

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 domain specific submodules. The supplementary materials provide additional examples and further outline details of the architecture and features of SymPy.

Keywords: symbolic, Python, computer algebra system

1 INTRODUCTION

SymPy is a full featured computer algebra system (CAS) written in the Python [28] programming language. It is free and open source software, licensed under the 3-clause BSD license [40]. 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 [36]. 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 [31]. SymPy is itself used by many libraries and tools to support research within a variety of domains, such as SageMath [46] (pure and applied mathematics), yt [49] (astronomy and astrophysics), PyDy [16] (multibody dynamics), and SfePy [10] (finite elements).

Unlike many CASs, SymPy does not invent its own programming language. Python itself is used both for the internal implementation and end user interaction. By using the operator overloading functionality of Python, SymPy follows the embedded domain specific language paradigm proposed by Hudak [21]. 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.

As 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 [25] 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 discusses the architecture of SymPy. Section 3 enumerates the features of SymPy and takes a closer look at some of the important ones. The section 4 looks at the numerical features of

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

100 SymPy and its dependency library, mpmath. Section 5 looks at the domain specific physics
101 submodules for performing symbolic and numerical calculations in classical mechanics and
102 quantum mechanics. Conclusions and future directions for SymPy are given in section 6. All
103 examples in this paper use SymPy version 1.0 and mpmath version 0.19.

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

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

107 All examples could be tested on the SymPy Live instance, that is an online Python shell,
108 which uses the Google App Engine to execute SymPy code.

109 2 ARCHITECTURE

110 Software architecture is of central importance in any large software project because it establishes
111 predictable patterns of usage and development [42]. This section describes the essential structural
112 components of SymPy, provides justifications for the design decisions that have been made, and
113 gives example user-facing code as appropriate.

114 2.1 Basic Usage

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

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

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

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

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

130 Importantly, SymPy expressions are immutable. This simplifies the design of SymPy by
131 allowing expression interning. It also enables expressions to be hashed, that is used to implement
132 caching in SymPy.

133 2.2 The Core

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

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.

³The 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.

In SymPy every symbolic expression is an instance of a Python `Basic` class,⁴ a superclass of all SymPy types providing common methods to all SymPy tree-elements, such as traversals. The children of a node in the tree are held in the `args` attribute. A terminal or leaf node in the expression tree has empty `args`.

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

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

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

```
>>> 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'>
>>> expr.args[0].args
()
```

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

```
>>> exp(1)
E
>>> exp(1).args
()
>>> x.args
()
```

A useful way to view an expression tree is using the `srepr` function, which returns a string representation of an expression as valid Python code⁵ with all the nested class constructor calls to create the given expression.

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

Every SymPy expression satisfies a key identity invariant:

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

This means that expressions are rebuildable from their `args`.⁶ Note that in SymPy the `==` operator represents exact structural equality, not mathematical equality. This allows testing if any two expressions are equal to one another as expression trees. For example, even though $(x+1)^2$ and $x^2 + 2x + 1$ are equal mathematically, SymPy gives

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

⁴Some internal classes, such as those used in the polynomial submodule, do not follow this rule for efficiency reasons.

⁵ 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.

⁶`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.

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

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

190 2.3 Assumptions

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

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

```
198 >>> t = Symbol('t')
199 >>> sqrt(t**2)
200 sqrt(t**2)
```

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

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

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

209 Some of the common assumptions that SymPy allows are `positive`, `negative`, `real`, `nonpositive`,
210 `integer`, `prime` and `commutative`.⁷ Assumptions on any object can be checked with the `is_assumption`
211 attributes, like `t.is_positive`.

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

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

220 `None` represents the "unknown" case. This could mean that given assumptions do not unam-
221 biguously specify the truth of an attribute. For instance, `Symbol('x', real=True).is_positive`
222 will give `None` because a real symbol might be positive or negative. The `None` could also mean
223 that not enough is known or implemented to compute the given fact. For instance, `(pi +`
224 `E).is_irrational` gives `None`, because determining whether $\pi + e$ is rational or irrational is an
225 open problem in mathematics [27].

226 Basic implications between the facts are used to deduce assumptions. For instance, the
227 assumptions system knows that being an integer implies being rational.

```
228 >>> i = Symbol('i', integer=True)
```

⁷SymPy 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.

```

229 >>> i.is_rational
230 True

```

231 Furthermore, expressions compute the assumptions on themselves based on the assumptions
232 of their arguments. For instance, if x and y are both created with `positive=True`, then $(x +$
233 $y).is_positive$ will be `True` whereas $(x - y).is_positive$ will be `None`.

