Automated Symbolic and Numerical Testing of DLMF Formulae using Computer Algebra Systems

Howard S. Cohl, André Greiner-Petter, and Moritz Schubotz

1 Applied and Computational Mathematics Division, National Institute of Standards and Technology, Mission Viejo, CA, U.S.A., howard.cohl@nist.gov
2 Dept. of Computer and Information Science, University of Konstanz, Konstanz, Germany, first.last@uni-konstanz.de

Abstract. We have developed an automated procedure for symbolic and numerical testing of formulae extracted from the NIST Digital Library of Mathematical Functions (DLMF). For the NIST Digital Repository of Mathematical Formulae, we have developed conversion tools from semantic LaTeX to the Computer Algebra System (CAS) MAPLE which relies on Youssef’s part-of-math tagger. We convert a test data subset of 4,078 semantic LaTeX DLMF formulae to the native CAS representation and then apply an automated scheme for symbolic and numerical testing and verification. Our framework is implemented using Java and MAPLE. We describe in detail the conversion process which is required so that the CAS can correctly interpret the mathematical representation of the formulae. We describe the improvement of the effectiveness of our automated scheme through incremental enhancement (making more precise) of the mathematical semantic markup for the formulae.

1 Problem and Current State

The NIST Digital Library of Mathematical Functions [7] (DLMF) is an online digital mathematics library which focuses on special functions and orthogonal polynomials. The DLMF is special in that it has been written like a book, but published online as a digital resource. The DLMF contains a table of contents which links to specific chapters (See Table 1 for a summary of the 36 DLMF Chapters) each of which has been written and edited by mathematicians who are experts in their specific field of focus. Furthermore, the DLMF is constantly being maintained (edited, corrected, updated) by a team of mathematicians and computer scientists who are determined to maintain and preserve the high standard of mathematical accuracy and exposition.

The DLMF has been developed in such a way that mathematical metadata is constantly being improved and restructured. For the organizational structure, semantic metadata has been incorporated at the document, chapter, section, subsection, and paragraph levels. An effort has been made to make more precise the nature of the objects which appear in the DLMF. The DLMF’s semantic realization of mathematical content has very much in common with the way mathematics is written using LaTeX, for the preparation of journal publications and actual physical books. In fact, for the construction of the DLMF, Bruce Miller has developed and actively maintains LaTeXxml [10], a program which is able to process a certain flavor of LaTeX and from it, generate a fully functional web site. We refer to this flavor of LaTeXxml as semantic LaTeX. The website is then generated using LaTeXxml, from a collection of semantic LaTeX source documents, and from other documents including Cascading Style Sheets (CSS), WebGL (Web Graphics Library) controls, Mathematical Markup Language (MathML), LaTeX style files, LaTeXxml binding files (LaTeXxml analogue of a style or class file), Java, JavaScript, etc. (see for instance [11]). The outcome is a highly sophisticated digital platform for accessing mathematical content on the web.

One main difference between LaTeX and semantic LaTeX is the latter’s ability to encapsulate mathematical knowledge in such a way that it can then be extracted by a computer program, namely LaTeXxml, to generate correctly formatted MathML (see [13] for further information about this). LaTeXxml is then able to interpret the content written in semantic LaTeX in order to generate
presentation (and content) MathML. This is then used to construct the DLMF web site and to, for instance, display metadata associated with the mathematical content. The mathematical semantic content of the DLMF includes mathematics which appears within the main body of the text, formulae (in various formulae environments), tables (in which mathematics is displayed in a tabular environment), figures (in which mathematics is visualized), operators, functions/symbols, variables (see [15] for a nice description), etc.

Even though there certainly exist methods to convert \LaTeX\ expressions into CAS formats, these in practice are only really effective if one is dealing with elementary functions defined in terms of compositions of powers-laws, sums, differences, products, quotients, trigonometric/hyperbolic functions, and exponential/logarithmic functions. If one is dealing with more complicated special functions like Bessel functions, hypergeometric functions, Airy functions, elliptic integrals, elliptic functions, etc., then effective conversions from \LaTeX\ to CAS really do not exist, and our implementation described below is the first to be able to handle situations such as these. Also, several differences in CAS vs. DLMF implementations must be captured in any effective translation, including: (1) the usage of $m = k^2$ for elliptic integrals/functions; (2) branch cuts for Legendre/Ferrers functions (and other functions); (3) and differences in normalizations of special functions. If one is unable to capture these subtleties in a translation process for the DLMF, which require careful and detailed mathematical knowledge and implementation, then the translation will fail.

