NRPyLaTeX: A LaTeX interface to computer algebra systems for general relativity

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Abstract. While each computer algebra system (CAS) contains its own unique syntax for inputting mathematical expressions, \textsc{LaTeX} is perhaps the most widespread language for typesetting mathematics. \textsc{NRPyLaTeX} (NL) enables direct \textsc{LaTeX} input of complex tensorial expressions (written in Einstein notation) relevant to general relativity and differential geometry into the \textsc{SymPy} CAS. As \textsc{SymPy} also supports output compatible with the \textsc{Mathematica} and \textsc{Maple} CASs, NL lowers the learning curve for inputting and manipulating tensorial expressions in three widely used CASs. \textsc{LaTeX} however is a typesetting language, and as such is not designed to resolve ambiguities in mathematical expressions. To address this, NL implements a convenient configuration interface that, e.g., defines variables with certain attributes. Configuration commands appear as \textsc{LaTeX} comments, so that entire NL workflows can fit seamlessly into the \textsc{LaTeX} source code of scientific papers without interfering with the rendered mathematical expressions. Further, NL adopts \textsc{NRPy}+'s rigid syntax for indexed symbols (e.g., tensors), which enables NL output to be directly converted into highly optimized C/C++ code kernels using \textsc{NRPy}+. Finally NL has robust and user-friendly error-handling, which catches common tensor indexing errors and reports unresolved ambiguities, further expediting the input and validation of \textsc{LaTeX} expressions into a CAS.

Keywords: \textsc{LaTeX}, parser-lexer, general relativity, numerical relativity, Einstein notation, differential geometry, \textsc{NRPy}+, \textsc{SymPy}, computer algebra

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1. Introduction

\LaTeX\ is perhaps the canonical markup language for communicating mathematical ideas in scientific papers, and most practitioners of general relativity and differential geometry are proficient in it. Further, computer algebra systems (CASs) like SymPy [1], Mathematica [2], or Maple [3] are often an essential resource in these fields, but to our knowledge there are currently no CASs or CAS add-on packages, except for Cadabra [4], that support the input of tensorial/indexed \LaTeX\ expressions adopting Einstein notation. Thus new practitioners are often required to learn one language for communicating mathematical ideas in scientific papers, and another to input & manipulate mathematical expressions in a CAS. As a result expressions developed within a CAS often need to be translated into \LaTeX\ or vice-versa when constructing a scientific paper, and human errors in transcription can become a menace to productivity and reproducibility of scientific results.

Various packages have been developed to ease the input of tensorial/indexed expressions using Einstein notation into CASs. For example, xTensor [5] is an open-source add-on package for the Mathematica CAS, greatly extending its capabilities for performing abstract tensor calculus. In short, xTensor enables the definition and manipulation of tensors with arbitrary symmetries on multiple manifolds. Upon declaring a metric for a given manifold, covariant, Lie, and other derivatives may be computed, and associated curvature tensors may be immediately defined. As it is an extremely powerful add-on to one of the most popular and powerful CASs, xTensor finds wide use across the community. Despite its success, perhaps the largest barrier to entry for new users is its dependency on the closed-source Mathematica, whose software licenses carry a price that can be too high for some users.

Cadabra is a powerful CAS for solving problems in field theory, with a similar design philosophy to \textsc{NRPy+}/\textsc{NRPyLaTeX}. Both Cadabra and \textsc{NRPy+}/\textsc{NRPyLaTeX} use the same three language system: \LaTeX\ for mathematics, Python for programming, and C/C++ for computation. In contrast, most CASs, e.g. SymPy, use a single language for each of those respective tasks. However, Cadabra and \textsc{NRPy+} differ in three main respects. First, \textsc{NRPyLaTeX} is intended for general relativity. As such, \textsc{NRPyLaTeX} makes certain convenient inferences about indexing, consistent with common conventions in the general relativity and numerical relativity literature. Specifically, Latin and Greek indices default to 3D and 4D, respectively. In addition, \textsc{NRPyLaTeX} adopts notations common to the field of general relativity for specifying covariant (e.g., $D_i$ or $\nabla_i$) and Lie (e.g., $\mathcal{L}_\beta$) derivative operators. Cadabra, on the other hand, is intended for more general field theory use, and thus requires more user input to remove ambiguities. Second, as detailed below \textsc{NRPyLaTeX} is natively compatible with numerical workflows through \textsc{NRPy+}'s C-code generation capabilities, as it adopts rigid syntax for naming indexed symbols (e.g., $v^i \equiv vU[i]$) and specifying derivatives that are to be computed numerically. In contrast, Cadabra is largely geared toward symbolic workflows. Third, \textsc{NRPyLaTeX} configurations (i.e., commands that users must input to remove ambiguities
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in the symbolic expressions, like specifying the symmetry properties of a tensor) exist as \LaTeX comments, so NRPyLaTeX workflows can be embedded completely inside of the source code of a \LaTeX document, eliminating the step of sharing these workflows through a separate document. As described below, this feature is particularly convenient in the context of scientific paper preprints on e.g., the arXiv, which are usually downloadable as \LaTeX source. Cadabra’s configuration, on the other hand, does not appear as \LaTeX comments, making it less convenient to share configurations.

