SUPPLEMENTARY MATERIALS: SYMPY: SYMBOLIC COMPUTING IN PYTHON

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As in the paper, all examples in the supplement assume that the following has been run:

```
>>> from sympy import *
>>> x, y, z = symbols('x y z')
```

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SM1. Limits: The Gruntz Algorithm. SymPy calculates limits using the Gruntz algorithm, as described in [SM7]. The basic idea is as follows: any limit can be converted to a limit $\lim_{x\to\infty} f(x)$ by substitutions like $x \to \frac{1}{x}$. Then the subexpression ω (that converges to zero as $x \to \infty$ faster than all other subexpressions) is identified in $f(x)$, and $f(x)$ is expanded into a series with respect to ω. Any positive powers of ω converge to zero (while negative powers indicate an infinite limit) and any constant term independent of ω determines the limit. When a constant term still dependends on x the Gruntz algorithm is applied again until a final numerical value is obtained as the limit.

To determine the most rapidly varying subexpression, the comparability classes must first be defined, by calculating L:

$$L \equiv \lim_{x\to\infty} \frac{\log|f(x)|}{\log|g(x)|} \tag{SM1}$$

The relations $<$, $>$, and $\sim$ are defined as follows: $f > g$ when $L = \pm\infty$ (it is said that f is more rapidly varying than g, i.e., f goes to ∞ or 0 faster than g), $f < g$ when $L = 0$ (f is less rapidly varying than g) and $f \sim g$ when $L \neq 0, \pm\infty$ (both f and g are bounded from above and below by suitable integral powers of the other). Note that if $f > g$, then $f > g^n$ for any n. Here are some examples of comparability classes:

$$2 < x < e^x < e^{x^2} < e^{e^x}$$

$$2 \sim 3 \sim -5$$

$$x \sim x^2 \sim x^3 \sim \frac{1}{x} \sim x^m \sim -x$$

$$e^x \sim e^{-x} \sim e^{2x} \sim e^{x+e^{-x}}$$

$$f(x) \sim \frac{1}{f(x)}$$

The Gruntz algorithm is now illustrated with the following example:

$$f(x) = e^{x+2e^{-x}} - e^x + \frac{1}{x}\,. \tag{SM2}$$

The goal is to calculate $\lim_{x\to\infty} f(x)$. First, the set of most rapidly varying subexpressions is determined—the so-called *mrv set*. For (SM2), the mrv set $\{e^x, e^{-x}, e^{x+2e^{-x}}\}$ is obtained. These are all subexpressions of (SM2) and they all belong to the same comparability class. This calculation can be done using SymPy as follows:

```
>>> from sympy.series.gruntz import mrv
>>> mrv(exp(x+2*exp(-x))-exp(x) + 1/x, x)[0].keys()
dict_keys([exp(x + 2*exp(-x)), exp(x), exp(-x)])
```

Next, an arbitrary item ω is taken from mrv that converges to zero for $x \to \infty$. The item $\omega = e^{-x}$ is obtained. If such a term is not present in the mrv set (i.e., all terms converge to infinity instead of zero), the relation $f(x) \sim \frac{1}{f(x)}$ can be used.

The next step is to rewrite the mrv set in terms of ω: $\{\frac{1}{\omega}, \omega, \frac{1}{\omega}e^{2\omega}\}$. Then the original subexpressions are substituted back into $f(x)$ and expanded with respect to ω:

$$f(x) = \frac{1}{x} - \frac{1}{\omega} + \frac{1}{\omega}e^{2\omega} = 2 + \frac{1}{x} + 2\omega + O(\omega^2) \tag{SM3}$$

Since ω is from the mrv set, then in the limit as $x \to \infty$, $\omega \to 0$, and so $2\omega + O(\omega^2) \to 0$ in (SM3):

$$f(x) = \frac{1}{x} - \frac{1}{\omega} + \frac{1}{\omega}e^{2\omega} = 2 + \frac{1}{x} + 2\omega + O(\omega^2) \to 2 + \frac{1}{x} \tag{SM4}$$

Since the result $(2 + \frac{1}{x})$ still depends on x, the above procedure is repeated until just a value independent of x is obtained. This is the final limit. In the above case the limit is 2, as can be verified by SymPy:

```
>>> limit(exp(x+2*exp(-x))-exp(x) + 1/x, x, oo)
2
```

In general, when $f(x)$ is expanded in terms of ω, the following is obtained:

$$f(x) = \underbrace{O\left(\frac{1}{\omega^3}\right)}_{\infty} + \underbrace{\frac{C_{-2}(x)}{\omega^2}}_{\infty} + \underbrace{\frac{C_{-1}(x)}{\omega}}_{\infty} + C_0(x) + \underbrace{C_1(x)\omega}_{0} + \underbrace{O(\omega^2)}_{0} \tag{SM5}$$

The positive powers of ω are zero. If there are any negative powers of ω, then the result of the limit is infinity, otherwise the limit is equal to $\lim_{x\to\infty} C_0(x)$. The expression $C_0(x)$ is simpler than $f(x)$ and so the algorithm always converges. A proof of this and further details on the algorithm are given in Gruntz's PhD thesis [SM7].

SM2. Series.