In a previous paper [5], we described the conversion process that we have developed to input semantic \LaTeX\ and output a corresponding \textsc{Maple}\ CAS representation. Not surprisingly, this conversion is continually in development. New ideas are being implemented in order to increase the semantic enhancement of the original source (see for instance [14]), as well as to improve the effectiveness of our conversion software. In order to do this, we are also contributing in order to assist in the development of the part-of-math (POM) tagger [15], which our conversion program relies upon.

In this paper, we describe the process of extracting mathematical formulae from the DLMF, and then take advantage of the powerful mathematical semantic coverage of semantic \LaTeX\ used in the DLMF to convert to CAS representations whose sole purpose is to drive an automated scheme for verification of DLMF formulae. In order to improve the precision of our DLMF formulae testing reported on in [5], we did the following: (1) we updated our test formulae dataset; (2) fixed numerous translation bugs; (3) implemented a new method for handling constraints; and (4) added configuration files which make it easier to change the setup of our symbolic and numerical testing.

2 Extraction of DLMF formulae

2.1 First extraction scan

In the first extraction scan, we extract mathematical formulae from 36 \LaTeX\ source files which summarize the content of the 36 DLMF chapters formulae are extracted out of formula environments, which are (some custom)

{\texttt{\{equation\}}, \texttt{\{equationmix\}}, \texttt{\{equationgroup\}}, \texttt{\{align\}}}. Each DLMF formula in the output text file is then represented as a single string on each line in semantic \LaTeX. In order to accomplish this, all lines of the source \LaTeX\ file are merged, except that the following character strings are removed: comments; space (and other) formatting commands (such as $\backslash$ (used to insert a small horizontal space), $\backslash!$ (used to remove horizontal space), $\backslash\{\ldots\}$ (used to introduce line breaks), & (used for alignment purposes), $\ast$ (used to force line breaking on multiplication), etc.);

\texttt{\backslash MarkNotation, \backslash origref, \backslash note, \backslash lRefDeclaration, \backslash index, \backslash source, \backslash authorproof}

Along with the semantic \LaTeX\ source for the formula, we also extract two pieces of metadata associated with that formula, a \texttt{\{constraint\}} environment, and also a \texttt{\{label\}} environment. The \texttt{\backslash constraint} and \texttt{\backslash label} environments contain any constraints and \LaTeX\ labels which have been directly associated with the formula within the semantic \LaTeX\ formula environment in which it was extracted. If more than one formula is associated with a \texttt{\backslash label} environment, we inherit that \texttt{\backslash label} to all of those formulae.

\textsuperscript{3} The mention of specific products, trademarks, or brand names is for purposes of identification only. Such mention is not to be interpreted in any way as an endorsement or certification of such products or brands by the National Institute of Standards and Technology, nor does it imply that the products so identified are necessarily the best available for the purpose. All trademarks mentioned herein belong to their respective owners.
There are also certain \LaTeX\ commands or replacement macros which are specifically defined in the preamble of certain chapter source files. These are replaced in order for our translator to be able to correctly understand the corresponding derived semantic \LaTeX\ (e.g., in Chapters AI, CH the entity \texttt{\textbackslash gamma} is replaced with the macro \texttt{\textbackslash EulerConstant} \cite{7, (5.2.3)}\textsuperscript{4}, in Chapters JA, MA, LA, EL, the entities $K$ and $K'$ are replaced with the semantic macros \texttt{\textbackslash CompEllIntKk@@{k}} and \texttt{\textbackslash CompEllIntKk'@@{k}} respectively\textsuperscript{5}, etc.). See Table 1 for a description of the DLMF chapter codes. An attempt is made to remove punctuation marks at the end of each formula since these are really not a part of the formula itself. One final time consuming task is the conversion, wherever required, for the replacement of the entities $i$, $e$, and the \LaTeX\ command \texttt{\textbackslash pi} to the semantic macros \texttt{\textbackslash iunit}, \texttt{\textbackslash exp}, and \texttt{\textbackslash cpi}\textsuperscript{6}. The result of this first round is to extract 9,919 formulae from the DLMF (see the F1 entries in Table 1 for a chapter specific description of this).