SymPy is another very powerful CAS used widely across the scientific community. Unlike Mathematica or Maple, SymPy is built upon Python and is open-source (under the permissive 3-Clause BSD license). While SymPy contains both basic support for tensors and differential geometry, as well as basic, experimental \LaTeX input capabilities, \LaTeX input of tensorial/indexed expressions is not currently supported\footnote{b}. Instead, to input and manipulate tensorial/indexed expressions found in general relativity and differential geometry contexts, a few add-on packages for SymPy have been developed. These packages are somewhat analogous to xTensor, but they benefit from the fact that SymPy possesses no expensive software license. EinsteinPy\footnote{a} is one such (open-source, free) package, which extends basic tensor support in SymPy to handle metrics and construction of their associated connections and curvature tensors (Riemann & Ricci). It also contains friendly Jupyter notebook documentation and functionality for e.g., plotting geodesics in various spacetimes. The GraviPy\footnote{a} add-on package to SymPy possesses similar basic tensor symbolic manipulation functionality as EinsteinPy, but in addition e.g., supports the construction of the Einstein tensor, as well as user-defined tensors and covariant derivatives.

While xTensor, EinsteinPy, and GraviPy are exemplary packages that effectively convert popular CASs into powerful tools for general relativity and differential geometry, each depends on its own custom, non-\LaTeX syntax for inputting tensorial expressions. As discussed, this adds a slight learning curve for new users, and opens the door to \LaTeX ↔ CAS transcription errors when preparing scientific papers.

Our new, open-source NRPyLaTeX package provides a multifaceted \LaTeX interface to SymPy, with general relativity and differential geometry workloads in mind. NRPyLaTeX enables the input of tensorial expressions exactly as they would appear in the \LaTeX source code of scientific papers, and it possesses native support for e.g., multiple metrics; custom tensors of arbitrary rank & dimension; index raising & lowering; and covariant, Lie, & partial derivatives.

As \LaTeX is a typesetting markup language, it is neither designed to resolve ambiguities in mathematical expressions, nor able to point out e.g., errors in Einstein notation. To address ambiguities (e.g., which rank-2 tensor represents the metric), NRPyLaTeX contains a robust and user-friendly configuration interface, which enables one to define variables, assign attributes, ignore substrings, and perform (syntactic) string replacement. For example, this includes the ability to declare variables, define

\footnote{a as of SymPy 1.9}
\footnote{b under the permissive 2-Clause BSD license}
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NRPyLaTeX provides a \LaTeX\ frontend to the \texttt{SymPy} CAS, supporting the input of tensorial expressions written in Einstein notation. It includes a number of features with general relativity and differential geometry applications in mind, including covariant and Lie derivatives; spacetime and reference metrics; Levi-Civita and Christoffel symbols; as well as metric inverses and determinants, just to name a few.

At its core the NRPyLaTeX frontend is a lexer/parser with a powerful configuration interface that addresses ambiguities (e.g., specifying which metric is associated with a covariant derivative, or the dimension of a tensor) and defines arbitrary variable/operator macros. Configuration options are input as \LaTeX\ comments so that all

c \texttt{NRPy+} is short for “Python-based code generation for numerical relativity... and beyond!”.
d \texttt{SymPy} provides a pipeline from NRPyLaTeX to Mathematica/Maple through their Printing module.
e NRPyLaTeX tokenizes the input \LaTeX, using substring pattern matching, and parses the resulting token iterator at a syntactic level, including proper handling of Einstein notation.

tensors, input into \texttt{SymPy} un-rendered equations, declare arbitrary operators, and provide aliases for variable names. Conveniently this configuration interface exists entirely within \LaTeX\ comments, enabling it to be interspersed with the rendered \LaTeX\ without itself being rendered. Thus it provides a means to share CAS worksheets \emph{within the source code of scientific papers}, while minimizing the chances of a transcription error when translating CAS input expressions to a \LaTeX\-ed scientific paper. It also provides a new means for inputting \LaTeX\-ed equations (found in e.g., scientific paper source codes on the arXiv) directly into CASs.

To address errors in Einstein notation (e.g., “indexing” errors) and to help guide the user in resolving ambiguities in mathematical expressions, NRPyLaTeX contains a comprehensive exception handling infrastructure. For example, this infrastructure will return errors when a \LaTeX\-ed tensorial expression written in Einstein notation contains a repeated “down” index, or an unbalanced free index across the equality, or the use of a covariant derivative without specifying the associated metric.

As its name implies, NRPyLaTeX falls under the umbrella of our \texttt{SymPy}-based NRPy+ framework \cite{8,9}; NRPyLaTeX can be used seamlessly for not only symbolic but also numerical workflows using \texttt{NRPy+}. In short, \texttt{NRPy+} builds upon and extends \texttt{SymPy}'s native capabilities, to convert often complex indexed expressions (e.g., tensorial expressions) directly into highly optimized C/C++-code kernels with common-subexpression elimination; single-instruction, multiple-data (SIMD); and finite-difference derivative code generation capabilities. C/C++-code kernels like these form the heart of numerical relativity codes.

