

SymPy: symbolic computing in Python

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ABSTRACT

48 SymPy is an open source computer algebra system written in pure Python. It is built with a focus on
49 extensibility and ease of use, through both interactive and programmatic applications. These characteristics
50 have led SymPy to become a popular symbolic library for the scientific Python ecosystem. This paper
51 presents the architecture of SymPy, a description of its features, and a discussion of select submodules.
52 The supplementary material provide additional examples and further outline details of the architecture and
53 features of SymPy.

54 1 INTRODUCTION

55 SymPy is a full featured computer algebra system (CAS) written in the Python [32] programming
56 language. It is free and open source software, licensed under the 3-clause BSD license [49].
57 The SymPy project was started by Ondřej Čertík in 2005, and it has since grown to over 500
58 contributors. Currently, SymPy is developed on GitHub using a bazaar community model [43].
59 The accessibility of the codebase and the open community model allow SymPy to rapidly respond
60 to the needs of users and developers.

61 Python is a dynamically typed programming language that has a focus on ease of use and
62 readability.¹ Due in part to this focus, it has become a popular language for scientific computing
63 and data science, with a broad ecosystem of libraries [37]. SymPy is itself used as a dependency by
64 many libraries and tools to support research within a variety of domains, such as SageMath [58]
65 (pure and applied mathematics), yt [64] (astronomy and astrophysics), PyDy [19] (multibody
66 dynamics), and SfePy [10] (finite elements).

67 Unlike many CAS's, SymPy does not invent its own programming language. Python itself
68 is used both for the internal implementation and end user interaction. By using the operator
69 overloading functionality of Python, SymPy follows the embedded domain specific language
70 paradigm proposed by Hudak [24]. The exclusive usage of a single programming language makes
71 it easier for people already familiar with that language to use or develop SymPy. Simultaneously,
72 it enables developers to focus on mathematics, rather than language design. SymPy officially
73 supports Python 2.6, 2.7 and 3.2–3.5.

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

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

83 The remainder of this paper discusses key components of the SymPy library. Section 2
84 enumerates the features of SymPy and takes a closer look at some of the important ones.
85 The section 3 looks at the numerical features of SymPy and its dependency library, mpmath.
86 Section 4 looks at the domain specific physics submodules for performing symbolic and numerical
87 calculations in classical mechanics and quantum mechanics. Section 5 discusses the architecture
88 of SymPy. Section 6 looks at a selection of packages that depend on SymPy. Conclusions and
89 future directions for SymPy are given in section 7. All examples in this paper use SymPy version
90 1.0 and mpmath version 0.19.

91 The following statement imports all SymPy functions into the global Python namespace.²
92 From here on, all examples in this paper assume that this statement has been executed.³

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

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

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

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

97 2 OVERVIEW OF CAPABILITIES

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

102 2.1 Basic Usage

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

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

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

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

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

118 2.2 List of Features

119 Although SymPy’s extensive feature set cannot be covered in depth in this paper, bedrock areas,
 120 that is, those areas that are used throughout the library, are discussed in their own subsections
 121 below. Additionally, Table 1 gives a compact listing of all major capabilities present in the
 122 SymPy codebase. This grants a sampling from the breadth of topics and application domains
 123 that SymPy services. Unless stated otherwise, all features noted in Table 1 are symbolic in
 124 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.
Category Theory (<code>sympy.categories</code>)	Representation of objects, morphisms, and diagrams. Tools for drawing diagrams with Xy-pic [48].
Code Generation (<code>sympy.printing</code> , <code>sympy.codegen</code>)	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.

there is one, shown on the next line.

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 identity $\sqrt{t^2} = t$ holds if t is nonnegative ($t \geq 0$). However, for general complex t , no such identity holds.

