumptions are `negative`, `real`, `nonpositive`, `integer`, `prime` and `commutative`.⁵ Assumptions on any SymPy 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`. Note that `False` is returned if the SymPy object doesn't or can't have the assumption. For example, both `I.is_real` and `I.is_prime` return `False` for the imaginary unit `I`.

`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. `None` could also mean that not enough is known or implemented to compute the given fact. For instance, `(pi + E).is_irrational` gives `None`—indeed, the rationality of $\pi + e$ is an open problem in mathematics [31].

Basic implications between the facts are used to deduce assumptions. Deductions are made using the Rete algorithm [13].⁶ For instance, the assumptions system knows that being an integer implies being rational.

```

169 >>> i = Symbol('i', integer=True)
170 >>> i.is_rational
171 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 `None`).

2.4 Simplification

The generic way to simplify an expression is by calling the `simplify` function. It must be emphasized that simplification is not a rigorously defined mathematical operation [34]. The `simplify` function applies several simplification routines along with heuristics to make the output expression “simple”.⁷

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.

Examples for these simplification functions can be found in section 10 of the supplementary material.

⁵SymPy assumes that two expressions A and B commute with each other multiplicatively, that is, $A \cdot B = B \cdot A$, unless they both have `commutative=False`. Many algorithms in SymPy require special consideration to work correctly with noncommutative products.

⁶For historical reasons, this algorithm is distinct from the `sympy.logic` submodule, which is discussed in section 3 of the supplementary material. SymPy also has an experimental assumptions system which stores facts separate from objects, and uses `sympy.logic` and a SAT solver for deduction. We will not discuss this system here.

⁷The `measure` parameter of the `simplify` function lets the user specify the Python function used to determine how complex an expression is. The default `measure` function returns the total number of operations in the expression.

Table 2. Some SymPy Simplification Functions

<code>expand</code>	expand the expression
<code>factor</code>	factor a polynomial into irreducibles
<code>collect</code>	collect polynomial coefficients
<code>cancel</code>	rewrite a rational function as p/q with common factors canceled
<code>apart</code>	compute the partial fraction decomposition of a rational function
<code>trigsimp</code>	simplify trigonometric expressions [18]
<code>hyperexpand</code>	expand hypergeometric functions [44, 45]

2.5 Calculus

SymPy provides all the basic operations of calculus, such as calculating limits, derivatives, integrals, or summations.

Limits are computed with the `limit` function, using the Gruntz algorithm [22] for computing symbolic limits and heuristics (a description of the Gruntz algorithm may be found in section 1 of the supplementary material). For example, the following computes $\lim_{x \rightarrow \infty} x \sin(\frac{1}{x}) = 1$. Note that SymPy denotes ∞ as `oo` (two lower case “o”s).

```
>>> limit(x*sin(1/x), x, oo)
1
```

As a more complex example, SymPy computes

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

```
>>> limit((2*exp((1-cos(x))/sin(x))-1)**(sinh(x)/atan(x)**2), x, 0)
E
```

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

```
>>> diff(sin(x)*exp(x), x)
exp(x)*sin(x) + exp(x)*cos(x)
```

Integrals are calculated with the `integrate` function. SymPy implements a combination of the Risch algorithm [7], table lookups, a reimplement of Manuel Bronstein’s “Poor Man’s Integrator” [6], and an algorithm for computing integrals based on Meijer G-functions [44, 45]. 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

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

```
>>> s, t = symbols('s t', positive=True)
>>> integrate(exp(-s*t)*log(t), (t, 0, oo)).simplify()
-(log(s) + EulerGamma)/s
>>> integrate((-2*x**2*(log(x) + 1)*exp(x**2) +
... (exp(x**2) + 1)**2)/(x*(exp(x**2) + 1)**2*(log(x) + 1)), x)
log(log(x) + 1) + 1/(exp(x**2) + 1)
```


Summations are computed with the `summation` function, which uses a combination of Gosper's algorithm [21], an algorithm that uses Meijer G-functions [44, 45], and heuristics. Products are computed with `product` function via a suite of heuristics.

```

212 >>> i, n = symbols('i n')
213 >>> summation(2**i, (i, 0, n - 1))
214 2**n - 1
215 >>> summation(i*factorial(i), (i, 1, n))
216 n*factorial(n) + factorial(n) - 1

```

Series expansions are computed with the `series` function. This example computes the power series of $\sin(x)$ around $x = 0$ up to x^6 .