The remainder of the paper is organized as follows. In Sec. 2 we discuss the basic features and internal structure of NRPyLaTeX; and in Sec. 3 present symbolic and numerical workflows, as well as usage and exception handling. Finally in Sec. 4 we summarize the basic results and present plans for future work.

2. Basic Features and Methodology

NRPyLaTeX provides a \LaTeX\ frontend to the \texttt{SymPy} CAS, supporting the input of tensorial expressions written in Einstein notation. It includes a number of features with general relativity and differential geometry applications in mind, including covariant and Lie derivatives; spacetime and reference metrics; Levi-Civita and Christoffel symbols; as well as metric inverses and determinants, just to name a few.

At its core the NRPyLaTeX frontend is a lexer/parser with a powerful configuration interface that addresses ambiguities (e.g., specifying which metric is associated with a covariant derivative, or the dimension of a tensor) and defines arbitrary variable/operator macros. Configuration options are input as \LaTeX\ comments so that all
information needed to construct symbolic expressions can be shared in, e.g., a scientific paper’s \LaTeX source code.

\textbf{NRPyLaTeX} adopts the \texttt{NRPy+} notation for indexed symbols, so that e.g., $g_{\mu\nu}$ is accessible as a nested list of \texttt{SymPy} symbols $gDD[\mu][\nu]$, where e.g., $g_{tt}$ is stored in $gDD[0][0]$. Here \texttt{D} denotes a covariant \textit{(down)} index. Similarly \texttt{U} is appended to the tensor name for each contravariant \textit{(up)} index. In fact, for each indexed symbol of dimension $n$ and rank $r$, \texttt{NRPyLaTeX} will create an $r$-dimensional array (or symbol) of size $n \times \ldots \times n = n^r$ using \texttt{NRPy+} notation.

As \texttt{NRPy+} is designed to convert \texttt{SymPy} expressions into highly optimized C/C++-code kernels, compatibility with \texttt{SymPy} and \texttt{NRPy+} enables \texttt{NRPyLaTeX} to interface well with symbolic and numerical workloads, respectively. For example, specifying that the partial derivative $g_{\mu\nu,\delta}$ should be evaluated numerically requires that one simply first define the variable $gDD$ with a placeholder differentiation type in a \texttt{NRPyLaTeX} configuration line. Once this is completed, all symbolic first derivatives of $g_{\mu\nu}$ will be accessed in the \texttt{NRPy+}-compatible syntax $gDD.dD[\mu][\nu][\delta]$, second derivatives as $gDD.dDD[\mu][\nu][\delta][\gamma]$, and so forth. \texttt{NRPy+} can interpret such partial derivative symbols as requiring numerical (finite-difference) differentiation and generate the appropriate C/C++-code kernel.

Finally, \texttt{NRPyLaTeX} is developed using modern software engineering techniques, including \texttt{git} version control, robust exception handling, interactive \texttt{Jupyter} notebook documentation, convenient \texttt{IPython/Jupyter} interfaces, and more than 80 code-validation unit tests. These tests check \texttt{NRPyLaTeX}'s exception handling, as well as a large number of challenging tensor parsing edge cases and use case examples. Perhaps the most sophisticated such use case is \texttt{NRPyLaTeX}'s ability to reproduce the entire covariant BSSN [8, 10–12] system of equations in a \texttt{NRPy+}-compatible form; the generated symbolic expressions have been validated against the handwritten \texttt{SymPy} expressions for the BSSN formalism appearing within \texttt{NRPy+}. Associated with the BSSN validation test is a \texttt{Jupyter} notebook tutorial that demonstrates precisely how to input such equations into \texttt{NRPyLaTeX}. All validation tests are run within a continuous integration infrastructure, which is triggered upon any commit to the \texttt{git} repository. Further \texttt{NRPyLaTeX} exists within the \texttt{Python} Package Index (PyPI) and thus can be installed from a standard \texttt{Python} installation via \texttt{pip install nrpylatex}. Though, for the purpose of reproducing results in this paper, one should specify version 1.1.1.

Next we demonstrate \texttt{NRPyLaTeX}'s basic features through real-world examples, highlighting both its ability to handle symbolic (Sec. 3.1) and numerical/\texttt{NRPy+} (Sec. 3.2) workloads, as well as its exception handling (Sec. 3.3).

\textit{f} \texttt{NRPyLaTeX} extends the \texttt{NRPy+} notation for differentiation, in order to support Lie derivatives with respect to an arbitrary vector $v^i$.\texttt{ld}(v)\texttt{D} and covariant derivatives (\texttt{cdD}, \texttt{cdU}, \texttt{cdDU}, etc.)

\textit{g} \texttt{NRPyLaTeX} source code can be downloaded from \url{https://github.com/zachetienne/nrpylatex}, though it is generally advisable to install \texttt{NRPyLaTeX} through \texttt{pip} via \texttt{pip install nrpylatex}.  

