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1 SymPy: Symbolic Computing in Python

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55 **ABSTRACT**

56 SymPy is an open source computer algebra system written in pure Python. It is built with a focus on
57 extensibility and ease of use, through both interactive and programmatic applications. These characteristics
58 have led SymPy to become a popular symbolic library for the scientific Python ecosystem. This paper
59 presents the architecture of SymPy, a description of its features, and a discussion of select domain specific
60 submodules. The supplementary materials provide additional examples and further outline details of the
61 architecture and features of SymPy.

62 **Keywords:** symbolic, Python, computer algebra system

63 **1 INTRODUCTION**

64 SymPy is a full featured computer algebra system (CAS) written in the Python programming
65 language [25]. It is free and open source software, licensed under the 3-clause BSD license [37].
66 The SymPy project was started by Ondřej Čertík in 2005, and it has since grown to over 500
67 contributors. Currently, SymPy is developed on GitHub using a bazaar community model [33].
68 The accessibility of the codebase and the open community model allow SymPy to rapidly respond
69 to the needs of users and developers.

70 Python is a dynamically typed programming language that has a focus on ease of use and
71 readability. Due in part to this focus, it has become a popular language for scientific computing
72 and data science, with a broad ecosystem of libraries [28]. SymPy is itself used by many libraries
73 and tools to support research within a variety of domains, such as Sage [40] (pure mathematics),
74 yt [45] (astronomy and astrophysics), PyDy [15] (multibody dynamics), and SfePy [10] (finite
75 elements).

76 Unlike many CASs, SymPy does not invent its own programming language. Python itself
77 is used both for the internal implementation and end user interaction. By using the operator
78 overloading functionality of Python, SymPy follows the embedded domain specific language
79 paradigm proposed by Hudak [20]. The exclusive usage of a single programming language makes
80 it easier for people already familiar with that language to use or develop SymPy. Simultaneously,
81 it enables developers to focus on mathematics, rather than language design.

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

87 As a library, SymPy does not have a built-in graphical user interface (GUI). However, SymPy
88 exposes a rich interactive display system, and supports registering printers with Jupyter [30]
89 frontends, including the Notebook and Qt Console, which will render SymPy expressions using
90 MathJax [9] or \LaTeX .

91 The remainder of this paper discusses key components of the SymPy software. Section 2
92 discusses the architecture of SymPy. Section 3 enumerates the features of SymPy and takes
93 a closer look at some of the important ones. The section 4 looks at the numerical features of
94 SymPy and its dependency library, mpmath. Section 5 looks at the domain specific physics
95 submodules for performing symbolic and numerical calculations in classical mechanics and
96 quantum mechanics. Conclusions and future directions for SymPy are given in section 6.

97 **2 ARCHITECTURE**

98 Software architecture is of central importance in any large software project because it establishes
99 predictable patterns of usage and development [39]. This section describes the essential structural

100 components of SymPy, provides justifications for the design decisions that have been made, and
 101 gives example user-facing code as appropriate.

102 2.1 Basic Usage

103 The following statement imports all SymPy functions into the global Python namespace. From
 104 here on, all examples in this paper assume that this statement has been executed.¹

```
105 >>> from sympy import *
```

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

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

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

116 Expressions are created from symbols using Python's mathematical syntax. For instance, the
 117 following Python code creates the expression $(x^2 - 2x + 3)/y$.

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

120 Importantly, SymPy expressions are immutable. This simplifies the design of SymPy by
 121 allowing expression interning. It also enables expressions to be hashed and stored in Python
 122 dictionaries, thereby permitting features such as caching.

123 2.2 The Core

124 A computer algebra system (CAS) represents mathematical expressions as data structures. For
 125 example, the mathematical expression $x + y$ is represented as a tree with three nodes, `+`, x , and
 126 y , where x and y are ordered children of `+`. As users manipulate mathematical expressions
 127 with traditional mathematical syntax, the CAS manipulates the underlying data structures.
 128 Automated optimizations and computations such as integration, simplification, etc. are all
 129 functions that consume and produce expression trees.