SM2.1. Series Expansion. SymPy is able to calculate the symbolic series expansion of an arbitrary series or expression involving elementary and special functions and multiple variables. For this it has two different implementations: the `series` method and Ring Series.

The first approach stores a series as an instance of the `Expr` class. Each function has its specific implementation of its expansion, which is able to evaluate the Puiseux series expansion about a specified point. For example, consider a Taylor expansion about 0:

```
>>> series(sin(x+y) + cos(x*y), x, 0, 2)
1 + sin(y) + x*cos(y) + O(x**2)
```

The newer and much faster approach called Ring Series makes use of the fact that a truncated Taylor series is simply a polynomial. Correspondingly, they may be represented by sparse polynomials which perform well in a under a wide range of cases. Ring Series also gives the user the freedom to choose the type of coefficients to use, resulting in faster operations on certain types.

For this, several low-level methods for expansion of trigonometric, hyperbolic and other elementary operations (like series inversion, calculating the nth root, etc.) are implemented using variants of the Newton Method [SM2]. All these support Puiseux series expansion. The following example demonstrates the use of an elementary function that calculates the Taylor expansion of the sine of a series.

```
>>> from sympy.polys.ring_series import rs_sin
>>> R, t = ring('t', QQ)
>>> rs_sin(t**2 + t, t, 5)
-1/2*t**4 - 1/6*t**3 + t**2 + t
```

The function `sympy.polys.rs_series` makes use of these elementary functions to expand an arbitrary SymPy expression. It does so by following a recursive strategy of expanding the lowermost functions first and then composing them recursively to calculate the desired expansion. Currently, it only supports expansion about 0 and

is under active development. Ring Series is several times faster than the default implementation with the speed difference increasing with the size of the series. The `sympy.polys.rs_series` takes as input any SymPy expression and hence there is no need to explicitly create a polynomial `ring`. An example demonstrating its use:

```
>>> from sympy.polys.ring_series import rs_series
>>> from sympy.abc import a, b
>>> rs_series(sin(a + b), a, 4)
-1/2*(sin(b))*a**2 + (sin(b)) - 1/6*a**3*(cos(b)) + a*(cos(b))
```

SM2.2. Formal Power Series. SymPy can be used for computing the formal power series of a function. The implementation is based on the algorithm described in the paper on formal power series [SM8]. The advantage of this approach is that an explicit formula for the coefficients of the series expansion is generated rather than just computing a few terms.

The following example shows how to use `fps`:

```
>>> f = fps(sin(x), x, x0=0)
>>> f.truncate(6)
x - x**3/6 + x**5/120 + O(x**6)
>>> f[15]
-x**15/1307674368000
```

SM2.3. Fourier Series. SymPy provides functionality to compute Fourier series of a function using the `fourier_series` function:

```
>>> L = symbols('L')
>>> expr = 2 * (Heaviside(x/L) - Heaviside(x/L - 1)) - 1
>>> f = fourier_series(expr, (x, 0, 2*L))
>>> f.truncate(3)
4*sin(pi*x/L)/pi + 4*sin(3*pi*x/L)/(3*pi) + 4*sin(5*pi*x/L)/(5*pi)
```

SM3. Logic. SymPy supports construction and manipulation of boolean expressions through the `sympy.logic` module. SymPy symbols can be used as propositional variables and subsequently be replaced with `True` or `False` values. Many functions for manipulating boolean expressions have been implemented in the `logic` module.

SM3.1. Constructing boolean expressions. A boolean variable can be declared as a SymPy `Symbol`. Python operators `&`, `|` and `~` are overridden when using SymPy objects to use the SymPy functionality for logical `And`, `Or`, and `Not`. Other logic functions are also integrated into SymPy, including `Xor` and `Implies`, which are constructed with `^` and `>>`, respectively. Expressions can therefore be constructed either by using the shortcut operator notation or by directly creating the relevant objects: `And()`, `Or()`, `Not()`, `Xor()`, `Implies()`, `Nand()`, `Nor()`, etc.:

```
>>> e = (x & y) | z
>>> e.subs({x: True, y: True, z: False})
True
```

SM3.2. CNF and DNF. Any boolean expression can be converted to conjunctive normal form, disjunctive normal form, or negation normal form. The API also exposes methods to check if a boolean expression is in any of the aforementioned forms.

```
>>> from sympy.logic.boolalg import is_dnf, is_cnf
>>> to_cnf((x & y) | z)
And(Or(x, z), Or(y, z))
```

```
>>> to_dnf(x & (y | z))
Or(And(x, y), And(x, z))
>>> is_cnf((x | y) & z)
True
>>> is_dnf((x & y) | z)
True
```

SM3.3. Simplification and Equivalence. The `sympy.logic` module supports simplification of given boolean expression by making deductions from the expression. Equivalence of two logical expressions can also be checked. In the case of equivalence, the function `bool_map` can be used to show which variables of the first expression correspond to which variables of the second one.

```
>>> a, b, c = symbols('a b c')
>>> e = a & (~a | ~b) & (a | c)
>>> simplify(e)
And(Not(b), a)
>>> e1 = a & (b | c)
>>> e2 = (x & y) | (x & z)
>>> bool_map(e1, e2)
(And(Or(b, c), a), {a: x, b: y, c: z})
```