3. Examples

3.1. Symbolic Workload Example: Schwarzschild Solution to Einstein’s Equations

```latex
\begin{align}
% attrib coord [t, r, \theta, \phi] \\
% vardef -const G, M \\
% vardef -zero gDD::4D % initialize every component of gDD to zero \\
g_{\mu\nu} &= -\left(1 - \frac{2GM}{r}\right) \\
\text{g}_{rr} &= \left(1 - \frac{2GM}{r}\right)^{-1} \\
\text{g}_{\theta\theta} &= r^2 \\
\text{g}_{\phi\phi} &= r^2 \sin^2\theta \\
% assign -metric gDD \\
\text{R}^\alpha{}_{\beta\mu\nu} &= \partial_\mu \Gamma^\alpha_{\beta\nu} - \partial_\nu \Gamma^\alpha_{\beta\mu} + \Gamma^\alpha_{\mu\gamma} \Gamma^\gamma_{\beta\nu} - \Gamma^\alpha_{\nu\sigma} \Gamma^\sigma_{\beta\mu} \\
\text{R}_{\beta\nu} &= \text{R}^{\alpha}_{\beta\alpha\nu} \\
\text{R} &= \text{g}^{\beta\nu} \text{R}_{\beta\nu} \\
\text{G}_{\beta\nu} &= \text{R}_{\beta\nu} - \frac{\text{R}}{2} \text{g}_{\beta\nu} \\
\text{K} &= \text{R}^{\alpha\beta\mu\nu} \text{R}_{\alpha\beta\mu\nu}. \\
\end{align}
```

Figure 1: Symbolic workload example: Schwarzschild solution of general relativity

In this example, we demonstrate \texttt{NRPyLaTeX}'s ability to handle symbolic workloads, by first defining the Schwarzschild metric, and then constructing the corresponding Riemann tensor $R^\alpha{}_{\beta\mu\nu}$, Ricci tensor $R_{\beta\nu}$, Ricci scalar $R$, Einstein tensor $G_{\beta\nu}$, and the Kretschmann scalar $K$. As shown in Fig. 1, Lns. 2–3, the coordinate system and all constants (ignored during differentiation) must first be specified in the \texttt{NRPyLaTeX} configuration. Then in Ln. 4, the 4-metric $g_{\mu\nu}$ is initialized to zero (this ensures off-diagonal terms are set).

The remainder of the example is almost entirely boilerplate \LaTeX, which one might find in the source code of a journal article. In Lns. 5–8 the diagonal components of the Schwarzschild metric are specified. Line 9 is the final configuration command, which assigns $g_{\mu\nu}$ as the metric, and in doing so automatically constructs the metric inverse $g^{\mu\nu}$ and the associated connection $\Gamma^\sigma_{\mu\nu}$, both of which are essential to define the Riemann curvature tensor $R^\alpha{}_{\beta\mu\nu}$, the Ricci curvature tensor $R_{\beta\nu}$, the Ricci scalar $R$, the Einstein tensor $G_{\beta\nu}$, and the Kretschmann scalar $K$:

\begin{align}
R^\alpha{}_{\beta\mu\nu} &= \partial_\mu \Gamma^\alpha_{\beta\nu} - \partial_\nu \Gamma^\alpha_{\beta\mu} + \Gamma^\alpha_{\mu\gamma} \Gamma^\gamma_{\beta\nu} - \Gamma^\alpha_{\nu\sigma} \Gamma^\sigma_{\beta\mu} \\
R_{\beta\nu} &= R^{\alpha}_{\beta\alpha\nu} \\
R &= g^{\beta\nu} R_{\beta\nu} \\
G_{\beta\nu} &= R_{\beta\nu} - \frac{R}{2} g_{\beta\nu} \\
K &= R^{\alpha\beta\mu\nu} R_{\alpha\beta\mu\nu}. \\
\end{align}

Upon parsing the contents of Fig. 1, \texttt{NRPyLaTeX} generates symbolic (\texttt{SymPy}) expressions for all defined tensors and scalars using \texttt{NRPy+} notation as described in Sec. 2, and injects these expressions into the local namespace. So for example one can immediately access $g_{\theta\theta}$ from $\text{gDD}[2][2]$, finding that indeed it stores $r^2$. Similarly, one
can immediately confirm that each component of the Einstein tensor $G_{\mu\nu}$, stored in the nested list `GDD[\mu][\nu]` is identically zero (this requires use of SymPy’s simplification routine), and that the Kretschmann scalar (stored within the local variable $K$) is equal to the known value for the Schwarzschild solution $K = 48(GM/r)^2$. Thus we are able to confirm that NRPyLaTeX is correctly parsing these complex symbolic expressions, verifying that the Schwarzschild metric indeed solves Einstein’s equations and that invariants take values consistent with the literature.

Next we move on to a workload in which the metric is only known numerically, and thus the metric and metric derivatives must be left in a general unspecified form. In this workload, the resulting expressions can be directly input into NRPy+, which outputs highly optimized C/C++-code kernels that can adopt finite-difference representations to approximate partial derivatives.