```

219 >>> series(sin(x), x, 0, 6)
220 x - x**3/6 + x**5/120 + O(x**6)

```

Section 2 of the supplementary material discusses series expansions methods in more depth. Integrals, derivatives, summations, products, and limits that cannot be computed return unevaluated objects. These can also be created directly if the user chooses.

```

224 >>> integrate(x**x, x)
225 Integral(x**x, x)
226 >>> Sum(2**i, (i, 0, n - 1))
227 Sum(2**i, (i, 0, n - 1))

```

2.6 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.⁸ 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) [8, 14, 15]. 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 [38], are better expressed when the representation is dense. The dense multivariate representation is specifically a recursively-dense representation, where polynomials in $K[x_0, x_1, \dots, x_n]$ are viewed as a polynomials in $K[x_0][x_1] \dots [x_n]$. 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` submodule can be found in section 10 of the supplementary material.

2.7 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

⁸In 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.

far. The `str` form of an expression is valid Python and roughly matches what a user would type to enter the expression.⁹

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

A two-dimensional (2D) textual representation of the expression can be printed with 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.

```
>>> pprint(Integral(sqrt(phi0 + 1), phi0))

$$\int \sqrt{\varphi_0 + 1} \, d(\varphi_0)$$

```

Alternately, the `use_unicode=False` flag can be set, which causes the expression to be printed using only ASCII characters.

```
>>> pprint(Integral(sqrt(phi0 + 1), phi0), use_unicode=False)
/
|
| _____
| \ / phi0 + 1 d(phi0)
|
/
```

The function `latex` returns a \LaTeX representation of an expression.

```
>>> print(latex(Integral(sqrt(phi0 + 1), phi0)))
\int \sqrt{\phi_0 + 1}\, d\phi_0
```

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 [40], 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, which allows extending any given printer, and also 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.

2.8 Solvers

SymPy has equation solvers that can handle ordinary differential equations, recurrence relationships, Diophantine equations¹⁰, 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

⁹Many Python libraries distinguish the `str` form of an object, which is meant to be human-readable, and the `repr` form, which is meant to be valid Python that recreates the object. In SymPy, `str(expr) == repr(expr)`. In other words, the string representation of an expression is designed to be compact, human-readable, and valid Python code that could be used to recreate the expression. As noted in section 5.1, the `srepr` function prints the exact, verbose form of an expression.

¹⁰See section 4 of the supplementary material for an in depth discussion on the Diophantine submodule.

```

296 solve(f, *symbols, **flags)
297 solveset(f, symbol, domain=S.Complexes)

```

298 The `domain` parameter can be any set from the `sympy.sets` module (see section 5 of the supplementary material for details on `sympy.sets`), but is typically either `S.Complexes` (the default) or `S.Reals`; the latter causes `solveset` to only return real solutions.

301 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.

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

306 `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`, including multivariate systems, and some transcendental equations.

309 Some examples for `solveset` and `solve` can be found in section 10 of the supplementary material.

311 2.9 Matrices

312 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.

```

315 >>> A = Matrix([[x, x + y], [y, x]])
316 >>> A
317 Matrix([
318 [x, x + y],
319 [y, x]])

```

320 SymPy matrices support common symbolic linear algebra manipulations, including matrix addition, multiplication, exponentiation, computing determinants, solving linear systems, singular values, and computing inverses using LU decomposition, LDL decomposition, Gauss-Jordan elimination, Cholesky decomposition, Moore-Penrose pseudoinverse, or adjugate matrices.

324 All operations are performed symbolically. For instance, eigenvalues are computed by generating the characteristic polynomial using the Berkowitz algorithm and then finding its zeros using polynomial routines.

```

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

```

329 Internally these matrices store the elements as Lists of Lists (LIL) [27], meaning the matrix is stored as a list of lists of entries (effectively, the input format used to create the matrix `A` above), making it a dense representation.¹¹ For storing sparse matrices, the `SparseMatrix` class can be used. Sparse matrices store their elements in Dictionary of Keys (DOK) format, meaning that the entries are stored as a `dict` of (`row`, `column`) pairs mapping to the elements.

334 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.

338 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`.

341 When symbolic matrices are combined with the assumptions submodule for logical inference, they provide powerful reasoning over invertibility, semi-definiteness, orthogonality, etc., which are valuable in the construction of numerical linear algebra systems [46].

344 More examples for `Matrix` and `BlockMatrix` may be found in section 10 of the supplementary material.

¹¹Similar to the polynomials submodule, dense here means that all entries are stored in memory, contrasted with a sparse representation where only nonzero entries are stored.

3 NUMERICS

While SymPy primarily focuses on symbolics, it is impossible to have a complete symbolic system without the ability to numerically evaluate expressions. Many operations directly use numerical evaluation, such as plotting a function, or solving an equation numerically. Beyond this, certain purely symbolic operations require numerical evaluation to effectively compute. For instance, determining the truth value of $e + 1 > \pi$ is most conveniently done by numerically evaluating both sides of the inequality and checking which is larger.

3.1 Floating-Point Numbers

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:

```
>>> Float(1.1)
1.1000000000000000
>>> Float(1.1, 30) # precision equivalent to 30 digits
1.100000000000000008881784197001
>>> Float("1.1", 30)
1.10000000000000000000000000000000
```

The `evalf` method converts a constant symbolic expression to a `Float` with the specified precision, here 25 digits:

```
>>> (pi + 1).evalf(25)
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 [20]. A notorious case is that of catastrophic cancellation:

```
>>> cos(exp(-100)).evalf(25) - 1
0
```

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 each sub-expression, and adaptively increases the working precision until the estimated accuracy of the final result matches the sought number of decimal digits:

```
>>> (cos(exp(-100)) - 1).evalf(25)
-6.919482633683687653243407e-88
```

The `evalf` method works with complex numbers and supports more complicated expressions, such as special functions, infinite series, and integrals. The internal error tracking does not provide rigorous error bounds (in the sense of interval arithmetic) and cannot be used to accurately track uncertainty in measurement data; the sole purpose is to mitigate loss of accuracy that typically occurs when converting symbolic expressions to numerical values.

3.2 The mpmath Library

The implementation of arbitrary-precision floating-point arithmetic is supplied by the `mpmath` library [26]. Originally, it was developed as a SymPy submodule 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:

4.1 Classical Mechanics

One of the core domains that SymPy supports is the physics of classical mechanics. This is in turn separated into two distinct components: vector algebra and mechanics.

4.1.1 Vector Algebra

The `sympy.physics.vector` submodule 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. The vector and dyadic objects both 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 [53]. 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 π , $\frac{\pi}{2}$, and $\frac{\pi}{3}$, 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 $\frac{\pi}{2}$.

```
>>> from sympy.physics.vector import ReferenceFrame
>>> A, B, C = symbols('A B C', cls=ReferenceFrame)
>>> B.orient(A, 'body', (pi, pi/3, pi/4), 'zxz')
>>> C.orient(B, 'axis', (pi/2, B.x))
>>> v = 1*A.x + 2*B.z + 3*C.y
>>> v
A.x + 2*B.z + 3*C.y
>>> v.express(A)
A.x + 5*sqrt(3)/2*A.y + 5/2*A.z
```

4.1.2 Mechanics

The `sympy.physics.mechanics` submodule utilizes the `sympy.physics.vector` submodule 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 submodule offers two automated methods for formulating the equations of motion based on Lagrangian Dynamics [30] and Kane's Method [28]. Lastly, there are automated linearization routines for constrained dynamical systems [41].

4.2 Quantum Mechanics

The `sympy.physics.quantum` submodule has extensive capabilities to solve problems in quantum mechanics, using Python objects to represent the different mathematical objects relevant in quantum theory [50]: 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
>>> A, B, C, D = symbols('A B C D', cls=Operator)
>>> a = Ket('a')
```

```

495 >>> comm = Commutator(A, B)
496 >>> comm
497 [A,B]
498 >>> qapply(Dagger(comm*a)).doit()
499 -<a|*(Dagger(A)*Dagger(B) - Dagger(B)*Dagger(A))

```

500 Commutators can be expanded using common commutator identities:

```

501 >>> Commutator(C+B, A*D).expand(commutator=True)
502 -[A,B]*D - [A,C]*D + A*[B,D] + A*[C,D]

```

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

- 505 • Many of the exactly solvable quantum systems, including simple harmonic oscillator states
506 and raising/lowering operators, infinite square well states, and 3D position and momentum
507 operators and states.
- 508 • Second quantized formalism of non-relativistic many-body quantum mechanics [16].
- 509 • Quantum angular momentum [65]. Spin operators and their eigenstates can be represented
510 in any basis and for any quantum numbers. A rotation operator representing the Wigner
511 D-matrix, which may be defined symbolically or numerically, is also implemented to rotate
512 spin eigenstates. Functionality for coupling and uncoupling of arbitrary spin eigenstates is
513 provided, including symbolic representations of Clebsch-Gordon coefficients and Wigner
514 symbols.
- 515 • Quantum information and computing [35]. Multidimensional qubit states, and a full
516 set of one- and two-qubit gates are provided and can be represented symbolically or as
517 matrices/vectors. With these building blocks, it is possible to implement a number of basic
518 quantum algorithms including the quantum Fourier transform, quantum error correction,
519 quantum teleportation, Grover's algorithm, dense coding, etc. In addition, any quantum
520 circuit may be plotted using the `circuit_plot` function (Figure 1).

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