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

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

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

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

```
138 >>> type(expr)  
139 <class 'sympy.core.add.Add'>  
140 >>> expr.args  
141 (2, x*y)
```

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

¹All examples in this paper use SymPy version 1.0.

```

145 >>> expr.args[0]
146 2
147 >>> type(expr.args[0])
148 <class 'sympy.core.numbers.Integer'>
149 >>> expr.args[0].args
150 ()

```

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

```

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

```

156 Every SymPy expression satisfies a key identity invariant:

```

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

```

158 This means that expressions are rebuildable from their `args`.² Note that in SymPy the `==`
 159 operator represents exact structural equality, not mathematical equality. This allows testing if
 160 any two expressions are equal to one another as expression trees. For example, even though
 161 $(x + 1)^2$ and $x^2 + 2x + 1$ are equal mathematically, SymPy gives

```

162 >>> (x + 1)**2 == x**2 + 2*x + 1
163 False

```

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

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

173 2.3 Assumptions

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

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

```

181 >>> t = Symbol('t')
182 >>> sqrt(t**2)
183 sqrt(t**2)

```

184 By assuming the most general case, that symbols are complex by default, SymPy avoids
 185 performing mathematically invalid operations. However, in many cases users will wish to simplify
 186 expressions containing terms like $\sqrt{t^2}$.

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

```

189 >>> t = Symbol('t', positive=True)
190 >>> sqrt(t**2)
191 t

```

²`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.

192 Some of the common assumptions that SymPy allows are `positive`, `negative`, `real`, `nonpositive`,
 193 `integer`, `prime` and `commutative`.³ Assumptions on any object can be checked with the `is_assumption`
 194 attributes, like `t.is_positive`.

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

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

203 `None` represents the “unknown” case. This could mean that given assumptions do not unam-
 204 biguously specify the truth of an attribute. For instance, `Symbol('x', real=True).is_positive`
 205 will give `None` because a real symbol might be positive or negative. The `None` could also mean
 206 that not enough is known or implemented to compute the given fact. For instance, `(pi +`
 207 `E).is_irrational` gives `None`, because determining whether $\pi + e$ is rational or irrational is an
 208 open problem in mathematics [24].

209 Basic implications between the facts are used to deduce assumptions. For instance, the assump-
 210 tions system knows that being an integer implies being rational, so `Symbol('x', integer=True).is_rational`
 211 returns `True`. Furthermore, expressions compute the assumptions on themselves based on the
 212 assumptions of their arguments. For instance, if `x` and `y` are both created with `positive=True`,
 213 then `(x + y).is_positive` will be `True` whereas `(x - y).is_positive` will be `None`.

214 2.4 Extensibility

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

220 The typical way to create a custom SymPy object is to subclass an existing SymPy class,
 221 usually `Basic`, `Expr`, or `Function`. All SymPy classes used for expression trees⁴ should be
 222 subclasses of the base class `Basic`, which defines some basic methods for symbolic expression trees.
 223 `Expr` is the subclass for mathematical expressions that can be added and multiplied together.
 224 Instances of `Expr` typically represent complex numbers, but may also include other “rings” like
 225 matrix expressions. Not all SymPy classes are subclasses of `Expr`. For instance, logic expressions
 226 such as `And(x, y)` are subclasses of `Basic` but not of `Expr`.

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

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

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

³If A and B are Symbols created with `commutative=False` then SymPy will keep $A \cdot B$ and $B \cdot A$ distinct.

