unyt: Handle, manipulate, and convert data with units in Python

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Summary

Software that processes real-world data or that models a physical system must have some way of managing units. This might be as simple as the convention that all floating point numbers are understood to be in the same physical unit system (for example, the SI MKS units system). While simple approaches like this do work in practice, they also are fraught with possible error, both by programmers modifying the code who unintentionally misinterpret the units, and by users of the software who must take care to supply data in the correct units or who need to infer the units of data returned by the software. Famously, NASA lost contact with the Mars Climate Orbiter spacecraft after it crash-landed on the surface of Mars due to the use of English Imperial units rather than metric units in the spacecraft control software (Board 1999).

The unyt library is designed both to aid quick calculations at an interactive python prompt and to be tightly integrated into a larger Python application or library. The top-level unyt namespace ships with a large number of predefined units and physical constants to aid setting up quick calculations without needing to look up unit data or the value of a physical constant. Using the unyt library as an interactive calculation aid only requires knowledge of basic Python syntax and awareness of a few of the methods of the unyt_array class - for example, the unyt_array.to() method to convert data to a different unit. As the complexity of the usage increases, unyt provides a number of optional features to aid these cases, including custom unit registries containing both predefined physical units as well as user-defined units, built-in output to disk via the pickle protocol and to HDF5 files using the h5py library (Collette 2013), and round-trip converters for unit objects defined by other popular Python unit libraries.

Physical units in the unyt class are defined in terms of the dimensions of the unit, a string representation, and a floating point scaling to the MKS unit system. Rather than implementing algebra for unit expressions, we rely on the SymPy symbolic algebra library (Meurer et al. 2017) to handle symbolic algebraic manipulation. The unyt.Unit object can represent arbitrary units formed out of base dimensions in the SI unit system: time, length, mass, temperature, luminance, and electric current. We currently treat units such as mol with the seventh SI base dimension, amount of substance, as dimensionless, although we are open to changing this based on feedback from users. In addition, unyt supports forming quantities defined in other unit systems - in particular CGS Gaussian units common in astrophysics as well as geometrized “natural” units common in relativistic calculations. In addition, unyt ships with a number of other useful predefined unit systems based, including imperial units, Planck units, a unit system for calculations in the solar system, and a “galactic” unit system based on the solar mass, kiloparsecs, and Myr, a convention common in galactic astronomy.
In addition to the \texttt{unyt.Unit} class, \texttt{unyt} also provides two subclasses of the NumPy (Oliphant 2006) `ndarray` (Walt, Colbert, and Varoquaux 2011), \texttt{unyt.unyt_array} and \texttt{unyt.unyt_quantity} to represent arrays and scalars with units attached, respectively. The \texttt{unyt} library also provides a \texttt{unyt.UnitRegistry} class to allow custom systems of units, for example to track the internal unit system used in a simulation. These subclasses are tightly integrated with the NumPy ufunc system, which ensures that algebraic calculations that include data with units automatically check to make sure the units are consistent, and allow automatic converting of the final answer of a calculation into a convenient unit.

We direct readers interested in usage examples and a guide for integrating \texttt{unyt} into an existing Python application or workflow to the \texttt{unyt} documentation hosted at \url{http://unyt.readthedocs.io/en/latest/}.

**Comparison with \texttt{Pint} and \texttt{astropy.units}**

The scientific Python ecosystem has a long history of efforts to develop a library to handle unit conversions and enforce unit consistency. For a relatively recent review of these efforts, see (Bekolay 2013). While we won’t exhaustively cover extant Python libraries for handling units in this paper, we will focus on \texttt{Pint} (Grecco 2018) and \texttt{astropy.units} (The Astropy Collaboration et al. 2018), which both provide a robust implementation of an array container with units attached and are commonly used in research software projects.

At time of writing a GitHub search for \texttt{import astropy.units} returns approximately 10,500 results and a search for \texttt{import pint} returns approximately 1,500 results.