234 2.4 Extensibility

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

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

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

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

260 As an example of the notions presented in this section, Listing 1 presents a minimal version
261 of the gamma function $\Gamma(x)$ from SymPy, which evaluates itself on positive integer arguments,
262 has the positive and real assumptions defined, can be rewritten in terms of factorial with
263 `gamma(x).rewrite(factorial)`, and can be differentiated. `self.func` is used throughout instead
264 of referencing `gamma` explicitly so that potential subclasses of `gamma` can reuse the methods.

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

```

265 from sympy import Integer, Function, floor, factorial, polygamma
266
267 class gamma(Function)
268     @classmethod
269     def eval(cls, arg):
270         if isinstance(arg, Integer) and arg.is_positive:
271             return factorial(arg - 1)
272
273     def _eval_is_positive(self):
274         x = self.args[0]
275         if x.is_positive:
276             return True
277         elif x.is_noninteger:
278             return floor(x).is_even
279
280     def _eval_is_real(self):

```

```

281         x = self.args[0]
282         # noninteger means real and not integer
283         if x.is_positive or x.is_noninteger:
284             return True
285
286     def _eval_rewrite_as_factorial(self, z):
287         return factorial(z - 1)
288
289     def fdiff(self, argindex=1):
290         from sympy.core.function import ArgumentIndexError
291         if argindex == 1:
292             return self.func(self.args[0])*polygamma(0, self.args[0])
293         else:
294             raise ArgumentIndexError(self, argindex)

```

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

297 2.5 Speed

298 Due to being written in pure Python, SymPy's speed is generally slower compared with its
299 commercial competitors. For many applications and uses of SymPy, that is not a problem, as
300 SymPy is able to return the answer quickly enough, but for some applications that require
301 handling of very long expressions and/or lots of small expressions, the speed becomes a problem.

302 For this reason, a new library called SymEngine [47] was started. It is a pure C++ library
303 with thin wrappers to other languages (Python, Ruby, Julia, ...) whose aim is to be the fastest
304 manipulation library. Preliminary benchmarks suggest that SymEngine is as fast or faster than
305 the commercial or open source competitors.

306 The development branch of SymPy recently started to use SymEngine as an optional backend,
307 initially in `sympy.mechanics` only. The plan is to allow more algorithms in SymPy to take
308 advantage of the speed of SymEngine.

309 3 FEATURES

310 Although SymPy's extensive feature set cannot be covered in-depth in this paper, calculus and
311 other bedrock areas are discussed in their own subsections. Additionally, Table 1 gives a compact
312 listing of all major capabilities present in the SymPy codebase. This grants a sampling from the
313 breadth of topics and application domains that SymPy services. Unless stated otherwise, all
314 features noted in Table 1 are symbolic in nature. Numeric features are discussed in Section 4.

Table 1. SymPy Features and Descriptions

Feature(submodules)	Description
Calculus (core, series, integrals)	Algorithms for computing derivatives, integrals, and limits.
Category Theory (categories)	Representation of objects, morphisms, and diagrams. Tools for drawing diagrams with Xy-pic.
Code Generation (printing, codegen)	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 (combinatorics)	Permutations, combinations, partitions, subsets, various permutation groups (such as polyhedral, Rubik, symmetric, and others), Gray codes [30], and Prufer sequences [4].