### 3.2. Numerical Workload Example: BSSN Hamiltonian Constraint for Vacuum Spacetimes with Unspecified Metric

The 3+1 Baumgarte-Shapiro-Shibata-Nakamura (BSSN) formalism of general relativity is perhaps the most widely used formulation within the numerical relativity community. Transcribing the BSSN equations into a hand-optimized C/C++/Fortran code can be a daunting task by itself, not to mention the debugging process. Here we present a NRPyLaTeX workflow aimed at generating a SymPy expression for the BSSN Hamiltonian constraint (i.e., the Hamiltonian constraint written in terms of BSSN variables) in vacuum. The resulting expression can be plugged directly into NRPy+ to generate highly optimized C/C++-code kernels.

We start by defining the BSSN conformal 3-metric $\bar{\gamma}_{ij}$, which is related to the the physical 3-metric $\gamma_{ij}$ via

$$\bar{\gamma}_{ij} = e^{-4\phi} \gamma_{ij}. \quad (6)$$

Further the BSSN formalism decomposes the physical extrinsic curvature $K_{ij}$ into its trace $K$ and its trace-free part $\bar{A}_{ij}$:

$$\bar{A}_{ij} = e^{-4\phi} \left( K_{ij} - \frac{1}{3} \gamma_{ij} K \right). \quad (7)$$

Given these definitions, the Hamiltonian constraint is written (Eq. 46 of [8])

$$H = \frac{2}{3} K^2 - \bar{A}_{ij} \bar{A}^{ij} + e^{-4\phi} \left( \bar{R} - 8 \bar{D}^i \phi \bar{D}_i \phi - 8 \bar{D}^2 \phi \right), \quad (8)$$

where $\bar{D}_i$ and $\bar{R}$ are the covariant derivative and Ricci scalar associated with $\bar{\gamma}_{ij}$, respectively.

The following example was written as a validation test against the same expression manually input into NRPy+ (and independently validated against other trusted BSSN codes). As such, it adopts the NRPy+ convention referring to the evolved "conformal
factor” variable as cf. NRPy+ natively supports three options for conformal variable, but following e.g., `[8, 11, 15]` instead of evolving φ or $e^{-4\phi}$ directly in a numerical relativity code when constructing the spacetime, the variable $cf = W = e^{-2\phi}$ is evolved. This variable is generally chosen as it is a smoother function near puncture black holes, resulting in lower truncation errors when evaluating numerical derivatives.

```latex
\begin{verbatim}
\% vardef -diff_type=dD -metric gammabarDD \% append _dD to each partial derivative
\% vardef -diff_type=dD -symmetry=sym01 AbarDD, RbarDD \% symmetry [i][j] == [j][i]
\% parse \bar{R} = \bar{\gamma}^{ij} \bar{R}_{ij} \%
\% internal calculation (no rendering)
\% vardef -diff_type=dD cf
\% srepl "e^{-4\phi}" -> "text{cf}^2" \%
\% srepl -persist "\partial _<1> \phi" -> "\partial _<1> \text{cf} \frac{-1}{2 \text{cf}}" \%
\% srepl "\bar{D}^2" -> "\bar{D}^i \bar{D} _i" \%
\%
H = \frac{2}{3} K^2 - \bar{A}_{ij} \bar{A}^{ij} + e^{-4\phi} \left(\bar{R} - 8 \bar{D}^i \phi \bar{D}_i \phi - 8 \bar{D}^2 \phi\right)
\end{verbatim}
```

Figure 2: Numerical NRPy+ workload example: The Hamiltonian constraint of the BSSN formalism

In Fig. 2 we demonstrate the procedure for constructing the Hamiltonian constraint in terms of BSSN variables using as input unspecified spacetime variables $W$, $K$, $\bar{A}_{ij}$, $\bar{\gamma}_{ij}$, and $\bar{R}_{ij}$, and any derivatives will be computed numerically (outside of NRPyLaTeX) from these given variables. By “unspecified”, we mean that e.g., each component of the conformal 3-metric is left completely symbolic (e.g. $\gamma_{01}$ would be the SymPy symbol `gammaDD01`, accessible from the local namespace variable `gammaDD[0][1]`). Further, unlike the example of Sec. 3.1 (Ln. 1), we do not specify a particular coordinate system as this expression is covariant.

Line 1 defines an unspecified, 3-dimensional metric $\bar{\gamma}_{ij}$ and changes the derivative type to append a suffix _dD instead of attempting to evaluate each derivative symbolically. The resulting symbolic expressions involving e.g., $\text{gammabarDD}_dD[j][k][i]$ (i.e., $\bar{\gamma}_{jki}$) can be passed into NRPy+, which generates C/C++-code kernels that evaluate the derivatives using finite differences. Next (Ln. 2) the symmetric tensors $AbarDD$ and $RbarDD$ are defined in a similar way (i.e., they each appear in the final expression). As $AbarDD$ and $RbarDD$ are unspecified (i.e., we assume they are computed independently, and thus used here as input into the expression), their symmetry in the first two indices “sym01” (i.e. $\bar{A}_{ij} = \bar{A}_{ji}$ and $\bar{R}_{ij} = \bar{R}_{ji}$) must be manually imposed. Then (Ln. 3) the scalar $Rbar$ is constructed by contracting $RbarDD$ with itself, i.e. $R_{ij} = \bar{R}_{ij}$.