```

524 >>> from sympy.physics.quantum.qubit import Qubit
525 >>> from sympy.physics.quantum.gate import XGate
526 >>> q = Qubit('0101')
527 >>> q
528 |0101>
529 >>> X = XGate(1)
530 >>> qapply(X*q)
531 |0111>

```

532 Qubit states can also be used in adjoint operations, tensor products, inner/outer products:

```

533 >>> Dagger(q)
534 <0101|
535 >>> ip = Dagger(q)*q
536 >>> ip
537 <0101|0101>
538 >>> ip.doit()
539 1

```

540 Quantum gates (unitary operators) can be applied to transform these states and then classical
541 measurements can be performed on the results:

```

542 >>> from sympy.physics.quantum.qubit import measure_all
543 >>> from sympy.physics.quantum.gate import H, X, Y, Z
544 >>> c = H(0)*H(1)*Qubit('00')
545 >>> c
546 H(0)*H(1)*|00>
547 >>> q = qapply(c)
548 >>> measure_all(q)
549 [(|00>, 1/4), (|01>, 1/4), (|10>, 1/4), (|11>, 1/4)]

```



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

550 Lastly, the following example demonstrates creating a three-qubit quantum Fourier transform,
 551 decomposing it into one- and two-qubit gates, and then generating a circuit plot for the sequence
 552 of gates (see Figure 1).

```

553 >>> from sympy.physics.quantum.qft import QFT
554 >>> from sympy.physics.quantum.circuitplot import circuit_plot
555 >>> fourier = QFT(0,3).decompose()
556 >>> fourier
557 SWAP(0,2)*H(0)*C((0),S(1))*H(1)*C((0),T(2))*C((1),S(2))*H(2)
558 >>> c = circuit_plot(fourier, nqubits=3)

```

559 5 ARCHITECTURE

560 Software architecture is of central importance in any large software project because it establishes
 561 predictable patterns of usage and development [51]. This section describes the essential structural
 562 components of SymPy, provides justifications for the design decisions that have been made, and
 563 gives example user-facing code as appropriate.

564 5.1 The Core

565 A computer algebra system stores mathematical expressions as data structures. For example,
 566 the mathematical expression $x + y$ is represented as a tree with three nodes, $+$, x , and y ,
 567 where x and y are ordered children of $+$. As users manipulate mathematical expressions with
 568 traditional mathematical syntax, the CAS manipulates the underlying data structures. Symbolic
 569 computations such as integration, simplification, etc. are all functions that consume and produce
 570 expression trees.

571 In SymPy every symbolic expression is an instance of the class **Basic**,¹² the superclass of all
 572 SymPy types providing common methods to all SymPy tree-elements, such as traversals. The

¹²Some internal classes, such as those used in the polynomial submodule, do not follow this rule for efficiency reasons.

573 children of a node in the tree are held in the `args` attribute. A leaf node in the expression tree
574 has empty `args`.

575 For example, consider the expression $xy + 2$:

```
576 >>> x, y = symbols('x y')
577 >>> expr = x*y + 2
```

578 By order of operations, the parent of the expression tree for `expr` is an addition. It is of type
579 `Add`. The child nodes of `expr` are 2 and `x*y`.

```
580 >>> type(expr)
581 <class 'sympy.core.add.Add'>
582 >>> expr.args
583 (2, x*y)
```

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

```
587 >>> expr.args[0]
588 2
589 >>> type(expr.args[0])
590 <class 'sympy.core.numbers.Integer'>
591 >>> expr.args[0].args
592 ()
```

593 Symbols or symbolic constants, like e or π , are other examples of leaf nodes.

```
594 >>> exp(1)
595 E
596 >>> exp(1).args
597 ()
598 >>> x.args
599 ()
```

600 A useful way to view an expression tree is using the `srepr` function, which returns a string
601 representation of an expression as valid Python code¹³ with all the nested class constructor calls
602 to create the given expression.