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

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

```

244 from sympy import Integer, Function, floor, factorial, polygamma
245
246 class gamma(Function)
247     @classmethod
248     def eval(cls, arg):
249         if isinstance(arg, Integer) and arg.is_positive:
250             return factorial(arg - 1)
251
252     def _eval_is_positive(self):
253         x = self.args[0]
254         if x.is_positive:
255             return True
256         elif x.is_noninteger:
257             return floor(x).is_even
258
259     def _eval_is_real(self):
260         x = self.args[0]
261         # noninteger means real and not integer
262         if x.is_positive or x.is_noninteger:
263             return True
264
265     def _eval_rewrite_as_factorial(self, z):
266         return factorial(z - 1)
267
268     def fdiff(self, argindex=1):
269         from sympy.core.function import ArgumentIndexError
270         if argindex == 1:
271             return self.func(self.args[0])*polygamma(0, self.args[0])
272         else:
273             raise ArgumentIndexError(self, argindex)

```

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

276 3 FEATURES

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

Table 1. SymPy Features and Descriptions

Feature	Description
Calculus	Algorithms for computing derivatives, integrals, and limits.
Category Theory	Representation of objects, morphisms, and diagrams. Tools for drawing diagrams with Xy-pic.
Code Generation	Generation of compilable and executable code in a variety of different programming languages from expressions directly. Target languages include C, Fortran, Julia, JavaScript, Mathematica, MATLAB and Octave, Python, and Theano.
Combinatorics & Group Theory	Permutations, combinations, partitions, subsets, various permutation groups (such as polyhedral, Rubik, symmetric, and others), Gray codes [27], and Prufer sequences [4].

Concrete Math	Summation, products, tools for determining whether summation and product expressions are convergent, absolutely convergent, hypergeometric, and for determining other properties; computation of Gosper's normal form [32] for two univariate polynomials.
Cryptography	Block and stream ciphers, including shift, Affine, substitution, Vigenère's, Hill's, bifid, RSA, Kid RSA, linear-feedback shift registers, and Elgamal encryption.
Differential Geometry	Representations of manifolds, metrics, tensor products, and coordinate systems in Riemannian and pseudo-Riemannian geometries [41].
Geometry	Representations of 2D geometrical entities, such as lines and circles. Enables queries on these entities, such as asking the area of an ellipse, checking for collinearity of a set of points, or finding the intersection between objects.
Lie Algebras	Representations of Lie algebras and root systems.
Logic	Boolean expressions, equivalence testing, satisfiability, and normal forms.
Matrices	Tools for creating matrices of symbols and expressions. Both sparse and dense representations, as well as symbolic linear algebraic operations (e.g., inversion and factorization), are supported.
Matrix Expressions	Matrices with symbolic dimensions (unspecified entries). Block matrices.
Number Theory	Prime number generation, primality testing, integer factorization, continued fractions, Egyptian fractions, modular arithmetic, quadratic residues, partitions, binomial and multinomial coefficients, prime number tools, hexadecimal digits of π , and integer factorization.
Plotting	Hooks for visualizing expressions via matplotlib [21] or as text drawings when lacking a graphical back-end. 2D function plotting, 3D function plotting, and 2D implicit function plotting are supported.
Polynomials	Polynomial algebras over various coefficient domains. Functionality ranges from simple operations (e.g., polynomial division) to advanced computations (e.g., Gröbner bases [1] and multivariate factorization over algebraic number domains).
Printing	Functions for printing SymPy expressions in the terminal with ASCII or Unicode characters and converting SymPy expressions to L ^A T _E X and MathML.
Quantum Mechanics	Quantum states, bra-ket notation, operators, basis sets, representations, tensor products, inner products, outer products, commutators, anticommutators, and specific quantum system implementations.
Series	Series expansion, sequences, and limits of sequences. This includes Taylor, Laurent, and Puiseux series as well as special series, such as Fourier and formal power series.
Sets	Representations of empty, finite, and infinite sets. This includes special sets such as for all natural, integer, and complex numbers. Operations on sets such as union, intersection, Cartesian product, and building sets from other sets are supported.
Simplification	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	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	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	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 [36].
Tensors	Symbolic manipulation of indexed objects.
Vectors	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”.⁵

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 [14]
<code>hyperexpand</code>	expand hypergeometric functions [34, 35]

3.2 Calculus

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

Limits are computed with the `limit` function, using the Gruntz algorithm [18] 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`.