Concrete Math (concrete)	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 [35] for two univariate polynomials.
Cryptography (crypto)	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 (diff-geom)	Representations of manifolds, metrics, tensor products, and coordinate systems in Riemannian and pseudo-Riemannian geometries [43].
Geometry (geometry)	Representations of 2D geometrical entities, such as lines and circles. Enables queries on these entities, such as asking the area of an ellipse, checking for collinearity of a set of points, or finding the intersection between objects.
Lie Algebras (liealgebras)	Representations of Lie algebras and root systems.
Logic (logic)	Boolean expressions, equivalence testing, satisfiability, and normal forms.
Matrices (matrices)	Tools for creating matrices of symbols and expressions. Both sparse and dense representations, as well as symbolic linear algebraic operations (e.g., inversion and factorization), are supported.
Matrix Expressions (matrixes.expressions)	Matrices with symbolic dimensions (unspecified entries). Block matrices.
Number Theory (nththeory)	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 (plotting)	Hooks for visualizing expressions via matplotlib [22] or as text drawings when lacking a graphical back-end. 2D function plotting, 3D function plotting, and 2D implicit function plotting are supported.
Polynomials (polys)	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 (printing)	Functions for printing SymPy expressions in the terminal with ASCII or Unicode characters and converting SymPy expressions to L ^A T _E X and MathML.
Quantum Mechanics (physics.quantum)	Quantum states, bra-ket notation, operators, basis sets, representations, tensor products, inner products, outer products, commutators, anticommutators, and specific quantum system implementations.
Series (series)	Series expansion, sequences, and limits of sequences. This includes Taylor, Laurent, and Puiseux series as well as special series, such as Fourier and formal power series.
Sets (sets)	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 (simplify)	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 (solvers)	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 (functions)	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 (stats)	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 [39].
Tensors (tensor)	Symbolic manipulation of indexed objects.
Vectors (vector)	Basic operations on vectors and differential calculus with respect to 3D Cartesian coordinate systems.

3.1 Simplification

The generic way to simplify an expression is by calling the `simplify` function. It must be emphasized that simplification is not a rigorously defined mathematical operation [8]. The `simplify` function applies several simplification routines along with heuristics to make the output expression “simple”.⁸

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

Table 2. Some SymPy Simplification Functions

<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 [15]
<code>hyperexpand</code>	expand hypergeometric functions [37, 38]

3.2 Calculus

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

⁸The `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.

Limits are computed with the `limit` function, using the Gruntz algorithm [19] 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`.

```
332 >>> limit(x*sin(1/x), x, oo)
333 1
```

As a more complex example, SymPy computes

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

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

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

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

Integrals are calculated with the `integrate` function. SymPy implements a combination of the Risch algorithm [6], table lookups, a reimplementation of Manuel Bronstein’s “Poor Man’s Integrator” [5], and an algorithm for computing integrals based on Meijer G-functions [37, 38]. 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

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

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

Summations are computed with `summation` using a combination of Gosper’s algorithm [18], an algorithm that uses Meijer G-functions [37, 38], and heuristics. Products are computed with `product` function via a suite of heuristics.

```
349 >>> i, n = symbols('i n')
350 >>> summation(2**i, (i, 0, n - 1))
351 2**n - 1
352 >>> summation(i*factorial(i), (i, 1, n))
353 n*factorial(n) + factorial(n) - 1
```

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

```
356 >>> integrate(x**x, x)
357 Integral(x**x, x)
358 >>> Sum(2**i, (i, 0, n - 1))
359 Sum(2**i, (i, 0, n - 1))
```

3.3 Polynomials

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

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

SymPy implements dense and sparse polynomial representations.⁹ Both are used in the univariate and multivariate cases. The dense representation is the default for univariate polynomials. For multivariate polynomials, the choice of representation is based on the application. The most common case for the sparse representation is algorithms for computing Gröbner bases (Buchberger, F4, and F5) [7, 11, 12]. This is because different monomial orderings can be expressed easily in this representation. However, algorithms for computing multivariate GCDs or factorizations, at least those currently implemented in SymPy [32], 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.

3.4 Printers

SymPy has a rich collection of expression printers. By default, an interactive Python session will render the `str` form of an expression, which has been used in all the examples in this paper so far. The `str` form of an expression is valid Python and roughly matches what a user would type to enter the expression.¹⁰

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

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

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

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

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

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

⁹In 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.

¹⁰Many 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 it was noted in section 2.2, the `srepr` function prints the exact, verbose form of an expression.

```

402 | _____
403 | \ / phi0 + 1 d(phi0)
404 |
405 /

```

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

```

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

```

409 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. 410 In the Jupyter Notebook or Qt Console [33], the \LaTeX printer is used to render expressions 411 using MathJax or \LaTeX , if it is installed on the system. The 2D text representation is used 412 otherwise. 413

414 Other printers such as MathML are also available. SymPy uses an extensible printer subsystem 415 for customizing any given printer, and allows custom objects to define their printing behavior for 416 any printer. The code generation functionality of SymPy relies on this subsystem to convert 417 expressions into code in various target programming languages.

418 3.5 Solvers

419 SymPy has equation solvers that can handle ordinary differential equations, recurrence relation- 420 ships, Diophantine equations, and algebraic equations. There is also rudimentary support for 421 simple partial differential equations.