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

```
>>> 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.

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

Some of the common assumptions are `negative`, `real`, `nonpositive`, `integer`, `prime` and `commutative`.⁴ Assumptions on any SymPy object can be checked with the `is_assumption`

⁴SymPy 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.

145 attributes, like `t.is_positive`.

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

150 The assumptions system additionally has deductive capabilities. The assumptions use a
 151 three-valued logic using the Python built in objects `True`, `False`, and `None`. Note that `False` is
 152 returned if the SymPy object doesn't or can't have the assumption. For example, both `I.is_real`
 153 and `I.is_prime` return `False` for the imaginary unit `I`.

154 `None` represents the “unknown” case. This could mean that given assumptions do not unam-
 155 biguously specify the truth of an attribute. For instance, `Symbol('x', real=True).is_positive`
 156 will give `None` because a real symbol might be positive or negative. `None` could also mean that not
 157 enough is known or implemented to compute the given fact. For instance, `(pi + E).is_irrational`
 158 gives `None`—indeed, the rationality of $\pi + e$ is an open problem in mathematics [31].

159 Basic implications between the facts are used to deduce assumptions. Deductions are made
 160 using the Rete algorithm [13].⁵ For instance, the assumptions system knows that being an integer
 161 implies being rational.

```
162 >>> i = Symbol('i', integer=True)
163 >>> i.is_rational
164 True
```

165 Furthermore, expressions compute the assumptions on themselves based on the assumptions
 166 of their arguments. For instance, if `x` and `y` are both created with `positive=True`, then `(x +`
 167 `y).is_positive` will be `True` (whereas `(x - y).is_positive` will be `None`).

168 2.4 Simplification

169 The generic way to simplify an expression is by calling the `simplify` function. It must be
 170 emphasized that simplification is not a rigorously defined mathematical operation [34]. The
 171 `simplify` function applies several simplification routines along with heuristics to make the output
 172 expression “simple”.⁶

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

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]

178

179 Examples for these simplification functions can be found in the supplement.

⁵For 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.

⁶The `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.

180 2.5 Calculus

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

183 Limits are computed with the `limit` function, using the Gruntz algorithm [22] for computing
184 symbolic limits and heuristics (a description of the Gruntz algorithm may be found in the
185 supplement). For example, the following computes $\lim_{x \rightarrow \infty} x \sin(\frac{1}{x}) = 1$. Note that SymPy denotes
186 ∞ as `oo`.

```
187 >>> limit(x*sin(1/x), x, oo)
188 1
```

As a more complex example, SymPy computes

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

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

191 Derivatives are computed with the `diff` function, which recursively uses the various differen-
192 tiation rules.

```
193 >>> diff(sin(x)*exp(x), x)
194 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 reimplementaion 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

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

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

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

```
204 >>> i, n = symbols('i n')
205 >>> summation(2**i, (i, 0, n - 1))
206 2**n - 1
207 >>> summation(i*factorial(i), (i, 1, n))
208 n*factorial(n) + factorial(n) - 1
```

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


```

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

```

213 The supplementary material discusses series expansions methods in more depth.

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

```

216 >>> integrate(x**x, x)
217 Integral(x**x, x)
218 >>> Sum(2**i, (i, 0, n - 1))
219 Sum(2**i, (i, 0, n - 1))

```

220 2.6 Polynomials

221 SymPy implements a suite of algorithms for polynomial manipulation, which ranges from
 222 relatively simple algorithms for doing arithmetic of polynomials, to advanced methods for
 223 factoring multivariate polynomials into irreducibles, symbolically determining real and complex
 224 root isolation intervals, or computing Gröbner bases.