\subsection{Second extraction scan}

In a second round of post processing, a subset of formulae are culled from the first extraction scan (described in the previous section). The formulae which are removed are those which contain the following \LaTeX\ commands \texttt{\textbackslash sum}, \texttt{\textbackslash int}, \texttt{\textbackslash prod}, \texttt{\textbackslash lim}, \texttt{\textbackslash dots} (including all variants), \texttt{\textbackslash sim}, or the semantic macros \texttt{\textbackslash BigO}, \texttt{\textbackslash littleo}, \texttt{\textbackslash fDiff}, \texttt{\textbackslash dDiff}, \texttt{\textbackslash cDiff}, \texttt{\textbackslash asymp}, or the environments \texttt{\{cases\}}, \texttt{\{array\}}, \texttt{\{bmatrix\}}, \texttt{\{matrix\}}, \texttt{\{Bmatrix\}}, \texttt{\{pmatrix\}}, \texttt{\{Matrix\}}, \texttt{\{Lattice\}}. This is because either our CAS translator is unable to translate these effectively, or the CAS is unable to verify mathematical objects such as these. See Section 2.3 below for ongoing strategies for handling

\begin{table}
\centering
\begin{tabular}{|c|c|c|c|}
\hline
\textbf{2C/Ch} & \textbf{Chapter Name} & \textbf{F1} & \textbf{F2} \\
\hline
\hline
AL & 1 Algebraic and Analytic Methods & 624 & 85 \\
AS & 2 Asymptotic Approximations & 375 & 56 \\
BM & 3 Numerical Methods & 428 & 41 \\
EF & 4 Elementary Functions & 529 & 166 \\
GA & 5 Gamma Function & 181 & 56 \\
RE & 6 Exponential, Logarithmic, Sine, and Cosine Integrals & 110 & 44 \\
IG & 7 Error Functions, Dawson’s and Fresnel Integrals & 158 & 80 \\
AI & 8 Incomplete Gamma and Related Functions & 272 & 120 \\
RS & 9 Airy and Related Functions & 250 & 160 \\
ST & 10 Bessel Functions & 904 & 355 \\
PC & 11 Struve and Related Functions & 168 & 83 \\
CH & 12 Parabolic Cylinder Functions & 205 & 109 \\
LE & 13 Confluent Hypergeometric Functions & 391 & 174 \\
HY & 14 Legendre and Related Functions & 294 & 173 \\
GH & 15 Hypergeometric Function & 206 & 174 \\
QH & 16 Generalized Hypergeometric Functions & 107 & 32 \\
\hline
\end{tabular}
\caption{Summary of DLMF chapters (Version 1.0.13, 2016-09-16, see Section 2.1) with corresponding 2-letter codes (2C), chapters numbers (Ch), chapter names of the DLMF chapters, chapter formulae extracted from the first extraction scan (F1), and second extraction scan (F2).}
\end{table}

\textsuperscript{4} The macro \texttt{\textbackslash EulerConstant} is just one of many (currently unpublished) semantic DLMF \LaTeX\ semantic macros which have been developed by Bruce Miller for utilization in the DLMF. In fact, the macro names used in this manuscript, have been more recently updated. However, the macro set we are utilizing, is for those in usage as of 9/16/2016.

\textsuperscript{5} These semantic macros represent the complete and complementary elliptic integrals of the first kind \cite{7, (19.2.8-9)}

\textsuperscript{6} These semantic macros represent the mathematical constants $i$, $e$ and $\pi$ \cite{7, (1.9.1), (4.2.11), (3.12.1)}.
We have also utilized a new semantically enhanced macro \texttt{\wron} for 72, two-argument Wronskian relations \cite[(1.13.4)]{7}, so that the variable which is differentiated against is precisely specified in an updated macro call. In fact, we have continued to develop many new semantically enhanced \LaTeX macros (such as \texttt{\wron}) which are not in use in the DLMF, but are in use for the NIST Digital Repository of Mathematical Formulae (see \cite[4]{4} for more details about this). (e.g., \texttt{\newcommand{\etpipm}[1]{\exp{\pm2 \pi i/#1}}} which occur in 65 separate lines). We also split equations with multiple equal \texttt{=} signs (e.g., $a = b = c$ is split into two formulae $a = b$ and $a = c$). Furthermore, we split environments which contain \texttt{\pm} (plus or minus) and \texttt{\mp} (minus or plus) commands into two separate formulae, each with their correct sign. We also remove mathematical expressions which do not contain any of the relation commands $\leq$, $\geq$, $\neq$, $\langle$, $\rangle$, $\equiv$, since their non-existence implies that there is no logical component for the mathematical expression to be verified against. The result of this second round is to extract 4,078 formulae from the DLMF (see the F2 entries in Table 1 for a chapter specific description of this).