SM3.4. SAT solving. The module also supports satisfiability (SAT) checking of a given boolean expression. If an expression is satisfiable, it is possible to return a variable assignment which satisfies it. The API also supports listing all possible assignments. The SAT solver has a clause learning DPLL algorithm implemented with a watch literal scheme and VSIDS heuristic [SM11].

```
>>> satisfiable(a & (~a | b) & (~b | c) & ~c)
False
>>> satisfiable(a & (~a | b) & (~b | c) & c)
{a: True, b: True, c: True}
```

SM4. Diophantine Equations. Diophantine equations play a central role in number theory. A Diophantine equation has the form, $f(x_1, x_2, \ldots, x_n) = 0$ where $n \geq 2$ and $x_1, x_2, \ldots, x_n$ are integer variables. If there are n integers $a_1, a_2, \ldots, a_n$ such that $x_1 = a_1, x_2 = a_2, \ldots, x_n = a_n$ satisfies the above equation, the equation is said to be solvable.

Currently, the following five types of Diophantine equations can be solved using SymPy's Diophantine module ($a_1, \ldots, a_{n+1}$, a, b, c, d, e, f, and k are explicitly given rational constants):

- Linear Diophantine equations: $a_1x_1 + a_2x_2 + \cdots + a_nx_n = b$
- General binary quadratic equation: $ax^2 + bxy + cy^2 + dx + ey + f = 0$
- Homogeneous ternary quadratic equation: $ax^2+by^2+cz^2+dxy+eyz+fzx = 0$
- Extended Pythagorean equation: $a_1x_1^2 + a_2x_2^2 + \cdots + a_nx_n^2 = a_{n+1}x_{n+1}^2$
- General sum of squares: $x_1^2 + x_2^2 + \cdots + x_n^2 = k$

The `diophantine` function factors the equation it is given (if possible), solves each factor separately, and combines the results to give a final solution set. The following examples illustrate some of the basic functionalities of the Diophantine module.

```
>>> from sympy.solvers.diophantine import *
>>> diophantine(2*x + 3*y - 5)
set([(3*t_0 - 5, -2*t_0 + 5)])
```

```
>>> diophantine(2*x + 4*y - 3)
set()

>>> diophantine(x**2 - 4*x*y + 8*y**2 - 3*x + 7*y - 5)
set([(2, 1), (5, 1)])

>>> diophantine(x**2 - 4*x*y + 4*y**2 - 3*x + 7*y - 5)
set([(-2*t**2 - 7*t + 10, -t**2 - 3*t + 5)])

>>> diophantine(3*x**2 + 4*y**2 - 5*z**2 + 4*x*y - 7*y*z + 7*z*x)
set([(-16*p**2 + 28*p*q + 20*q**2,
3*p**2 + 38*p*q - 25*q**2,
4*p**2 - 24*p*q + 68*q**2)])

>>> x1, x2, x3, x4, x5, x6 = symbols('x1, x2, x3, x4, x5, x6')
>>> diophantine(9*x1**2 + 16*x2**2 + x3**2 + 49*x4**2 + 4*x5**2 - 25*x6**2)
set([(70*t1**2 + 70*t2**2 + 70*t3**2 + 70*t4**2 - 70*t5**2, 105*t1*t5,
420*t2*t5, 60*t3*t5, 210*t4*t5,
42*t1**2 + 42*t2**2 + 42*t3**2 + 42*t4**2 + 42*t5**2)])

>>> a, b, c, d = symbols('a:d')
>>> diophantine(a**2 + b**2 + c**2 + d**2 - 23)
set([(2, 3, 3, 1)])
```

SM5. Sets. SymPy supports representation of a wide variety of mathematical sets. This is achieved by first defining abstract representations of atomic set classes and then combining and transforming them using various set operations.

Each of the set classes inherits from the base class `Set` and defines methods to check membership and calculate unions, intersections, and set differences. When these methods are not able to evaluate to atomic set classes, they are represented as abstract unevaluated objects.

SymPy has the following atomic set classes:

- `EmptySet` represents the empty set $\emptyset$.
- `UniversalSet` is an abstract "universal set" of which everything is a member. The union of the universal set with any set gives the universal set and the intersection gives the other set itself.
- `FiniteSet` is functionally equivalent to Python's built in `set` object. Its members can be any SymPy object including other sets.
- `Integers` represents the set of integers $\mathbb{Z}$.
- `Naturals` represents the set of natural numbers $\mathbb{N}$, i.e., the set of positive integers.
- `Naturals0` represents the set of whole numbers $\mathbb{N}_0$, which are all the non-negative integers.
- `Range` represents a range of integers. A range is defined by specifying a start value, an end value, and a step size. The enumeration of a `Range` object is functionally equivalent to Python's `range` except it supports infinite endpoints, allowing the representation of infinite ranges.
- `Interval` represents an interval of real numbers. It is defined by giving the start and the end points and by specifying if the interval is open or closed on the respective ends.

Other than unevaluated classes of `Union`, `Intersection`, and `Complement` operations, SymPy has the following set classes.