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

As a more complex example, SymPy computes

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

⁵The `measure` parameter of the `simplify` function lets 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.

```

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

```

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

```

305 >>> diff(sin(x)*exp(x), x)
306 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 reimplement of Manuel Bronstein's "Poor Man's Integrator" [5], and an algorithm for computing integrals based on Meijer G-functions [34, 35]. 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

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

```

307 >>> s, t = symbols('s t', positive=True)
308 >>> integrate(exp(-s*t)*log(t), (t, 0, oo)).simplify()
309 -(log(s) + EulerGamma)/s
310 >>> integrate((-2*x**2*(log(x) + 1)*exp(x**2) +
311 ... (exp(x**2) + 1)**2)/(x*(exp(x**2) + 1)**2*(log(x) + 1)), x)
312 log(log(x) + 1) + 1/(exp(x**2) + 1)

```

Summations are computed with `summation` using a combination of Gosper's algorithm [17], an algorithm that uses Meijer G-functions [34, 35], and heuristics. Products are computed with `product` function via a suite of heuristics.

```

316 >>> i, n = symbols('i n')
317 >>> summation(2**i, (i, 0, n - 1))
318 2**n - 1
319 >>> summation(i*factorial(i), (i, 1, n))
320 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.

```

323 >>> integrate(x**x, x)
324 Integral(x**x, x)
325 >>> Sum(2**i, (i, 0, n - 1))
326 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

336 algorithms are used to solve the problem. The solutions to the original problem are subsequently
 337 recovered from the results. This is a common scheme in symbolic integration or summation
 338 algorithms.

339 SymPy implements dense and sparse polynomial representations.⁶ Both are used in the uni-
 340 variate and multivariate cases. The dense representation is the default for univariate polynomials.
 341 For multivariate polynomials, the choice of representation is based on the application. The most
 342 common case for the sparse representation is algorithms for computing Gröbner bases (Buchberger,
 343 F4, and F5) [7, 11, 12]. This is because different monomial orderings can be expressed easily in
 344 this representation. However, algorithms for computing multivariate GCDs or factorizations, at
 345 least those currently implemented in SymPy [29], are better expressed when the representation
 346 is dense. The dense multivariate representation is specifically a recursively-dense representation,
 347 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
 348 that despite this, the coefficient domain K , can be a multivariate polynomial domain as well.
 349 The dense recursive representation in Python gets inefficient as the number of variables increases.

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

351 3.4 Printers

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

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

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

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

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

```

363
 364 Alternately, the `use_unicode=False` flag can be set, which causes the expression to be printed
 365 using only ASCII characters.

```
366 >>> pprint(Integral(sqrt(phi0 + 1), phi0), use_unicode=False)
367 /
368 |
369 | _____
370 | \sqrt{phi0 + 1} d(phi0)
371 |
372 /
```

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

```
374 >>> print(latex(Integral(sqrt(phi0 + 1), phi0)))
375 \int \sqrt{\phi_{0} + 1}\lambda, d\phi_{0}
```

376 Users are encouraged to run the `init_printing` function at the beginning of interactive
 377 sessions, which automatically enables the best pretty printing supported by their environment.
 378 In the Jupyter Notebook or Qt Console [30], the \LaTeX printer is used to render expressions

⁶In 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.

379 using MathJax or L^AT_EX, if it is installed on the system. The 2D text representation is used
380 otherwise.

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

385 3.5 Solvers

386 SymPy has a module of equation solvers that can handle ordinary differential equations, recurrence
387 relationships, Diophantine equations, and algebraic equations. There is also rudimentary support
388 for simple partial differential equations.