422 There are two functions for solving algebraic equations in SymPy: `solve` and `solveset`. 423 `solveset` has several design changes with respect to the older `solve` function. This distinction 424 is present in order to resolve the usability issues with the previous `solve` function API while 425 maintaining backward compatibility with earlier versions of SymPy. `solveset` only requires 426 essential input information from the user. The function signatures of `solve` and `solveset` are

```

427 solve(f, *symbols, **flags)
428 solveset(f, symbol, domain=S.Complexes)

```

429 The `domain` parameter is typically either `S.Complexes` (the default) or `S.Reals`; the latter causes 430 `solveset` to only return real solutions.

431 An important difference between the two functions is that the output API of `solve` varies 432 with input (sometimes returning a Python list and sometimes a Python dictionary) whereas 433 `solveset` always returns a SymPy set object.

434 Both functions implicitly assume that expressions are equal to 0. For instance, `solveset(x - 435 1, x)` solves $x - 1 = 0$ for x .

436 `solveset` is under active development as a planned replacement for `solve`. There are certain 437 features which are implemented in `solve` that are not yet implemented in `solveset`, including 438 multivariate systems, and some transcendental equations.

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

440 3.6 Matrices

441 Besides being an important feature in its own right, computations on matrices with symbolic 442 entries are important for many algorithms within SymPy. The following code shows some basic 443 usage of the `Matrix` class.

```

444 >>> A = Matrix([[x, x + y], [y, x]])
445 >>> A
446 Matrix([
447 [x, x + y],
448 [y, x]])

```

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

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

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

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

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

474 **4 NUMERICS**

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

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

[illegible]

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

```
489 >>> (pi + 1).evalf(25)
490 4.141592653589793238462643
```

491 **Float** numbers do not track their accuracy, and should be used with caution within symbolic
492 expressions since familiar dangers of floating-point arithmetic apply [17]. A notorious case is
493 that of catastrophic cancellation:

```
494 >>> cos(exp(-100)).evalf(25) - 1
495 0
```

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.

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

```
500 >>> (cos(exp(-100)) - 1).evalf(25)
501 -6.919482633683687653243407e-88
```

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

507 4.1 The mpmath library

The implementation of arbitrary-precision floating-point arithmetic is supplied by the `mpmath` library [23]. Originally, it was developed as a `SymPy` submodule but has subsequently been moved to a standalone pure-Python package. The basic datatypes in `mpmath` are `mpf` and `mpc`, which respectively act as multiprecision substitutes for Python’s `float` and `complex`. The floating-point precision is controlled by a global context:

```

513 >>> import mpmath
514 >>> mpmath.mp.dps = 30      # 30 digits of precision
515 >>> mpmath.mpf("0.1") + mpmath.exp(-50)
516 mpf('0.1000000000000000000000000000192874984794')
517 >>> print(_)               # pretty-printed
518 0.1000000000000000000000000000192874985

```

Like SymPy, mpmath is a pure Python library. A design decision of SymPy is to keep it and its required dependencies pure Python. This is a primary advantage of mpmath over other multiple precision libraries such as GNU MPFR [14], which is much more feature-rich and fast. Like SymPy, mpmath is also BSD licensed (GNU MPFR is licensed under the GNU Lesser General Public License [40]).

Internally, `mpmath` represents a floating-point number $(-1)^s x \cdot 2^y$ by a tuple (s, x, y, b) where x and y are arbitrary-size Python integers and the redundant integer b stores the bit length of x for quick access. If GMPY [20] is installed, `mpmath` automatically uses the `gmpy.mpz` type for x , and GMPY methods for rounding-related operations, improving performance.

Most mpmath and SymPy functions use the same naming scheme, although this is not true in every case. For example, the symbolic SymPy summation expression `Sum(f(x), (x, a, b))` representing $\sum_{x=a}^b f(x)$ is represented in mpmath as `nsum(f, (a, b))`, where `f` is a numeric Python function.

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

The double exponential (tanh-sinh) quadrature is used for numerical integration by default. For smooth integrands, this algorithm usually converges extremely rapidly, even when the integration interval is infinite or singularities are present at the endpoints [45, 2]. However, for good performance, singularities in the middle of the interval must be specified by the user. To evaluate slowly converging limits and infinite series, mpmath automatically tries Richardson extrapolation and the Shanks transformation (Euler-Maclaurin summation can also be used) [3]. A function to evaluate oscillatory integrals by means of convergence acceleration is also available.