- `ProductSet` defines the Cartesian product of two or more sets. The product set is useful when representing higher dimensional spaces. For example, to represent a three-dimensional space, SymPy uses the Cartesian product of three real sets.
- `ImageSet` represents the image of a function when applied to a particular set. The image set of a function F with respect to a set S is $\{F(x) \mid x \in S\}$. SymPy uses image sets to represent sets of infinite solutions of equations such as $\sin(x) = 0$.
- `ConditionSet` represents a subset of a set whose members satisfy a particular condition. The subset of set S given by the condition H is $\{x \mid H(x), x \in S\}$. SymPy uses condition sets to represent the set of solutions of equations and inequalities, where the equation or the inequality is the condition and the set is the domain over which it is being solved.

A few other classes are implemented as special cases of the classes described above. The set of real numbers, `Reals`, is implemented as a special case of `Interval`. `ComplexRegion` is implemented as a special case of `ImageSet`. `ComplexRegion` supports both polar and rectangular representation of regions on the complex plane.

SM6. Statistics. The `sympy.stats` module provides random variable types and methods for computing of statistical properties of expressions involving random variables, which can be either continuous or discrete, the latter ones being further divided into finite and infinite. The variables are associated with probability densities on corresponding domains and internally defined in terms of probability spaces. Apart from the possibility of defining the random variables from user supplied density distribution, SymPy provides definitions of most common distributions, including `Uniform`, `Poisson`, `Normal`, `Binomial`, `Bernoulli`, and many others.

Properties of random expressions can be calculated using, e.g., `expectation` (abbreviated `E`) and `variance` to calculate expectation and variance. Internally, these functions generate integrals and summations, which are automatically evaluated. The evaluation can be suppressed using `evaluate=False` keyword argument.

Conditions on random variables can be defined with inequalities, equalities, and logical operators and their overall probabilities are obtained using `P`. The features can be illustrated on a model of two dice throws:

```
>>> from sympy.stats import Die, P, E
>>> X, Y = Die("X"), Die("Y")
>>> P(Eq(X, 6) & Eq(Y, 6))
1/36
>>> P(X>Y)
5/12
```

The conditions can also be supplied as a second parameter to `E`, `P`, and other methods to calculate the property given the condition:

```
>>> E(X, X+Y<5)
5/3
```

Using the facilities of the `sympy.stats` module, one can, for example, calculate the well known properties of maxwellian velocity distribution

```
>>> from sympy.stats import Maxwell, density
>>> kT, m, x = symbols("kT m x", positive=True)
>>> v = Maxwell("v", sqrt(kT/m))
```

```
>>> E(v)                                # mean velocity
2*sqrt(2)*sqrt(kT)/(sqrt(pi)*sqrt(m))
>>> E(v, evaluate=False)                # unevaluated mean velocity
Integral(sqrt(2)*m**(3/2)*v**3*exp(-m*v**2/(2*kT))/(sqrt(pi)*kT**(3/2)),
(v, 0, oo))
>>> E(m*v**2/2)                         # mean energy
3*kT/2
>>> solve(density(v)(x).diff(x), x)[0]  # most probable velocity
sqrt(2)*sqrt(kT)/sqrt(m)
```

More information on the `sympy.stats` module can be found in [SM13].

SM7. Category Theory. SymPy includes a module for dealing with categories—abstract mathematical objects representing classes of structures as classes of objects (points) and morphisms (arrows) between the objects. The module was designed with the following two goals in mind:

1. automatic typesetting of diagrams given by a collection of objects and of morphisms between them, and
2. specification and semi-automatic derivation of properties using commutative diagrams.

As of version 1.0, SymPy only implements the first goal, while a partially working draft of implementation of the second goal is available at https://github.com/scolobb/sympy/tree/ct4-commutativity.

In order to achieve the two goals, the module `sympy.categories` defines several classes representing some of the essential concepts: objects, morphisms, categories, and diagrams. In category theory, the inner structure of objects is often discarded in the favor of studying the properties of morphisms, so the class `Object` is essentially a synonym of the class `Symbol`. There are several morphism classes which do not have a particular internal structure either, though an exception is `CompositeMorphism`, which essentially stores a list of morphisms.

The class `Diagram` captures the properties of morphisms. This class stores a family of morphisms, the corresponding source and target objects, and, possibly, some properties of the morphisms. Generally, no restrictions are imposed on what the properties may be—for example, one might use strings of the form "forall", "exists", "unique", etc. Furthermore, the morphisms of a diagram are grouped into *premises* and *conclusions* in order to be able to represent logical implications of the form "for a collection of morphisms P with properties $p : P \to \Omega$ (the premises), there exists a collection of morphisms C with properties $c : C \to \Omega$ (the conclusions)", where Ω is the universal collection of properties. Finally, the class `Category` includes a collection of diagrams which are deemed commutative and which therefore define the properties of this category.

Automatic typesetting of diagrams takes a `Diagram` and produces LaTeX code using the `Xy-pic` package. Typesetting is done in two stages: layout and generation of `Xy-pic` code. The layout stage is taken care of by the class `DiagramGrid`, which takes a `Diagram` and lays out the objects in a grid, trying to reduce the average length of the arrows in the final picture. By default, `DiagramGrid` uses a series of triangle-based heuristics to produce a rectangular grid. A linear layout can also be imposed. Furthermore, groups of objects can be given; in this case, the groups will be treated as atomic cells, and the member objects will be typeset independently of the other objects.