```
603 >>> srepr(expr)
604 "Add(Mul(Symbol('x'), Symbol('y')), Integer(2))"
```

605 Every SymPy expression satisfies a key identity invariant:

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

607 This means that expressions are rebuildable from their `args`.¹⁴ Note that in SymPy the `==`
608 operator represents exact structural equality, not mathematical equality. This allows testing if
609 any two expressions are equal to one another as expression trees. For example, even though
610 $(x+1)^2$ and $x^2 + 2x + 1$ are equal mathematically, SymPy gives

```
611 >>> (x + 1)**2 == x**2 + 2*x + 1
612 False
```

¹³ The `dotprint` function from the `sympy.printing.dot` submodule prints output to dot format, which can be rendered with Graphviz to visualize expression trees graphically.

¹⁴`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.

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

615 Another important property of SymPy expressions is that they are immutable. This simplifies
616 the design of SymPy, and enables expression interning. It also enables expressions to be hashed,
617 which allows expressions to be used as keys in Python dictionaries, and is used to implement
618 caching in SymPy.

619 Python allows classes to override mathematical operators. The Python interpreter translates
620 the above $x*y + 2$ to, roughly, `(x.__mul__(y)).__add__(2)`. Both `x` and `y`, returned from the
621 `symbols` function, are `Symbol` instances. The `2` in the expression is processed by Python as a
622 literal, and is stored as Python's built in `int` type. When `2` is passed to the `__add__` method
623 of `Symbol`, it is converted to the SymPy type `Integer(2)` before being stored in the resulting
624 expression tree. In this way, SymPy expressions can be built in the natural way using Python
625 operators and numeric literals.

626 5.2 Extensibility

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

632 The typical way to create a custom SymPy object is to subclass an existing SymPy class,
633 usually `Basic`, `Expr`, or `Function`. As it was stated before, all SymPy classes used for expression
634 trees should be subclasses of the base class `Basic`. `Expr` is the `Basic` subclass for mathematical
635 objects that can be added and multiplied together. The most commonly seen classes in SymPy
636 are subclasses of `Expr`, including `Add`, `Mul`, and `Symbol`. Instances of `Expr` typically represent
637 complex numbers, but may also include other “rings”, like matrix expressions. Not all SymPy
638 classes are subclasses of `Expr`. For instance, logic expressions, such as `And(x, y)`, are subclasses
639 of `Basic` but not of `Expr`.¹⁵

640 The `Function` class is a subclass of `Expr` which makes it easier to define mathematical functions
641 called with arguments. This includes named functions like $\sin(x)$ and $\log(x)$ as well as undefined
642 functions like $f(x)$. Subclasses of `Function` should define a class method `eval`, which returns
643 an evaluated value for the function application (usually an instance of some other class, e.g., a
644 `Number`), or `None` if for the given arguments it should not be automatically evaluated.

645 Many SymPy functions perform various evaluations down the expression tree. Classes
646 define their behavior in such functions by defining a relevant `_eval_*` method. For instance,
647 an object can indicate to the `diff` function how to take the derivative of itself by defining the
648 `_eval_derivative(self, x)` method, which may in turn call `diff` on its args. (Subclasses of
649 `Function` should implement the `fdiff` method instead; it returns the derivative of the function
650 without considering the chain rule.) The most common `_eval_*` methods relate to the assumptions:
651 `_eval_is_assumption` is used to deduce *assumption* on the object.

652 Listing 1 presents an example of this extensibility. It gives a stripped down version of the
653 `gamma` function $\Gamma(x)$ from SymPy. The methods defined allow it to evaluate itself on positive
654 integer arguments, define the real assumption, allow it to be rewritten in terms of factorial (with
655 `gamma(x).rewrite(factorial)`), and allow it to be differentiated. `self.func` is used throughout
656 instead of referencing `gamma` explicitly so that potential subclasses of `gamma` can reuse the methods.

Listing 1. A minimal implementation of `sympy.gamma`.

```
657 from sympy import Function, Integer, factorial, polygamma
658
659 class gamma(Function):
660     @classmethod
661     def eval(cls, arg):
662         if isinstance(arg, Integer) and arg.is_positive:
663             return factorial(arg - 1)
```

¹⁵See section 3 of the supplementary material for more information on the `sympy.logic` submodule.