A wide array of higher mathematical functions is implemented with full support for complex values of all parameters and arguments, including complete and incomplete gamma functions, Bessel functions, orthogonal polynomials, elliptic functions and integrals, zeta and polylogarithm functions, the generalized hypergeometric function, and the Meijer G-function. The Meijer G-function instance $G_{1,3}^{3,0}(0; \frac{1}{2}, -1, -\frac{3}{2}|x)$ is a good test case [48]; past versions of both Maple and

Mathematica produced incorrect numerical values for large $x > 0$. Here, mpmath automatically removes an internal singularity and compensates for cancellations (amounting to 656 bits of precision when $x = 10000$), giving correct values:

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

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

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

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

5 DOMAIN SPECIFIC SUBMODULES

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

5.1 Classical Mechanics

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

5.1.1 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. Both of these objects can be written in very compact notation that make it easy to express the vectors and dyadics in terms of multiple reference frames with arbitrarily defined relative orientations. The vectors are used to specify the positions, velocities, and accelerations of points; orientations, angular velocities, and angular accelerations of reference frames; and forces and torques. The dyadics are essentially reference frame-aware 3×3 tensors [44]. 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 = ReferenceFrame('A')
>>> B = ReferenceFrame('B')
>>> C = ReferenceFrame('C')
>>> 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
```

5.1.2 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 [26] and Kane's Method [24]. Lastly, there are automated linearization routines for constrained dynamical systems [34].

5.2 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 [41]: 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 = Operator('A')
>>> B = Operator('B')
>>> C = Operator('C')
>>> D = Operator('D')
>>> 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 [13].
- Quantum angular momentum [50]. 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 [29]. 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:

```
651 >>> from sympy.physics.quantum.qubit import Qubit
652 >>> from sympy.physics.quantum.gate import XGate
653 >>> q = Qubit('0101')
654 >>> q
655 |0101>
656 >>> X = XGate(1)
657 >>> qapply(X*q)
658 |0111>
```

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

```
660 >>> Dagger(q)
661 <0101|
662 >>> ip = Dagger(q)*q
663 >>> ip
664 <0101|0101>
665 >>> ip.doit()
666 1
```

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

```
669 >>> from sympy.physics.quantum.qubit import measure_all
670 >>> from sympy.physics.quantum.gate import H, X, Y, Z
671 >>> c = H(0)*H(1)*Qubit('00')
672 >>> c
673 H(0)*H(1)*|00>
674 >>> q = qapply(c)
675 >>> measure_all(q)
676 [(|00>, 1/4), (|01>, 1/4), (|10>, 1/4), (|11>, 1/4)]
```

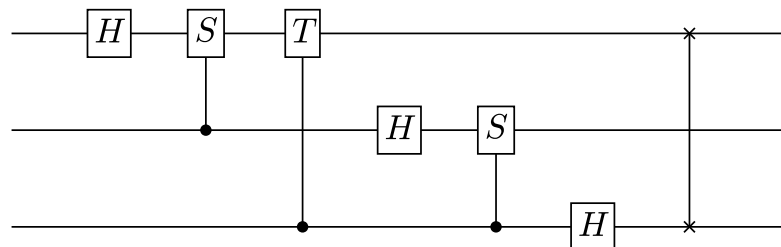


Figure 1. The circuit diagram for a three-qubit quantum Fourier transform generated by SymPy.

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

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

686 6 CONCLUSION AND FUTURE WORK

687 SymPy is a robust computer algebra system that provides a wide spectrum of features both in
 688 traditional computer algebra and in a plethora of scientific disciplines. This allows SymPy to be
 689 used in a first-class way with other Python projects, including the scientific Python stack. Unlike
 690 many other CASSs, SymPy is designed to be used in an extensible way: both as an end-user
 691 application and as a library.

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

696 SymPy supports a wide array of mathematical facilities. This includes functions for simplify-
 697 ing expressions, performing common calculus operations, pretty printing expressions, solving
 698 equations, and representing symbolic matrices. Other supported facilities include discrete math,
 699 concrete math, plotting, geometry, statistics, polynomials, sets, series, vectors, combinatorics,
 700 group theory, code generation, tensors, Lie algebras, cryptography, and special functions. Ad-
 701 ditionally, SymPy contains submodules targeting certain specific domains, such as classical
 702 mechanics and quantum mechanics. This breadth of domains has been engendered by a strong
 703 and vibrant user community. Anecdotaly, these users likely chose SymPy because of its ease of
 704 access.

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

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