The second phase of diagram typesetting consists in actually drawing the picture and is carried out by the class `XypicDiagramDrawer`. An example of a diagram automatically typeset by `DiagramgGrid` and `XypicDiagramDrawer` in given in Figure SM1.

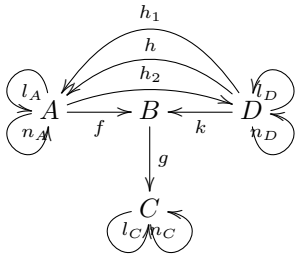

Fig. SM1: An automatically typeset commutative diagram

As far as the second main goal of the module is concerned, the principal idea consists in automatically deciding whether a diagram is commutative or not, given a collection of "axioms": diagrams known to be commutative. The implementation is based on graph embeddings (injective maps): whenever an embedding of a commutative diagram into a given diagram is found, one concludes that the subdiagram is commutative. Deciding commutativity of the whole diagram is therefore based (theoretically) on finding a "cover" of the target diagram by embeddings of the axioms. The naïve implementation proved to be prohibitively slow; a better optimized version is therefore in order, as well as application of heuristics.

SM8. SymPy Gamma. SymPy Gamma is a simple web application that runs on Google App Engine. It executes and displays the results of SymPy expressions as well as additional related computations, in a fashion similar to that of Wolfram|Alpha. For instance, entering an integer will display its prime factors, digits in the base-10 expansion, and a factorization diagram. Entering a function will display its docstring; in general, entering an arbitrary expression will display its derivative, integral, series expansion, plot, and roots.

SymPy Gamma also has several features beyond just computing the results using SymPy.

- SymPy Gamma displays integration and differentiation steps in detail, which can be viewed in Figure SM2:

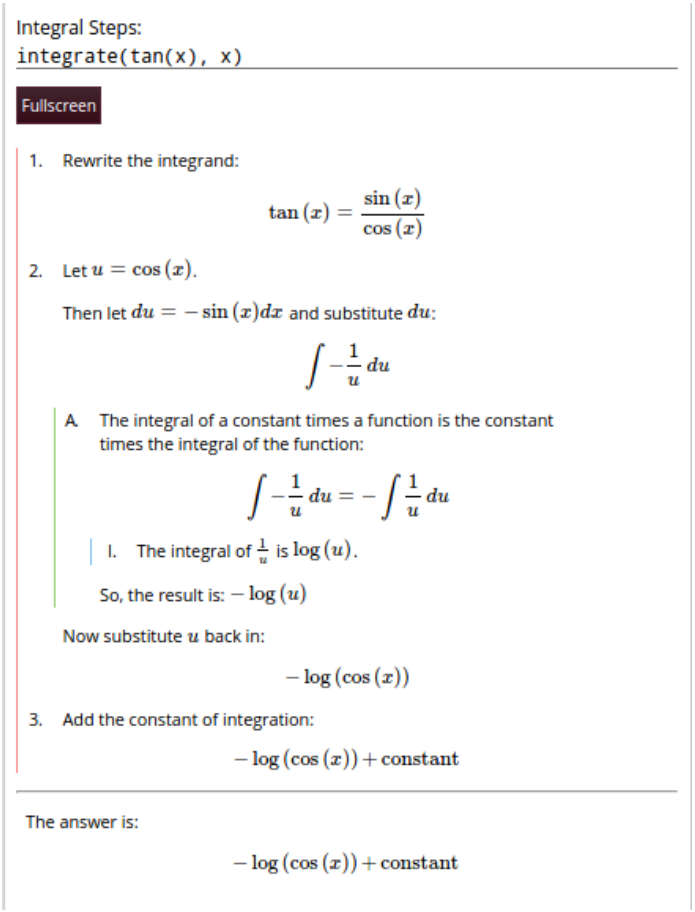

Fig. SM2: Integral steps of $\tan(x)$

- SymPy Gamma displays the factor tree diagrams for different numbers.
- SymPy Gamma saves user search queries, and offers many such similar features for free, which Wolfram|Alpha only offers to its paid users.

Every input query from the user on SymPy Gamma is first parsed by its own parser capable of handling several different forms of function names which SymPy as a library does not support. For instance, SymPy Gamma supports queries like `sin x`, whereas SymPy will only recognise `sin(x)`.

This parser converts the input query to the equivalent SymPy readable code, which is then processed by SymPy, and the result is finally printed with the built-in LaTeX output and rendered by the SymPy Gamma web application.

SM9. SymPy Live. SymPy Live is an online Python shell, which uses the Google App Engine to executes SymPy code. It is integrated in the SymPy documentation examples at http://docs.sympy.org.

This is accomplished by providing a HTML/JavaScript GUI for entering source code and visualization of output, and a server that evaluates the requested source code. It is an interactive AJAX shell that runs SymPy code using Python on the server.

SM10. Comparison with Mathematica. Wolfram Mathematica is a popular proprietary CAS that features highly advanced algorithms, has a core written in C++ [SM16], and interprets its own programming language, Wolfram Language.