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

```
394 solve(f, *symbols, **flags)
395 solveset(f, symbol, domain=S.Complexes)
```

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

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

401 Both functions implicitly assume that expressions are equal to 0. For instance, `solveset(x -
402 1, x)` solves $x - 1 = 0$ for x .

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

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

407 3.6 Matrices

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

```
411 >>> A = Matrix(2, 2, [x, x + y, y, x])
412 >>> A
413 Matrix([
414 [x, x + y],
415 [y, x]])
```

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

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

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

425 Internally these matrices store the elements as lists of lists, making it a dense representation.⁷
426 For storing sparse matrices, the `SparseMatrix` class can be used. Sparse matrices store their
427 elements as a dictionary of keys.

⁷Similar to the polynomials module, dense here means that all entries are stored in memory, contrasted with a sparse representation where only nonzero entries are stored.

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 symbolics and mechanics.

5.1.1 Vector Algebra

The `sympy.physics.vector` package provides reference frame-, time-, and space-aware vector and dyadic objects that allow for three-dimensional operations such as addition, subtraction, scalar multiplication, inner and outer products, and cross products. Both of these objects can be written in very compact notation that make it easy to express the vectors and dyadics in terms of multiple reference frames with arbitrarily defined relative orientations. The vectors are used to specify the positions, velocities, and accelerations of points; orientations, angular velocities, and angular accelerations of reference frames; and forces and torques. The dyadics are essentially reference frame-aware 3×3 tensors [42]. 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 $\frac{\pi}{3}$ rad, respectively, whereas the C frame is oriented with respect to the B frame through a simple rotation about the B frame's X unit vector through $\frac{\pi}{2}$ rad.

```

546 >>> from sympy.physics.vector import ReferenceFrame
547 >>> A = ReferenceFrame('A')
548 >>> B = ReferenceFrame('B')
549 >>> C = ReferenceFrame('C')
550 >>> B.orient(A, 'body', (pi, pi/3, pi/4), 'zxyz')
551 >>> C.orient(B, 'axis', (pi/2, B.x))
552 >>> v = 1*A.x + 2*B.z + 3*C.y
553 >>> v
554 A.x + 2*B.z + 3*C.y
555 >>> v.express(A)
556 A.x + 5*sqrt(3)/2*A.y + 5/2*A.z

```

5.1.2 Mechanics

The `sympy.physics.mechanics` package utilizes the `sympy.physics.vector` package to populate time-aware particle and rigid-body objects to fully describe the kinematics and kinetics of a rigid multi-body system. These objects store all of the information needed to derive the ordinary differential or differential algebraic equations that govern the motion of the system, i.e., the equations of motion. These equations of motion abide by Newton's laws of motion and can handle arbitrary kinematic constraints or complex loads. The package offers two automated methods for formulating the equations of motion based on Lagrangian Dynamics [23] and Kane's Method [22]. Lastly, there are automated linearization routines for constrained dynamical systems [31].

5.2 Quantum Mechanics

The `sympy.physics.quantum` package has extensive capabilities for performing symbolic quantum mechanics, using Python objects to represent the different mathematical objects relevant in quantum theory [38]: 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.

```

576 >>> from sympy.physics.quantum import Commutator, Dagger, Operator
577 >>> from sympy.physics.quantum import Ket, qapply

```

```

578 >>> A = Operator('A')
579 >>> B = Operator('B')
580 >>> C = Operator('C')
581 >>> D = Operator('D')
582 >>> a = Ket('a')
583 >>> comm = Commutator(A, B)
584 >>> comm
585 [A,B]
586 >>> qapply(Dagger(comm*a)).doit()
587 -<a|*(Dagger(A)*Dagger(B) - Dagger(B)*Dagger(A))

```

588 Commutators can be expanded using common commutator identities:

```

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