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

232 SymPy implements dense and sparse polynomial representations.⁷ Both are used in the uni-
 233 variate and multivariate cases. The dense representation is the default for univariate polynomials.
 234 For multivariate polynomials, the choice of representation is based on the application. The most
 235 common case for the sparse representation is algorithms for computing Gröbner bases (Buchberger,
 236 F4, and F5) [8, 14, 15]. This is because different monomial orderings can be expressed easily in
 237 this representation. However, algorithms for computing multivariate GCDs or factorizations, at
 238 least those currently implemented in SymPy [38], are better expressed when the representation
 239 is dense. The dense multivariate representation is specifically a recursively-dense representation,
 240 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
 241 that despite this, the coefficient domain K , can be a multivariate polynomial domain as well.
 242 The dense recursive representation in Python gets inefficient as the number of variables increases.

243 Some examples for the `sympy.polys` submodule can be found in the supplement.

244 2.7 Printers

245 SymPy has a rich collection of expression printers. By default, an interactive Python session will
 246 render the `str` form of an expression, which has been used in all the examples in this paper so
 247 far. The `str` form of an expression is valid Python and roughly matches what a user would type
 248 to enter the expression.⁸

```

249 >>> phi0 = Symbol('phi0')
250 >>> str(Integral(sqrt(phi0), phi0))
251 'Integral(sqrt(phi0), phi0)'

```

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

⁷In 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.

⁸Many 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.


```

256 >>> pprint(Integral(sqrt(phi0 + 1), phi0))
257
258 
$$\int \sqrt{\varphi_0 + 1} \, d(\varphi_0)$$


```

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

```

259 >>> pprint(Integral(sqrt(phi0 + 1), phi0), use_unicode=False)
260 /
261 |
262 | _____
263 | \ / phi0 + 1 d(phi0)
264 |
265 /

```

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

```

267 >>> print(latex(Integral(sqrt(phi0 + 1), phi0)))
268 \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 equations⁹, 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

```

287 solve(f, *symbols, **flags)
288 solveset(f, symbol, domain=S.Complexes)

```

The `domain` parameter can be any set from the `sympy.sets` module (see 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.

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

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

`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.

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

⁹See the supplementary material for an in depth discussion on the Diophantine submodule.

2.9 Matrices

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

```
>>> A = Matrix([[x, x + y], [y, x]])
>>> A
Matrix([
[x, x + y],
[y,      x]])
```

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.

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

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

Internally these matrices store the elements as Lists of Lists (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.¹⁰ For storing sparse matrices, the `SparseMatrix` class can be used. Sparse matrices store their elements in Dictionary of Keys (DOK) format, meaning entries are stored as a `dict` of (`row`, `column`) pairs mapping to the elements.

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

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

When symbolic matrices are combined with the `assumptions` 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].

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

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:

¹⁰Similar 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.

397 representing $\sum_{x=a}^b f(x)$ is represented in mpmath as `nsum(f, (a, b))`, where `f` is a numeric
398 Python function.

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

403 The double exponential (tanh-sinh) quadrature is used for numerical integration by default.
404 For smooth integrands, this algorithm usually converges extremely rapidly, even when the
405 integration interval is infinite or singularities are present at the endpoints [54, 2]. However, for
406 good performance, singularities in the middle of the interval must be specified by the user. To
407 evaluate slowly converging limits and infinite series, mpmath automatically tries Richardson
408 extrapolation and the Shanks transformation (Euler-Maclaurin summation can also be used) [3].
409 A function to evaluate oscillatory integrals by means of convergence acceleration is also available.

410 A wide array of higher mathematical functions is implemented with full support for complex
411 values of all parameters and arguments, including complete and incomplete gamma functions,
412 Bessel functions, orthogonal polynomials, elliptic functions and integrals, zeta and polylogarithm
413 functions, the generalized hypergeometric function, and the Meijer G-function. The Meijer
414 G-function instance $G_{1,3}^{3,0}(0; \frac{1}{2}, -1, -\frac{3}{2}|x)$ is a good test case [63]; past versions of both Maple and
415 Mathematica produced incorrect numerical values for large $x > 0$. Here, mpmath automatically
416 removes an internal singularity and compensates for cancellations (amounting to 656 bits of
417 precision when $x = 10000$), giving correct values:

```
418 >>> mpmath.mp.dps = 15
419 >>> mpmath.meijerg([], [0], [[-0.5, -1, -1.5], []], 10000)
420 mpf('2.4392576907199564e-94')
```

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

```
422 >>> meijerg([], [0], [[-S(1)/2, -1, -S(3)/2], []], 10000).evalf()
423 2.43925769071996e-94
```

424 Symbolic integration and summation often produce hypergeometric and Meijer G-function
425 closed forms (see section 2.5); numerical evaluation of such special functions is a useful complement
426 to direct numerical integration and summation.

427 4 PHYSICS SUBMODULE

428 SymPy includes several submodules that allow users to solve domain specific physics problems.
429 For example, a comprehensive physics submodule is included that is useful for solving problems
430 in mechanics, optics, and quantum mechanics along with support for manipulating physical
431 quantities with units.

432 4.1 Classical Mechanics

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

435 4.1.1 Vector Algebra

436 The `sympy.physics.vector` submodule provides reference frame-, time-, and space-aware vector
437 and dyadic objects that allow for three-dimensional operations such as addition, subtraction,
438 scalar multiplication, inner and outer products, and cross products. The vector and dyadic
439 objects both can be written in very compact notation that make it easy to express the vectors
440 and dyadics in terms of multiple reference frames with arbitrarily defined relative orientations.
441 The vectors are used to specify the positions, velocities, and accelerations of points; orientations,
442 angular velocities, and angular accelerations of reference frames; and forces and torques. The
443 dyadics are essentially reference frame-aware 3×3 tensors [53]. The vector and dyadic objects
444 can be used for any one-, two-, or three-dimensional vector algebra, and they provide a strong
445 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')
>>> comm = Commutator(A, B)
>>> comm
[A,B]
>>> qapply(Dagger(comm*a)).doit()
-<a|*(Dagger(A)*Dagger(B) - Dagger(B)*Dagger(A))
```

Commutators can be expanded using common commutator identities:

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

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

- Many of the exactly solvable quantum systems, including simple harmonic oscillator states and raising/lowering operators, infinite square well states, and 3D position and momentum operators and states.

- Second quantized formalism of non-relativistic many-body quantum mechanics [16].
- Quantum angular momentum [65]. Spin operators and their eigenstates can be represented in any basis and for any quantum numbers. A rotation operator representing the Wigner D-matrix, which may be defined symbolically or numerically, is also implemented to rotate spin eigenstates. Functionality for coupling and uncoupling of arbitrary spin eigenstates is provided, including symbolic representations of Clebsch-Gordon coefficients and Wigner symbols.
- Quantum information and computing [35]. Multidimensional qubit states, and a full set of one- and two-qubit gates are provided and can be represented symbolically or as matrices/vectors. With these building blocks, it is possible to implement a number of basic quantum algorithms including the quantum Fourier transform, quantum error correction, quantum teleportation, Grover's algorithm, dense coding, etc. In addition, any quantum circuit may be plotted using the `circuit_plot` function (Figure 1).

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

```
>>> from sympy.physics.quantum.qubit import Qubit
>>> from sympy.physics.quantum.gate import XGate
>>> q = Qubit('0101')
>>> q
|0101>
>>> X = XGate(1)
>>> qapply(X*q)
|0111>
```

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

```
>>> Dagger(q)
<0101|
>>> ip = Dagger(q)*q
>>> ip
<0101|0101>
>>> ip.doit()
1
```

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

```
>>> from sympy.physics.quantum.qubit import measure_all
>>> from sympy.physics.quantum.gate import H, X, Y, Z
>>> c = H(0)*H(1)*Qubit('00')
>>> c
H(0)*H(1)*|00>
>>> q = qapply(c)
>>> measure_all(q)
[ (|00>, 1/4), (|01>, 1/4), (|10>, 1/4), (|11>, 1/4) ]
```

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

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



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

5 ARCHITECTURE

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

5.1 The Core

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

In SymPy every symbolic expression is an instance of the class `Basic`,¹¹ the superclass of all SymPy types providing common methods to all SymPy tree-elements, such as traversals. The children of a node in the tree are held in the `args` attribute. A leaf node in the expression tree has empty `args`.

