

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 ?? discusses the Gruntz algorithm, which SymPy uses to calculate symbolic limits. Sections ??–?? of the supplement discuss the series, logic, Diophantine equations, sets, statistics, category theory, tensor, and numerical simplification submodules of SymPy, respectively. Supplement section ?? provides additional examples for topics discussed in the main paper. Supplement section ?? discusses the SymPy Gamma project. Finally, section ?? of the

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

97 supplement contains a 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://www.sympy.org/en/index.html), 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 the supplement.

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 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 the supplement). 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 reimplementation 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.

```
>>> i, n = symbols('i n')
>>> summation(2**i, (i, 0, n - 1))
2**n - 1
>>> summation(i*factorial(i), (i, 1, n))
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 .

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

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.

```
>>> integrate(x**x, x)
Integral(x**x, x)
>>> Sum(2**i, (i, 0, n - 1))
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 the supplement.

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.

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

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

259 A two-dimensional (2D) textual representation of the expression can be printed with
 260 monospace fonts via `pprint`. Unicode characters are used for rendering mathematical sym-
 261 bols such as integral signs, square roots, and parentheses. Greek letters and subscripts in symbol
 262 names that have Unicode code points associated are also rendered automatically.

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

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

```

263
 264 Alternately, the `use_unicode=False` flag can be set, which causes the expression to be printed
 265 using only ASCII characters.

```
266 >>> pprint(Integral(sqrt(phi0 + 1), phi0), use_unicode=False)
267 /
268 |
269 | _____
270 | \ / phi0 + 1 d(phi0)
271 |
272 /
```

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

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

276 Users are encouraged to run the `init_printing` function at the beginning of interactive
 277 sessions, which automatically enables the best pretty printing supported by their environment.
 278 In the Jupyter Notebook or Qt Console [40], the \LaTeX printer is used to render expressions
 279 using MathJax or \LaTeX , if it is installed on the system. The 2D text representation is used
 280 otherwise.

281 Other printers such as MathML are also available. SymPy uses an extensible printer subsystem,
 282 which allows extending any given printer, and also allows custom objects to define their printing
 283 behavior for any printer. The code generation functionality of SymPy relies on this subsystem
 284 to convert expressions into code in various target programming languages.

285 2.8 Solvers

286 SymPy has equation solvers that can handle ordinary differential equations, recurrence relation-
 287 ships, Diophantine equations¹⁰, and algebraic equations. There is also rudimentary support for
 288 simple partial differential equations.

289 There are two functions for solving algebraic equations in SymPy: `solve` and `solveset`.
 290 `solveset` has several design changes with respect to the older `solve` function. This distinction
 291 is present in order to resolve the usability issues with the previous `solve` function API while
 292 maintaining backward compatibility with earlier versions of SymPy. `solveset` only requires
 293 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 the supplementary material for an in depth discussion on the Diophantine submodule.

```

294 solve(f, *symbols, **flags)
295 solveset(f, symbol, domain=S.Complexes)

```

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

299 An important difference between the two functions is that the output API of `solve` varies
 300 with input (sometimes returning a Python list and sometimes a Python dictionary) whereas
 301 `solveset` always returns a SymPy set object.

302 Both functions implicitly assume that expressions are equal to 0. For instance, `solveset(x -`
 303 `1, x)` solves $x - 1 = 0$ for x .

304 `solveset` is under active development as a planned replacement for `solve`. There are certain
 305 features which are implemented in `solve` that are not yet implemented in `solveset`, including
 306 multivariate systems, and some transcendental equations.

307 Some examples for `solveset` and `solve` can be found in the supplement.

308 2.9 Matrices

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

```

312 >>> A = Matrix([[x, x + y], [y, x]])
313 >>> A
314 Matrix([
315 [x, x + y],
316 [y,      x]])

```

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

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

```

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

```

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

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

335 Block matrices are also implemented in SymPy. `BlockMatrix` elements can be any matrix ex-
 336 pression, including explicit matrices, matrix symbols, and other block matrices. All functionalities
 337 of matrix expressions are also present in `BlockMatrix`.

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

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

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.

342 3 NUMERICS

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

349 3.1 Floating-Point Numbers

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

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

```
356 >>> Float(1.1)
357 1.1000000000000000
358 >>> Float(1.1, 30) # precision equivalent to 30 digits
359 1.100000000000000008881784197001
360 >>> Float("1.1", 30)
361 1.100000000000000000000000000000
```

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

```
364 >>> (pi + 1).evalf(25)
365 4.141592653589793238462643
```

366 `Float` numbers do not track their accuracy, and should be used with caution within symbolic
367 expressions since familiar dangers of floating-point arithmetic apply [20]. A notorious case is
368 that of catastrophic cancellation:

```
369 >>> cos(exp(-100)).evalf(25) - 1
370 0
```

371 Applying the `evalf` method to the whole expression solves this problem. Internally, `evalf`
372 estimates the number of accurate bits of the floating-point approximation for each sub-expression,
373 and adaptively increases the working precision until the estimated accuracy of the final result
374 matches the sought number of decimal digits:

```
375 >>> (cos(exp(-100)) - 1).evalf(25)
376 -6.919482633683687653243407e-88
```

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

382 3.2 The mpmath Library

383 The implementation of arbitrary-precision floating-point arithmetic is supplied by the mpmath
384 library [26]. Originally, it was developed as a SymPy submodule but has subsequently been
385 moved to a standalone pure-Python package. The basic datatypes in mpmath are `mpf` and
386 `mpc`, which respectively act as multiprecision substitutes for Python's `float` and `complex`. The
387 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')
```

```

491 >>> comm = Commutator(A, B)
492 >>> comm
493 [A,B]
494 >>> qapply(Dagger(comm*a)).doit()
495 -<a|*(Dagger(A)*Dagger(B) - Dagger(B)*Dagger(A))

```

496 Commutators can be expanded using common commutator identities:

```

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

```

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

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

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

```

520 >>> from sympy.physics.quantum.qubit import Qubit
521 >>> from sympy.physics.quantum.gate import XGate
522 >>> q = Qubit('0101')
523 >>> q
524 |0101>
525 >>> X = XGate(1)
526 >>> qapply(X*q)
527 |0111>

```

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

```

529 >>> Dagger(q)
530 <0101|
531 >>> ip = Dagger(q)*q
532 >>> ip
533 <0101|0101>
534 >>> ip.doit()
535 1

```

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

```

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

```

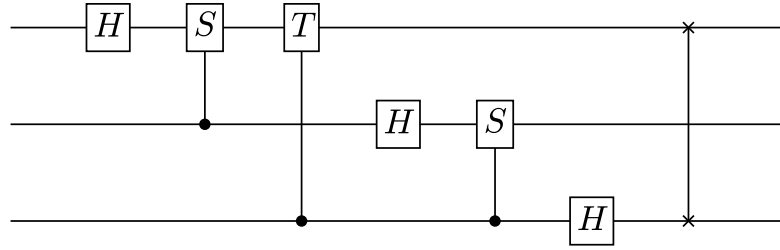


Figure 1. The circuit diagram for a three-qubit quantum Fourier transform generated by SymPy.

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

```

549 >>> from sympy.physics.quantum.qft import QFT
550 >>> from sympy.physics.quantum.circuitplot import circuit_plot
551 >>> fourier = QFT(0,3).decompose()
552 >>> fourier
553 SWAP(0,2)*H(0)*C((0),S(1))*H(1)*C((0),T(2))*C((1),S(2))*H(2)
554 >>> c = circuit_plot(fourier, nqubits=3)

```

555 5 ARCHITECTURE

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

560 5.1 The Core

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

567 In SymPy every symbolic expression is an instance of the class `Basic`,¹² the superclass of all
568 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.

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

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

```
572 >>> x, y = symbols('x y')
573 >>> expr = x*y + 2
```

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

```
576 >>> type(expr)
577 <class 'sympy.core.add.Add'>
578 >>> expr.args
579 (2, x*y)
```

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

```
583 >>> expr.args[0]
584 2
585 >>> type(expr.args[0])
586 <class 'sympy.core.numbers.Integer'>
587 >>> expr.args[0].args
588 ()
```

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

```
590 >>> exp(1)
591 E
592 >>> exp(1).args
593 ()
594 >>> x.args
595 ()
```

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

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

601 Every SymPy expression satisfies a key identity invariant:

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

603 This means that expressions are rebuildable from their `args`.¹⁴ Note that in SymPy the `==`
604 operator represents exact structural equality, not mathematical equality. This allows testing if
605 any two expressions are equal to one another as expression trees. For example, even though
606 $(x+1)^2$ and $x^2 + 2x + 1$ are equal mathematically, SymPy gives

```
607 >>> (x + 1)**2 == x**2 + 2*x + 1
608 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.

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

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

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

622 5.2 Extensibility

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

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

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

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

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

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

```
653 from sympy import Function, Integer, factorial, polygamma
654
655 class gamma(Function):
656     @classmethod
657     def eval(cls, arg):
658         if isinstance(arg, Integer) and arg.is_positive:
659             return factorial(arg - 1)
```

¹⁵See the supplement for more information on the `sympy.logic` submodule.

```

660
661     def _eval_is_real(self):
662         x = self.args[0]
663         # noninteger means real and not integer
664         if x.is_positive or x.is_noninteger:
665             return True
666
667     def _eval_rewrite_as_factorial(self, z):
668         return factorial(z - 1)
669
670     def fdiff(self, argindex=1):
671         from sympy.core.function import ArgumentIndexError
672         if argindex == 1:
673             return self.func(self.args[0])*polygamma(0, self.args[0])
674         else:
675             raise ArgumentIndexError(self, argindex)

```

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

678 5.3 Performance

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

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

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

695 6 PROJECTS THAT DEPEND ON SYMPY

696 There are several projects that depend on SymPy as a library for implementing a part of their
697 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 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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