```

664
665     def _eval_is_real(self):
666         x = self.args[0]
667         # noninteger means real and not integer
668         if x.is_positive or x.is_noninteger:
669             return True
670
671     def _eval_rewrite_as_factorial(self, z):
672         return factorial(z - 1)
673
674     def fdiff(self, argindex=1):
675         from sympy.core.function import ArgumentIndexError
676         if argindex == 1:
677             return self.func(self.args[0])*polygamma(0, self.args[0])
678         else:
679             raise ArgumentIndexError(self, argindex)

```

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

682 5.3 Performance

683 Due to being written in pure Python without the use of extension modules, SymPy's performance
684 characteristics are generally poorer than that of its commercial competitors. For many appli-
685 cations, the performance of SymPy, as measured by clock cycles, memory usage, and memory
686 layout, is sufficient. However, the boundaries for when SymPy's pure Python strategy becomes
687 insufficient are when the user requires handling of very long expressions or many small expressions.
688 Where this boundray lies depends on the system at hand, but tends to be within the range of
689 10^4 – 10^6 symbols for modern computers.

690 For this reason, a new project called SymEngine [60] has been started. The aim of this
691 project is to develop a library with better performance characteristics for symbolic manipulation.
692 SymEngine is a pure C++ library, which allows it fine-grained control over the memory layout
693 of expressions. SymEngine has thin wrappers to other languages (Python, Ruby, Julia, etc.). Its
694 aim is to be the fastest symbolic manipulation library. Preliminary benchmarks suggest that
695 SymEngine performs as well as its commercial and open source competitors.

696 The development version of SymPy has recently started to use SymEngine as an optional
697 backend, initially in `sympy.physics.mechanics` only. Future work will involve allowing more
698 algorithms in SymPy to use SymEngine as a backend.

699 6 PROJECTS THAT DEPEND ON SYMPY

700 There are several projects that depend on SymPy as a library for implementing a part of their
701 functionality. A selection of these projects are listed in Table 3.

Table 3. Selected projects that depend on SymPy.

Project name	Description
SymPy Gamma	An open source analog of Wolfram Alpha that uses SymPy [61]. There is more information about SymPy Gamma in section 11 of the supplementary material.
Cadabra	A CAS designed specifically for the resolution of problems encountered in field theory [39].
GNU Octave Symbolic Package	An implementation of a symbolic toolbox for Octave using SymPy [59].
SymPy.jl	A Julia interface to SymPy, provided using PyCall [62].
Mathics	A free, online CAS featuring Mathematica compatible syntax and functions [56].

Mathpix	An iOS App that detects handwritten math as input and uses SymPy Gamma to evaluate the math input and generate the relevant steps to solve the problem [33].
IKFast	A robot kinematics compiler provided by OpenRAVE [12].
SageMath	A free open-source mathematics software system, which builds on top of many existing open-source packages, including SymPy [58].
PyDy	Multibody Dynamics with Python [19].
galgebra	A Python package for geometric algebra (previously <code>sympy.galgebra</code>) [5].
yt	A Python package for analyzing and visualizing volumetric data [64].
SfePy	A Python package for solving partial differential equations (PDEs) in 1D, 2D, and 3D by the finite element (FE) method [66, 10].
Quameon	Quantum Monte Carlo in Python [57].
Lcapy	An experimental Python package for teaching linear circuit analysis [55].

7 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. It can be used in a first-class way with other Python projects, including the scientific Python stack.

SymPy supports a wide array of mathematical facilities. These include functions for assuming and deducing common mathematical facts, simplifying expressions, performing common calculus operations, manipulating polynomials, pretty printing expressions, solving equations, and representing symbolic matrices. Other supported facilities include discrete math, concrete math, plotting, geometry, statistics, sets, series, vectors, combinatorics, group theory, code generation, tensors, Lie algebras, cryptography, and special functions. SymPy has strong support for arbitrary precision numerics, backed by the mpmath package. Additionally, SymPy contains submodules targeting certain specific physics domains, such as classical mechanics and quantum mechanics. This breadth of domains has been engendered by a strong and vibrant user community. Anecdotally, many of these users chose SymPy because of its ease of access. SymPy is a dependency of many external projects across a wide spectrum of domains.

SymPy expressions are immutable trees of Python objects. Unlike many other CAS's, SymPy is designed to be used in an extensible way: both as an end-user application and as a library. SymPy uses Python both as the internal language and the user language. This permits users to access the same methods used by the library itself in order to extend it for their needs.

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

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