Analogous to Lisp S-expressions, Mathematica uses its own style of M-expressions, which are arrays of either atoms or other M-expressions. The first element of the expression identifies the type of the expression and is indexed by zero, and the first argument is indexed starting with one. In SymPy, expression arguments are stored in a Python tuple (that is, an immutable array), while the expression type is identified by the type of the object storing the expression.

Mathematica can associate attributes to its atoms. Attributes may define mathematical properties and behavior of the nodes associated to the atom. In SymPy, the usage of static class fields is roughly similar to Mathematica's attributes, though other programming patterns may also be used to achieve an equivalent behavior such as class inheritance.

Unlike SymPy, Mathematica's expressions are mutable: one can change parts of the expression tree without the need of creating a new object. The mutability of Mathematica expressions allows for a lazy updating of any references to a given data structure.

Products in Mathematica are determined by some built in node types, such as `Times`, `Dot`, and others. `Times` is a representation of the `*` operator, and is always meant to represent a commutative product operator. The other notable product is `Dot`, which represents the `.` operator. This product represents matrix multiplication. It is not commutative. Unlike Mathematica, SymPy determines commutativity with respect to multiplication from the expression type of the factors. Mathematica puts the `Orderless` attribute on the expression type.

Regarding associative expressions, SymPy handles associativity of sums and products by automatically flattening them, Mathematica specifies the `Flat` attribute on the expression type.

Mathematica relies heavily on pattern matching—even the so-called equivalent of function declaration is in reality the definition of a pattern generating an expression tree transformation on input expressions. Mathematica's pattern matching is sensitive to associative, commutative, and one-identity properties of its expression tree nodes. SymPy has various ways to perform pattern matching. All of them play a lesser role in the CAS than in Mathematica and are basically available as a tool to rewrite expressions. The differential equation solver in SymPy somewhat relies on pattern matching to identify differential equation types, but it is envisaged to replace that strategy with analysis of Lie symmetries in the future. Mathematica's real advantage is the ability to add (at runtime) new overloading to the expression builder or specific subnodes. Consider for example:

```
In[1]:= Unprotect[Plus]
Out[1]= {Plus}

In[2]:= Sin[x_]^2 + Cos[y_]^2 := 1

In[3]:= x + Sin[t]^2 + y + Cos[t]^2
Out[3]= 1 + x + y
```

This expression in Mathematica defines a substitution rule that overloads the functionality of the `Plus` node (the node for additions in Mathematica). A symbol with a trailing underscore is treated as a wildcard. Although one may wish to keep this identity unevaluated, this example clearly illustrates the potential to define one's own

immediate transformation rules. In SymPy, the operations constructing the addition node in the expression tree are Python class constructors and cannot be modified at runtime.[1] The way SymPy deals with extending the missing runtime overloadability functionality is by subclassing the node types: subclasses may redefine the class constructor to yield the proper extended functionality.

Unlike SymPy, Mathematica does not support type inheritance or polymorphism [SM4]. SymPy relies heavily on class inheritance, but for the most part, class inheritance is used to make sure that SymPy objects inherit the proper methods and implement the basic hashing system.

While Mathematica interprets nested lists as matrices whenever the sublists have the same length, matrices in SymPy are a type in their own right, allowing ordinary operators and functions (like multiplication and exponentiation) to be used as they traditionally are in mathematics.

```
>>> exp(Matrix([[1, 1],[0, 2]])) * Matrix([a, b])
Matrix([
[E*a + b*(-E + exp(2))],
[             b*exp(2)]])
```

Using the standard multiplication in Mathematica performs an element-wise product and calling the exponential function `Exp` on a matrix returns an element-wise exponentiation of its elements.

Unevaluated expressions in Mathematica can be achieved in various ways, most commonly with the `HoldForm` or `Hold` nodes, that block the evaluation of subnodes by the parser. Such a node cannot be expressed in Python because of greedy evaluation. Whenever needed in SymPy, it is necessary to add the parameter `evaluate=False` to all subnodes.

In Mathematica, the operator `==` returns a boolean whenever it is able to immediately evaluate the truth of the equality, otherwise it returns an `Equal` expression. In SymPy, `==` means structural equality and is always guaranteed to return a boolean expression. To express a mathematical equality in SymPy it is necessary to explicitly construct an instance of the `Equality` class.

SymPy, in accordance with Python (and unlike the usual programming convention), uses ** to express the power operator, while Mathematica uses the more common ^.

SymPy's use of floating-point numbers is similar to that of most other CASs, including Maple and Maxima. By contrast, Mathematica uses a form of significance arithmetic [SM14] for approximate numbers. This offers further protection against numerical errors, although it comes with its own set of problems (for a critique of significance arithmetic, see Fateman [SM4]). Internally, SymPy's `evalf` method works similarly to Mathematica's significance arithmetic, but the semantics are isolated from the rest of the system.

SM11. Other Projects that use SymPy. There are several projects that use SymPy as a library for implementing a part of their functionality. Some of them are listed below:

- **Cadabra**: Cadabra is a CAS designed specifically for the resolution of problems encountered in field theory.
- **Octave Symbolic**: The Octave-Forge Symbolic package adds symbolic calculation features to GNU Octave. These include common CAS tools such as

[1] Nonetheless, Python supports monkey patching but it is a discouraged programming pattern.

algebraic operations, calculus, equation solving, Fourier and Laplace transforms, variable precision arithmetic, and other features.