Next, we apply a two-step procedure to replace every instance of $\phi$ with the chosen evolved “conformal factor” variable $cf = W = e^{-2\phi}$. First, we define the conformal factor $cf$ (Ln. 4) and replace every instance of $e^{-4\phi}$ with $cf^2$ (Ln. 5). Note that this and all `srepl` replacements are done on the syntactic level, and are not string replacements.

i Note, we could also use $R = \bar{R}^i$ instead of $R = \bar{R}_{ij}$ since NRPyLaTeX performs automatic index raising and lowering using the metric.
Second (Ln. 6), we replace each partial derivative of the form $\partial_{(1)}\phi$ for any index $\langle 1 \rangle$ with the expression $(-1/2)\c f^{-1}\partial_{(1)}\c f$, as implied by the chain rule:

$$\partial_{(1)}\c f = \partial_{(1)}e^{-2\phi} = -2e^{-2\phi}\partial_{(1)}\phi \Rightarrow \partial_{(1)}\phi = -\frac{1}{2}\c f^{-1}\partial_{(1)}\c f.$$ 

Line 6 also enables the `-persist` option, which ensures this replacement is made inside of each covariant derivative expansion.

Finally (Ln. 7), `srepl` is used one more time to define a custom contraction operator $\bar{D}^2 := \bar{D}^i \bar{D}_i$. `NRPyLaTeX` expands each covariant derivative using the metric $\bar{\gamma}_{ij}$ and the associated, internally generated connection $\bar{\Gamma}^i_{jk}$. All components of $\bar{\Gamma}^i_{jk}$ are available to the user in their local namespace, as well as the covariant derivatives (represented with the suffix `_cd[UD]..[UD]`; the .. notation here denotes repetition to match the rank, or number of indices, of an indexed symbol). All this defined, the Hamiltonian constraint is immediately constructed in a form ready for `NRPy+ C/C++`-code kernel generation.

### 3.3. Example 3: `NRPyLaTeX` Exception Handling and Index Checking

| Line | Code | Error Message |
|------|------|---------------|
| 1    | `%load_ext nrpylatex.extension` | |
| 2    | `%%parse_latex` | |
| 3    | `...: % vardef gUD, vD` | |
| 4    | `...: v^a = g^a_b v_b` | TensorError: illegal bound index 'b' in vU |
| 5    | `...: % vardef gUU` | |
| 6    | `...: v^a = g^{cb} v_b` | TensorError: unbalanced free index {'a', 'c'} in vU |
| 7    | `%%parse_latex` | |
| 8    | `...: ? v^a = g^{a*} v_b` | ParseError: v^a = g^{a*} v_b ^ unexpected '*' at position 10 |
| 9    | `%%parse_latex` | |
| 10   | `...: % vardef g_wD` | |
| 11   | `...: v^a = g^a_x v_x` | ParseError: v^a = g^a_x v_x ^ cannot index undefined tensor 'v0' at position 30 |
| 12   | `%%parse_latex` | |
| 13   | `...: % vardef g_bD` | |
| 14   | `...: v^a = g^a_\omega v_\omega` | ParseError: v^a = g^a_\omega v_\omega ^ cannot index undefined tensor '\omega0' at position 32 |

Figure 3: Examples of exception handling within an `IPython` (interactive `Python`)/`Jupyter` session of `NRPyLaTeX` 

Fig.3 demonstrates `NRPyLaTeX`’s robust system for index checking and generic exception handling, implemented using its own `TensorError` and `ParseError` algorithms, respectively. In short these algorithms report ambiguities in mathematical expressions, violations of Einstein notation, and problems at the syntactic level with error reporting that is human-friendly, both being descriptive and pointing to the exact location of the error in either the `NRPyLaTeX` configuration or `\LaTeX` expressions.
NRPyLaTeX will raise its TensorError exception upon violation of the Einstein summation convention. In Fig 3, Cell 1 we load the custom IPython/Jupyter extension module nrpylatex.extension using the built-in load_ext magic command. In Cell 2 we attempt to parse the equation $v^a = g^{ab}v_b$, which is invalid as Einstein notation requires that a repeated (“bound”) index may appear only once as a superscript and exactly once as a subscript in any given term. NRPyLaTeX thus raises a TensorError exception for an ‘illegal bound index’, which occurred since the index $b$ appeared twice in the down position. Next, in Cell 3 we attempt to parse the equation $v^a = g^{ab}v_b$, proper Einstein summation notation requires a free index to appear in every term with the same (“up” or “down”) position and cannot be summed over in any term. NRPyLaTeX checks for this and raises a TensorError exception for an ‘unbalanced free index’, which occurred since index $a$ and index $c$ appeared only once on each side of the equation.