While \texttt{unyt} provides functionality that overlaps with \texttt{astropy.units} and \texttt{Pint}, there are important differences which we elaborate on below. In addition, it is worth noting that all three codebases had origins at roughly the same time period. \texttt{Pint} initially began development in 2012 according to the git repository logs. Likewise \texttt{astropy.units} began development in 2012 and was released as part of \texttt{astropy} 0.2 in 2013, although the initial implementation was adapted from the \texttt{pynbody} library (Pontzen et al. 2013), which started its units implementation in 2010 according to the git repository logs. In the case of \texttt{unyt}, it originated via the \texttt{dimensionful} library (Stark 2012) in 2012. Later, \texttt{dimensionful} was elaborated on and improved to become \texttt{yt.units}, the unit system for the \texttt{yt} library (Turk et al. 2011) at a \texttt{yt} developer workshop in 2013 and was subsequently released as part of \texttt{yt} 3.0 in 2014. One of the design goals for the \texttt{yt} unit system was the ability to dynamically define “code” units (e.g. units internal to data loaded by \texttt{yt}) as well as units that depend on details of the dataset - in particular cosmological comoving units and the “little \texttt{h}” factor, used to parameterize the Hubble constant in cosmology calculations (Croton 2013). For cosmology simulations in particular, comparing data with different unit systems can be tricky because one might want to use data from multiple outputs in a time series, with each output having a different mapping from internal units to physical units. This despite the fact that each output in the time series represents the same physical system and common workflows involve combining data from multiple outputs. This requirement to manage complex custom units and interoperate between custom unit systems drove the \texttt{yt} community to independently develop a custom unit system solution. We have decided to repackage and improve \texttt{yt.units} in the form of \texttt{unyt} to both make it easier to work on and improve the unit system and encourage use of the unit system for scientific python users who do not want to install a heavy-weight dependency like \texttt{yt}.

Below we present a table comparing \texttt{unyt} with \texttt{astropy.units} and \texttt{Pint}. Estimates for lines of code in the library were generated using the \texttt{cloc} tool (Danial 2018); blank and comment lines are excluded from the estimate. Test coverage was estimated using the \texttt{coveralls} output for \texttt{Pint} and \texttt{astropy.units} and using the \texttt{codecov.io} output for \texttt{unyt}.

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Goldbaum, (2018). \texttt{unyt}: Handle, manipulate, and convert data with units in Python. \textit{Journal of Open Source Software}, xxx(xxx), xxx. 

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We offer lines of code as a very rough estimate for the “hackability” of the codebase. In general, smaller codebases with higher test coverage have fewer defects (Lipow 1982; Koru, Zhang, and Liu 2007; Gopinath, Jensen, and Groce 2014). This comparison is somewhat unfair in favor of unyt in that astropy.units only depends on NumPy and Pint has no dependencies, while unyt depends on both SymPy and NumPy. Much of the reduction in the size of the unyt library can be attributed to offloading the handling of algebra to SymPy rather than needing to implement the algebra of unit symbols directly in unyt. For potential users who are wary of adding SymPy as a dependency, that might argue in favor of using Pint in favor of unyt.

astropy.units

The astropy.units subpackage provides a PrefixUnit class, a Quantity class that represents both scalar and array data with attached units, and a large number of predefined unit symbols. The preferred way to create Quantity instances is via multiplication with a PrefixUnit instance. Similar to unyt, the Quantity class is implemented via a subclass of the NumPy ndarray class. Indeed, in many ways the everyday usage patterns of astropy.units and unyt are similar, although unyt is not quite a drop-in replacement for astropy.units as there are some API differences. The main functional difference between astropy.units and unyt is that astropy.units is a subpackage of the larger astropy package. This means that depending on astropy.units requires installing a large collection of astronomically focused software included in the astropy package, including a substantial amount of compiled C code. This presents a barrier to usage for potential users of astropy.units who are not astronomers or do not need the observational astronomy capabilities provided by astropy.

Pint

The Pint package provides a different API for accessing units compared with unyt and astropy.units. Rather than making units immediately importable from the Pint namespace, Pint instead requires users to instantiate a UnitRegistry instance (unrelated to the unyt.UnitRegistry class), which in turn has Unit instances as attributes. Just like with unyt and astropy.units, creating a Quantity instance requires multiplying an array or scalar by a Unit instance. Exposing the UnitRegistry directly to all users like this does force users of the library to think about which system of units they are working with, which may be beneficial in some cases, however it also means that users have a bit of extra cognitive overhead they need to deal with every time they use Pint.