- **SymPy.jl**: Provides a Julia interface to SymPy using PyCall.
- **Mathics**: Mathics is a free, general-purpose online CAS featuring Mathematica compatible syntax and functions. It is backed by highly extensible Python code, relying on SymPy for most mathematical tasks.
- **Mathpix**: An iOS App, that detects handwritten math as input, and uses SymPy Gamma to evaluate the math input and generate the relevant steps to solve the problem.
- **IKFast**: IKFast is a robot kinematics compiler provided by OpenRAVE. It analytically solves robot inverse kinematics equations and generates optimized C++ files. It uses SymPy for its internal symbolic mathematics.
- **Sage**: A CAS, visioned to be a viable free open source alternative to Magma, Maple, Mathematica and MATLAB. Sage includes many open source mathematical libraries, including SymPy.
- **SageMathCloud**: SageMathCloud is a web-based cloud computing and course management platform for computational mathematics.
- **PyDy**: Multibody Dynamics with Python.
- **galgebra**: Geometric algebra (previously `sympy.galgebra`).
- **yt**: Python package for analyzing and visualizing volumetric data (`yt.units` uses SymPy).
- **SfePy**: Simple finite elements in Python, see section SM11.1.
- **Quameon**: Quantum Monte Carlo in Python.
- **Lcapy**: Experimental Python package for teaching linear circuit analysis.
- **Quantum Programming in Python**: Quantum 1D Simple Harmonic Oscillator and Quantum Mapping Gate.
- **LaTeX Expression project**: Easy LaTeX typesetting of algebraic expressions in symbolic form with automatic substitution and result computation.
- **Symbolic statistical modeling**: Adding statistical operations to complex physical models.

SM11.1. SfePy. **SfePy** (Simple finite elements in Python), cf. [SM3], is a Python package for solving partial differential equations (PDEs) in 1D, 2D and 3D by the finite element (FE) method [SM17]. SymPy is used within this package mostly for code generation and testing, namely:

- generation of the hierarchical FE basis module, involving generation and symbolic differentiation of 1D Legendre and Lobatto polynomials, constructing the FE basis polynomials [SM15] and generating the C code;
- generation of symbolic conversion formulas for various groups of elastic constants [SM6]: provide any two of the Young's modulus, Poisson's ratio, bulk modulus, Lamé's first parameter, shear modulus (Lamé's second parameter) or longitudinal wave modulus and get the other ones;
- simple physical unit conversions, generation of consistent unit sets;
- testing FE solutions using method of manufactured (analytical) solutions: the differential operator of a PDE is symbolically applied and a symbolic right-hand side is created, evaluated in quadrature points, and subsequently used to obtain a numerical solution that is then compared to the analytical one;
- testing accuracy of 1D, 2D and 3D numerical quadrature formulas (cf. [SM1]) by generating polynomials of suitable orders, integrating them, and comparing the results with those obtained by the numerical quadrature.

SM12. Tensors. Ongoing work to provide the capabilities of tensor computer algebra has so far produced the `tensor` module. It comprises three submodules whose purposes are quite different: `sympy.tensor.indexed` and `sympy.tensor.indexed_methods` support indexed symbols, `sympy.tensor.array` contains facilities to operate on symbolic N-dimensional arrays, and finally `sympy.tensor.tensor` is used to define abstract tensors. The abstract tensors submodule is inspired by xAct [SM10] and Cadabra [SM12]. Canonicalization based on the Butler-Portugal [SM9] algorithm is supported in SymPy. Tensor support in SymPy is currently limited to polynomial tensor expressions.

SM13. Numerical simplification. The `nsimplify` function in SymPy (a wrapper of `identify` in mpmath) attempts to find a simple symbolic expression that evaluates to the same numerical value as the given input. It works by applying a few simple transformations (including square roots, reciprocals, logarithms and exponentials) to the input and, for each transformed value, using the PSLQ algorithm [SM5] to search for a matching algebraic number or optionally a linear combination of user-provided base constants (such as π).

```
>>> t = 1 / (sin(pi/5)+sin(2*pi/5)+sin(3*pi/5)+sin(4*pi/5))**2
>>> nsimplify(t)
-2*sqrt(5)/5 + 1
>>> nsimplify(pi, tolerance=0.01)
22/7
>>> nsimplify(1.783919626661888, [pi], tolerance=1e-12)
pi/(-1/3 + 2*pi/3)
```

SM14. Examples.

SM14.1. Simplification.

- `expand`:
  ```
  >>> expand((x + y)**3)
  x**3 + 3*x**2*y + 3*x*y**2 + y**3
  ```
- `factor`:
  ```
  >>> factor(x**3 + 3*x**2*y + 3*x*y**2 + y**3)
  (x + y)**3
  ```
- `collect`:
  ```
  >>> collect(y*x**2 + 3*x**2 - x*y + x - 1, x)
  x**2*(y + 3) + x*(-y + 1) - 1
  ```
- `cancel`:
  ```
  >>> cancel((x**2 + 2*x + 1)/(x**2 - 1))
  (x + 1)/(x - 1)
  ```
- `apart`:
  ```
  >>> apart((x**3 + 4*x - 1)/(x**2 - 1))
  x + 3/(x + 1) + 2/(x - 1)
  ```
- `trigsimp`:
  ```
  >>> trigsimp(cos(x)**2*tan(x) - sin(2*x))
  -sin(2*x)/2
  ```

SM14.2. Polynomials.