NRPyLaTeX will raise the custom ParseError exception upon identifying a syntax error in the argument string of the parse_latex function or magic command. In Cell 4, we attempt to parse the equation $v^a = g^{ab}v_b$, but NRPyLaTeX raised a ParseError exception for an ‘unexpected’ lexeme as NRPyLaTeX did not recognize a valid index. NRPyLaTeX could also raise a ParseError exception for an ‘expected’ token if only that exact token would satisfy a production rule (e.g. $\sqrt{0.2}\{\ldots}$ would raise that exception since NRPyLaTeX would expect an integer for the root). In Cell 5, we attempt to parse the equation $T_{ab} = v_a w_b$, but NRPyLaTeX raises a ParseError exception for indexing an ‘undefined’ symbol $wD$, which occurred because the indexed symbol $wD$ has not been defined (i.e., NRPyLaTeX did not find the indexed symbol $wD$ in the namespace). This exception can be addressed by defining $wD$ with the vardef macro. In Cell 6 we attempt to parse the equation $J^a = (4\pi k)^{-1}\nabla_b F^{ab}$, but NRPyLaTeX raised a ParseError exception since a covariant derivative cannot be generated without first defining a metric. For covariant derivatives without a diacritic, NRPyLaTeX searches the namespace for the metric $gDD$ (or $gUU$) and did not find it, thus throwing the error. The Appendix describes more generally which metric is assumed to be associated with a given covariant derivative.

4. Conclusions & Future Work

NRPyLaTeX provides a \LaTeX interface for the free and open source SymPy CAS, and includes native support for Einstein notation. As \LaTeX is widely used in the scientific community and the NRPyLaTeX infrastructure is completely free and open source, the learning curve for new users is minimized; the financial barrier to entry is eliminated; and anyone is free to modify and extend NRPyLaTeX (within the confines of its permissive 2-Clause BSD license). In addition to Einstein notation, NRPyLaTeX can, provided a metric, dynamically perform index raising and lowering, and automatically generate the metric inverse, determinant, and connection. Moreover, NRPyLaTeX expands covariant

\footnote{In a standard Python environment, we would instead import the parse_latex function from the nrpylatex module using the import keyword.}
and Lie derivatives; and generates the Levi-Civita symbol (of arbitrary rank).

NRPyLaTeX's configuration consists of a command system modeled on the POSIX command syntax, aiming to reduce the learning curve. In brief, the command system defines variables, keywords, and ignore commands; assigns properties and attributes; and performs (syntactic) string replacement. To prevent rendering of NRPyLaTeX commands, we embed each command inside of a \texttt{\LaTeX} comment; i.e., in text that follows a single percent symbol. This enables entire NRPyLaTeX workflows to be stored seamlessly within a scientific paper’s \texttt{\LaTeX} source code.

In summary, use cases for NRPyLaTeX range from symbolic manipulation of complex tensorial expressions in Jupyter notebooks, numerical code generation (e.g., when combined with its sister code NRPy+), and sharing of mathematical workflows directly within the \LaTeX source code of a scientific paper.

In the future, we plan on expanding the integration with NRPy+ to include reference metric support. This will enable one to choose from the broad class of curvilinear coordinate systems that NRPy+ supports \cite{8}, to output covariant expressions in a particular coordinate system. In addition, we plan to incorporate native support for Post-Newtonian (PN) notation. In the current build of NRPyLaTeX, we are capable of parsing PN notation using the \texttt{srepl} command to remap the PN notation for the dot/cross products of vectors to their definitions in Einstein notation. However, this approach requires too many \texttt{srepl} replacements to be both robust and feasible. Instead, we are targeting native PN support for a future release of NRPyLaTeX. Finally, we plan on adding a direct pipeline for parsing \LaTeX to optimized C/C++-code using NRPy+.

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Appendix (NRPyLaTeX v1.1.1 Reference Manual)

This Appendix serves both to ensure completeness in the exposition of NRPyLaTeX features and to provide a quick reference guide for NRPyLaTeX.
Appendix A.1. PARSE_LATEX Function

The parse_latex function provides a frontend interface to NRPyLaTeX, accepting a \LaTeX\ string, preferably a Python raw string to avoid unwanted character escaping, and returning either a SymPy expression or a namespace dictionary containing every variable defined by the vardef command and/or a \LaTeX\ equation. Note, NRPyLaTeX injects every instantiated variable into the local namespace (i.e. the local scope of the parse_latex function call) to avoid redundant variable assignment. Further, to eliminate constant redefining of common symbols/tensors, NRPyLaTeX automatically expands Levi-Civita symbols (of arbitrary rank), covariant derivatives, and Lie derivatives with their appropriate Einstein notation definitions using an operator inference system. In addition to parsing expressions/equations in Einstein notation, NRPyLaTeX also supports the \LaTeX\ align environment for parsing multiple equations in a single parse_latex function call. NRPyLaTeX also supports comma/semicolon notation for specifying partial/covariant derivatives, respectively. Finally, NRPyLaTeX provides an IPython/Jupyter extension module nrpylatex.extension that includes a parse_latex (line and cell) magic command, which aliases to the \%\latex\ cell magic for displaying and the parse_latex function for processing.
Appendix A.2. PARSE Command

The `parse` command parses an equation without typesetting in a `.tex` document or a Jupyter Notebook. Typically, we use the `parse` command to perform an intermediate calculation that we deem necessary but trivial; e.g., a contraction to reduce rank.