```

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

- 593 • Many of the exactly solvable quantum systems, including simple harmonic oscillator states
594 and raising/lowering operators, infinite square well states, and 3D position and momentum
595 operators and states.
- 596 • Second quantized formalism of non-relativistic many-body quantum mechanics [13].
- 597 • Quantum angular momentum [46]. Spin operators and their eigenstates can be represented
598 in any basis and for any quantum numbers. A rotation operator representing the Wigner-D
599 matrix, which may be defined symbolically or numerically, is also implemented to rotate
600 spin eigenstates. Functionality for coupling and uncoupling of arbitrary spin eigenstates is
601 provided, including symbolic representations of Clebsch-Gordon coefficients and Wigner
602 symbols.
- 603 • Quantum information and computing [26]. Multidimensional qubit states, and a full
604 set of one- and two-qubit gates are provided and can be represented symbolically or as
605 matrices/vectors. With these building blocks, it is possible to implement a number of basic
606 quantum algorithms including the quantum Fourier transform, quantum error correction,
607 quantum teleportation, Grover's algorithm, dense coding, etc. In addition, any quantum
608 circuit may be plotted using the `circuit_plot` function (Figure 1).

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

```

612 >>> from sympy.physics.quantum.qubit import Qubit
613 >>> from sympy.physics.quantum.gate import XGate
614 >>> q = Qubit('0101')
615 >>> q
616 |0101>
617 >>> X = XGate(1)
618 >>> qapply(X*q)
619 |0111>

```

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

```

621 >>> Dagger(q)
622 <0101|
623 >>> ip = Dagger(q)*q
624 >>> ip
625 <0101|0101>
626 >>> ip.doit()
627 1

```


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

```
630 >>> from sympy.physics.quantum.qubit import measure_all
631 >>> from sympy.physics.quantum.gate import H, X, Y, Z
632 >>> c = H(0)*H(1)*Qubit('00')
633 >>> c
634 H(0)*H(1)*|00>
635 >>> q = qapply(c)
636 >>> measure_all(q)
637 [(|00>, 1/4), (|01>, 1/4), (|10>, 1/4), (|11>, 1/4)]
```

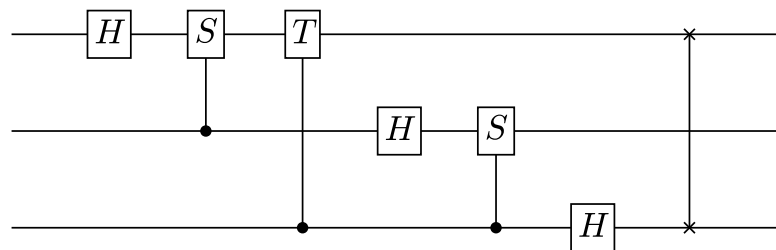


Figure 1. The circuit diagram for a three-qubit quantum Fourier transform generated by SymPy.

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

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

647 6 CONCLUSION AND FUTURE WORK

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

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

657 SymPy has submodules for many areas of mathematics. This includes functions for simplify-
658 ing expressions, performing common calculus operations, pretty printing expressions, solving
659 equations, and representing symbolic matrices. Other included areas are discrete math, concrete
660 math, plotting, geometry, statistics, polynomials, sets, series, vectors, combinatorics, group
661 theory, code generation, tensors, Lie algebras, cryptography, and special functions. Additionally,
662 SymPy contains submodules targeting certain specific domains, such as classical mechanics and

663 quantum mechanics. This breadth of domains has been engendered by a strong and vibrant user
664 community. Anecdotally, these users likely chose SymPy because of its ease of access.

665 Some of the planned future work for SymPy includes work on improving code generation,
666 improvements to the speed of SymPy (one area of work in this direction is SymEngine, a C++
667 symbolic manipulation library that is planned to be usable as a alternative core for SymPy),
668 improving the assumptions system, and improving the solvers module.

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