In addition, the Quantity class provided by Pint is not a subclass of NumPy’s ndarray. Instead, it is a wrapper around an internal ndarray buffer. This simplifies the implementation of Pint by avoiding the somewhat arcane process for creating an ndarray subclass, although the Pint Quantity class must also be careful to emulate the full NumPy ndarray API so that it can be a drop-in replacement for ndarray.

Finally, in comparing the output of our benchmarks of Pint, astropy.units, and unyt, we found that in-place operations making use of a NumPy ufunc will unexpectedly strip units in Pint. For example, if a and b are Pint Quantity instances, np.add(a, b, out=out)) will operate on a and b as if neither have units attached. Interestingly, without the out
Figure 1: A benchmark comparing the ratio of the time to apply units to lists and NumPy ndarray instances to the time to interpret the same list or ndarray to an ndarray. This ratio, $T_{\text{package}}/T_{\text{numpy}}$, corresponds to the overhead of converting data to work with one of the three packages. Values close to unity correspond to zero or negligible overhead, while values larger than unity correspond to measurable overhead. Optimally all values would be near zero. In practice, applying units to small arrays incurs substantial overhead. Each test is shown for three different sizes of input data, including inputs with size 3, 1,000, and 1,000,000. The black lines at the top of the bars indicate the sample standard deviation. The $T_{\text{numpy}}$ time is calculated by benchmarking the time to perform `np.asarray(data)` where data is either a list or an ndarray.

Goldbaum, (2018). unyt: Handle, manipulate, and convert data with units in Python. Journal of Open Source Software, xxx(xxx), xxx.
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Figure 2: A benchmark comparing the time to square an array and to take the square root of an array. See Figure 1 for a detailed explanation of the plot style.

keyword, Pint does get the correct answer, so it is possible that this is a bug in Pint, and we have reported it as such upstream (see https://github.com/hgrecco/pint/issues/644).

Performance Comparison

Checking units will always add some overhead over using hard-coded unit conversion factors. Thus a library that is entrusted with checking units in an application should incur the minimum possible overhead to avoid triggering performance regressions after integrating unit checking into an application. Optimally, a unit library will add zero overhead regardless of the size of the array. In practice that is not the case for any of the three libraries under consideration, and there is a minimum array size above which the overhead of doing a mathematical operation exceeds the overhead of checking units. It is thus worth benchmarking unit libraries in a fair manner, comparing with the same operation implemented using plain NumPy.

Here we present such a benchmark. We made use of the perf (Stinner 2018) Python benchmarking tool, which not only provides facilities for establishing the statistical significance of a benchmark run, but also can tune a linux system to turn off operating system and hardware features like CPU throttling that might introduce variance in a benchmark. We made use of a Dell Latitude E7270 laptop equipped with an Intel i5-6300U CPU clocked at 2.4 Ghz. The testing environment was based on Python 3.6.3 and had NumPy 1.14.2, sympy 1.1.1, fastcache 1.0.2, Astropy 3.0.1, and Pint 0.8.1 installed. fastcache (Brady 2017) is an optional dependency of SymPy that provides an optimized LRU cache implemented in C that can substantially speed up SymPy. The system was instrumented using perf system tune to turn off CPU features that might interfere with stable benchmarks. We did not make any boot-time Linux kernel parameter
Figure 3: A benchmark comparing the time to perform various binary arithmetic operations on input operands that have different but dimensionally compatible units. See Figure 1 for a detailed explanation of the plot style.

changes.

For each of the benchmarks below, we show the ratio of the time to perform an operation with one of `unyt`, `Pint`, and `astropy.units`, $T_{package}$, to the time it takes for `NumPy` to perform the equivalent operation, $T_{numpy}$. For example, for the comparison of the performance of `np.add(a, b)` where `a` and `b` have different units with the same dimension, the corresponding benchmark to generate $T_{numpy}$ would use the code `np.add(a, c*b)` where `a` and `b` would be `ndarray` instances and `c` would be the floating point conversion factor between the units of `a` and `b`. Much of the time in $T_{package}$ relative to $T_{numpy}$ is spent in the respective packages calculating the appropriate conversion factor $c$. Thus the comparisons below depict very directly the overhead for using a unit library over an equivalent operation that uses hard-coded unit-conversion factors.