Appendix A.3. IGNORE Command

The `ignore` command ignores a \LaTeX command or substring during parsing, so that one can sanitize \LaTeX typesetting for input into NRPyLaTeX. Note, the following formatting commands are ignored by default: `\left`, `\right`, `{}`, and `&`. Furthermore, the `ignore` command and the empty replacement (`% srepl "..." -> ""`) are interchangeable. Finally, we remark that an equation cannot be split across a line break, and hence we suggest appending a percent symbol `%` to the end of a line break, creating a custom line break `\%`, and then removing that substring using the `ignore` command.
Appendix A.4. VARDEF Command

The **vardef** command defines a variable, including optional assignment of a metric (for index raising/lowering), derivative type, tensor weight, and (anti)symmetry option. In addition to assigning attributes and properties, we can label the variable a scalar constant, Kronecker delta, or metric tensor. Note, the **metric** option symmetrizes the variable and generates the metric inverse, determinant, and connection. In **NRPyLaTeX**, every variable in the namespace has an associated metric to automatically perform index raising and lowering on that variable, with the default metric following from the diacritic (or lack thereof) in the variable name (e.g., $v_i$, $\hat{v}_i$, $\bar{v}_i$, $\tilde{v}_i$). Note, **NRPyLaTeX** also supports diacritics on covariant derivatives (e.g., $D_i$, $\hat{D}_i$, $\bar{D}_i$, $\tilde{\nabla}_i$), which determines the metric used in the expansion of those covariant derivatives.

If we wanted to change the derivative type of a specific subexpression, we could use the **vphantom** command, a pseudo in-line \LaTeX comment for **NRPyLaTeX**, to prefix that subexpression with a derivative type. However, a priority system need be established between the derivative type of a variable and that specified by a **vphantom** command. In general, **vphantom** takes precedence over each variable in the subexpression with the
exception of a variable explicitly assigned a symbolic derivative type. Finally, if \( \mathbf{v} \) and \( \mathbf{vU} \), for example, are both in the namespace and we attempt to parse the expression \( \mathbf{v}^2 \), the output from \texttt{NRPyLaTeX} will be \( \mathbf{vU}[2] \) (the third component of \( \mathbf{vU} \)). To resolve that indexing ambiguity between \( \mathbf{vU}[2] \) and \( \mathbf{v}^{*2} \) (\( \mathbf{v} \) squared), we suggest using the notation \( \mathbf{v}^\{2\} \) since \( \mathbf{v}^2 \) and \( \mathbf{v}^\{2\} \) are typeset identically in \LaTeX. Similarly, if \( \mathbf{v} \) and \( \mathbf{vD} \) are both in the namespace and we are parsing the symbol \( \mathbf{v}_2 \), we suggest replacing \( \mathbf{v}_2 \) with \( \texttt{text}\{\mathbf{v}_2\} \) using the \texttt{srepl} macro to construct a compound symbol in \texttt{NRPyLaTeX} and preserve the \LaTeX typesetting of \( \mathbf{v}_2 \).

**Appendix A.5. ATTRIB Command**

![attrib]

The **attrib** command overrides global properties of \texttt{NRPyLaTeX}, called **attributes**, e. g., the coordinate system or index ranges (for looping or summation). To enable symbolic differentiation without imposing a specific coordinate system, \texttt{NRPyLaTeX} implements a generalized coordinate system \( \{x_0, \ldots, x_n\} \) capable of dynamic dimension adjustment, with a default dimension of three. However, a specific coordinate system can be imposed on \texttt{NRPyLaTeX} using the **attrib** command, allowing for coordinate indexing and symbolic differentiation with respect to a specific coordinate system. In addition to defining a coordinate system, the **attrib** command can also override the default range of an index used in Einstein summation notation, making it useful for mixed dimension indexing.
Appendix A.6. ASSIGN Command

The **assign** command assigns a **vardef** option to an already existing variable in the namespace, which can be useful for assigning attributes to variables created through equation parsing.

Appendix A.7. SREPL Command

The **srepl** command performs string replacement, ignoring whitespace, with lexeme capture group support, allowing for dynamic variable renaming, expansion/replacement of subexpressions, custom operator definitions, custom superscript/subscript definitions.
(e.g., ’, +, or -), and much more. However, unlike their regular expression counterpart, `srepl` capture groups can capture either a single lexeme or a sequence of lexemes. If we use a continuous capture group, then `srepl` captures lexemes continuously until reaching the lexeme immediately following the capture group in the replacement pattern, e.g. \( x^{<1..>} \) captures everything inside of the curly braces. Finally, the `persist` option instructs `NRPyLaTeX` to perform (syntactic) string replacement on each `parse_latex` function call, including those functions calls internal to `NRPyLaTeX` that generate \( \LaTeX \).

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\(*) Consider the following pattern: `\partial_t \phi = <1..> \.` Now, suppose that instead of the `srepl` capture group `<1..>` we use a regex capture group `([^\\]+)`. In that case, the string replacement would fail for substrings containing backslashes (a common occurrence in \( \LaTeX \)).