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

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

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

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

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

```
>>> expr.args[0]
2
>>> type(expr.args[0])
<class 'sympy.core.numbers.Integer'>
```

¹¹Some internal classes, such as those used in the polynomial submodule, do not follow this rule for efficiency reasons.


```

580 >>> expr.args[0].args
581 ()

```

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

```

583 >>> exp(1)
584 E
585 >>> exp(1).args
586 ()
587 >>> x.args
588 ()

```

589 A useful way to view an expression tree is using the `srepr` function, which returns a string
 590 representation of an expression as valid Python code¹² with all the nested class constructor calls
 591 to create the given expression.

```

592 >>> srepr(expr)
593 "Add(Mul(Symbol('x'), Symbol('y')), Integer(2))"

```

594 Every SymPy expression satisfies a key identity invariant:

```

595 expr.func(*expr.args) == expr

```

596 This means that expressions are rebuildable from their `args`.¹³ Note that in SymPy the `==`
 597 operator represents exact structural equality, not mathematical equality. This allows testing if
 598 any two expressions are equal to one another as expression trees. For example, even though
 599 $(x+1)^2$ and x^2+2x+1 are equal mathematically, SymPy gives

```

600 >>> (x + 1)**2 == x**2 + 2*x + 1
601 False

```

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

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

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

615 5.2 Extensibility

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

621 The typical way to create a custom SymPy object is to subclass an existing SymPy class,
 622 usually `Basic`, `Expr`, or `Function`. As it was stated before, all SymPy classes used for expression
 623 trees should be subclasses of the base class `Basic`. `Expr` is the `Basic` subclass for mathematical
 624 objects that can be added and multiplied together. The most commonly seen classes in SymPy

¹² 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.

¹³ `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.

are subclasses of `Expr`, including `Add`, `Mul`, and `Symbol`. Instances of `Expr` typically represent complex numbers, but may also include other “rings”, like matrix expressions. Not all SymPy classes are subclasses of `Expr`. For instance, logic expressions, such as `And(x, y)`, are subclasses of `Basic` but not of `Expr`.¹⁴

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

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

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

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

```

646 from sympy import Function, Integer, factorial, polygamma
647
648 class gamma(Function):
649     @classmethod
650     def eval(cls, arg):
651         if isinstance(arg, Integer) and arg.is_positive:
652             return factorial(arg - 1)
653
654     def _eval_is_real(self):
655         x = self.args[0]
656         # noninteger means real and not integer
657         if x.is_positive or x.is_noninteger:
658             return True
659
660     def _eval_rewrite_as_factorial(self, z):
661         return factorial(z - 1)
662
663     def fdiff(self, argindex=1):
664         from sympy.core.function import ArgumentIndexError
665         if argindex == 1:
666             return self.func(self.args[0])*polygamma(0, self.args[0])
667         else:
668             raise ArgumentIndexError(self, argindex)

```

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

5.3 Performance

Due to being written in pure Python without the use of extension modules, SymPy’s performance characteristics are generally poorer than its commercial competitors. For many applications, the performance of SymPy, as measured by clock cycles, memory usage, and memory layout, is sufficient. However, the boundaries for when SymPy’s pure Python strategy becomes insufficient

¹⁴See the supplement for more information on the `sympy.logic` submodule.

are when the user requires handling of very long expressions or many small expressions. Where this boundary lies depends on the system at hand, but tends to be within the range of 10^4 – 10^6 symbols for modern computers.

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

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

6 PROJECTS THAT DEPEND ON SYMPY

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