**Applying units to data**

In Figure 1 we plot the overhead for applying units to data, showing both Python lists and NumPy `ndarray` instances as the input to apply data to. Since all three libraries eventually convert input data to a NumPy `ndarray`, the comparison with array inputs more explicitly shows the overhead for *just* applying units to data. When applying units to a list, all three libraries as well as NumPy need to first copy the contents of the list into a NumPy array or a subclass of `ndarray`. This explains why the overhead is systematically lower when starting with a list.

In all cases, `unyt` either is fastest by a statistically significant margin, or ties with `astropy`. Even for large input arrays, `Pint` still has statistically significant overhead, while both

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Figure 4: A benchmark comparing the time to perform various binary arithmetic operations on input operands that have the same units. See Figure 1 for a detailed explanation of the plot style.

unyt and astropy.units have negligible overhead once the input array size reaches $10^6$ elements.

**Unary arithmetic operations**

Expressions involving powers of data with units, including integer and fractional powers, are very common in the physical sciences. It is therefore very important for a library that handles units to be able to track this case in a performant way. In Figure 2 we present a benchmark comparing Pint, unyt, and astropy.units for the squaring and square root operation. In all cases, unyt has the lowest overhead, with Pint coming in second, and astropy.units trailing. Note that the y-axis is plotted on a log scale, so astropy is as much as 4 times slower than unyt for these operations.

**Binary arithmetic operations**

Binary operations form the core of arithmetic. It is vital for a library that handles unit manipulation to both transparently convert units when necessary and to ensure that expressions involving quantities with units are dimensionally consistent. In Figure 3 and 4 we present benchmarks for binary arithmetic expressions, both with input data that has the same units and with input data with different units but the same dimensions. In most cases, unyt has less overhead than both astropy and Pint, although there are a few anomalies that are worth explaining in more detail. For comparison operations, Pint exhibits a slowdown even on large input arrays. This is not present for other binary operations, so it is possible that this overhead might be eliminated with a code change in Pint. For multiplication on large arrays, all three libraries have measured overhead of

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Figure 5: A benchmark comparing the overhead for computing various NumPy ufunc operations. The operands of all binary ufuncs have the same units. See Figure 1 for a detailed explanation of the plot style.
Figure 6: The same as Figure 5, but with in-place ufunc operations. See Figure 1 for a detailed explanation of the plot style.

~ 0.5 than that of the “equivalent” Numpy operation. That is because all three libraries produce results with units given by the product of the input units. That is, there is no need to multiply the result of the multiplication operation by an additional constant, while a pure NumPy implementation would need to multiply the result by a constant to ensure both operands of the operation are in the same units. Finally, for division, both Pint and astropy.units exhibit the same behavior as for multiplication, and for similar reasons: the result of the division operation is output with units given by the ratio of the input units. On the other hand, unyt will automatically cancel the dimensionally compatible units in the ratio and return a result with dimensionless units.

NumPy ufunc performance

Lastly, In Figures 4 and 5, we present benchmarks of NumPy ufunc operations. A NumPy ufunc is a fast C implementation of a basic mathematical operation. This includes arithmetic operators as well as trigonometric and special functions. By using a ufunc directly, one bypasses the Python object protocol and short-circuits directly to the low-level NumPy math kernels. We show both directly using the NumPy ufunc operators (Figure 4) as well as using the same operators with a pre-allocated output array to benchmark in-place operations.

As for the other benchmarks, unyt tends to have the lowest amount of overhead, although there are some significant exceptions. For np.power, Pint has the lowest overhead, except for very large input arrays, where the overhead for all three libraries is negligible. On the other hand, for np.sqrt, np.equal, np.add, and np.subtract, Pint still has statistically significant overhead for large input arrays. Finally, for the in-place ufunc comparison, Pint has the lowest overhead for all operations. However, as discussed above, this is
because of a bug in Pint which causes the library to ignore units when calling a ufunc with the out keyword set.

Conclusions

In this paper we present the unyt library, giving background on the reasons for its existence and some historical context for its origin. We also present a set of benchmarks for common arithmetic operations, comparing the performance of unyt with Pint and astropy.units. In general, we find that unyt either outperforms or matches the performance astropy.units and Pint, depending on the operation and size of the input data. We also demonstrate that the unyt library constitutes a smaller codebase with higher test coverage than both Pint and astropy.units.

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