- Factorization:
  ```
  >>> t = symbols('t')
  >>> f = (2115*x**4*y + 45*x**3*z**3*t**2 - 45*x**3*t**2 -
  ...      423*x*y**4 - 47*x*y**3 + 141*x*y*z**3 + 94*x*y*z*t -
  ```

```
...      9*y**3*z**3*t**2 + 9*y**3*t**2 - y**2*z**3*t**2 +
...      y**2*t**2 + 3*z**6*t**2 +  2*z**4*t**3 - 3*z**3*t**2 -
...      2*z*t**3)
>>> factor(f)
(t**2*z**3 - t**2 + 47*x*y)*(2*t*z + 45*x**3 - 9*y**3 - y**2 +
 3*z**3)
```

- Gröbner bases:

```
>>> x0, x1, x2 = symbols('x:3')
>>> I = [x0 + 2*x1 + 2*x2 - 1,
...      x0**2 + 2*x1**2 + 2*x2**2 - x0,
...      2*x0*x1 + 2*x1*x2 - x1]
>>> groebner(I, order='lex')
GroebnerBasis([7*x0 - 420*x2**3 + 158*x2**2 + 8*x2 - 7,
7*x1 + 210*x2**3 - 79*x2**2 + 3*x2,
84*x2**4 - 40*x2**3 + x2**2 + x2], x0, x1, x2, domain='ZZ',
order='lex')
```

- Root isolation:

```
>>> f = 7*z**4 - 19*z**3 + 20*z**2 + 17*z + 20
>>> intervals(f, all=True, eps=0.001)
([],
 [((-425/1024 - 625*I/1024, -1485/3584 - 2185*I/3584), 1),
  ((-425/1024 + 2185*I/3584, -1485/3584 + 625*I/1024), 1),
  ((3175/1792 - 2605*I/1792, 1815/1024 - 10415*I/7168), 1),
  ((3175/1792 + 10415*I/7168, 1815/1024 + 2605*I/1792), 1)])
```

SM14.3. Solvers.

- Single solution:

```
>>> solveset(x - 1, x)
{1}
```

- Finite solution set, quadratic equation:

```
>>> solveset(x**2 - pi**2, x)
{-pi, pi}
```

- No solution:

```
>>> solveset(1, x)
EmptySet()
```

- Interval solution:

```
>>> solveset(x**2 - 3 > 0, x, domain=S.Reals)
(-oo, -sqrt(3)) U (sqrt(3), oo)
```

- Infinitely many solutions:

```
>>> solveset(x - x, x, domain=S.Reals)
(-oo, oo)
>>> solveset(x - x, x, domain=S.Complexes)
S.Complexes
```

- Linear systems (`linsolve`)

```
>>> A = Matrix([[1, 2, 3], [4, 5, 6], [7, 8, 10]])
>>> b = Matrix([3, 6, 9])
>>> linsolve((A, b), x, y, z)
{(-1, 2, 0)}
>>> linsolve(Matrix(([1, 1, 1, 1], [1, 1, 2, 3])), (x, y, z))
{(-y - 1, y, 2)}
```

Below are examples of `solve` applied to problems not yet handled by `solveset`.

- Nonlinear (multivariate) system of equations (the intersection of a circle and a parabola):

```
>>> solve([x**2 + y**2 - 16, 4*x - y**2 + 6], x, y)
[(-2 + sqrt(14), -sqrt(-2 + 4*sqrt(14))),
 (-2 + sqrt(14), sqrt(-2 + 4*sqrt(14))),
 (-sqrt(14) - 2, -I*sqrt(2 + 4*sqrt(14))),
 (-sqrt(14) - 2, I*sqrt(2 + 4*sqrt(14)))]
```

- Transcendental equations:

```
>>> solve((x + log(x))**2 - 5*(x + log(x)) + 6, x)
[LambertW(exp(2)), LambertW(exp(3))]
>>> solve(x**3 + exp(x))
[-3*LambertW((-1)**(2/3)/3)]
```

SM14.4. Matrices.

- Matrix expressions

```
>>> m, n, p = symbols('m n p', integer=True)
>>> R = MatrixSymbol('R', m, n)
>>> S = MatrixSymbol('S', n, p)
>>> T = MatrixSymbol('T', m, p)
>>> U = R*S + 2*T
>>> U.shape
(m, p)
>>> U[0, 1]
2*T[0, 1] + Sum(R[0, _k]*S[_k, 1], (_k, 0, n - 1))
```

- Block Matrices

```
>>> n, m, l = symbols('n m l')
>>> X = MatrixSymbol('X', n, n)
>>> Y = MatrixSymbol('Y', m ,m)
>>> Z = MatrixSymbol('Z', n, m)
>>> B = BlockMatrix([[X, Z], [ZeroMatrix(m, n), Y]])
>>> B
Matrix([
[X, Z],
[0, Y]])
>>> B[0, 0]
X[0, 0]
>>> B.shape
(m + n, m + n)
```

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