2.3 Ongoing semantic enhancement for second extraction scan.

As mentioned above, we are currently not able to convert \LaTeX commands such as \texttt{\sum}, \texttt{\int}, \texttt{\prod}, \texttt{\lim}, which represent sums, integrals, products and limits, respectively. In this case, one draws (presentation) subscripts and superscripts in order to provide critical semantic information for these mathematical operators. In this case, there is no certainty in the specificity of the mathematical operation.

Another notation in which semantic capture is challenged is with the prime (e.g., $f'$), double prime (e.g., $f''$), triple prime (e.g., $f'''$) or superscript parenthetical (e.g., $f^{(iv)}$) notations for differentiation a given number of times. This is the same issue that was encountered previously with the Wronskian relation. In order for a CAS to be able to translate expressions such as these, we must provide the variable that one is differentiating with respect to. This is an example where a human is often able to read a formula, and by knowing the context, be able to surmise what the variable is that one is differentiating with respect to. Sometimes there is more than one variable in an expression that one is differentiating with respect to, and if one does not provide the variable, then a translator is unable to disambiguate the expression. It is interesting to note that we were able to enhance the semantics of 74 Wronskian relations by rewriting the macro so that it included the variable that derivatives are taken with respect to as a parameter. A similar semantic enhancement is possible for another 284 formulae where the potentially ambiguous prime notation $''$ is used for derivatives.

The powerful tool used by the DLMF, \LaTeX, is often able to guess a syntax tree when the \LaTeX commands \texttt{\sum}, \texttt{\int}, \texttt{\prod}, and \texttt{\lim} are used. This is due to, for instance, the utilization of the semantic \LaTeX \texttt{\diff} macro for integrals. This is quite effective, since it makes available the variable that one is integrating with respect to. For instance, one may mark up a definite integral such as

\[
\int_a^b f(x,y)dx.
\]

by using semantic \LaTeX as follows \texttt{\int_{a}^{b} f(x,y) \diff{x}}, which provides the variable of integration $x$. This information is essential for disambiguation of the involved operation variable, and therefore for converting the definite integral to a CAS representation. Such content is not always easily accessible. For instance, one is still unable to easily guess the variable of differentiation when prime (etc.) notations for derivatives are used. One is able to facilitate the extraction of semantic content in formulae which contain mathematical \LaTeX such as described above, by making the semantic content more easily available. We would like to see this type of semantic content made more fully available for translators, and this is an ongoing effort.

It is possible to incrementally enhance mathematical semantic expressions through optimization and broader usage and development of semantic \LaTeX macros. Take for instance the formula with the label \{eq:OP.CP.SV.LR.1a\} \cite[(18.8.21)]{7}, given by

\[
\lim_{\beta \to \infty} \text{JacobiP}(\alpha)\beta(n)\left(1-\left(2x/\beta\right)\right) = \text{LaguerreL}(\alpha)\beta(x).
\]
In this example, our semantic enhancement process is made more effective by developing and utilizing a new mathematical semantic \LaTeX macro with separate parameters and arguments (before and after the \@ sign respectively) which is described as
\[ \text{\textbackslash Lim\{#1\}\@\{#2\}@\{#3\} := } \lim_{#1 \to #2} #3. \]

Here the first parameter of the macro call \#1 is the variable the limit is taken over, the second parameter of the macro call \#2 is the destination of the limit for \#1, and the argument \#3 is the expression that the limit is taken over. Utilizing this new macro, the above formula is then written with enhanced semantics as:
\[ \text{\textbackslash Lim\{\beta\}\@\{\infty\}@\{\text{\textbackslash JacobiP\{\alpha\}\@\{\beta\}@\{n\}@\{1-(\text{\textfrac{2x}{\beta}})\}\}\} } = \text{\textbackslash LaguerreL\{\alpha\}@\{n\}@\{x\}.} \]

This new formula will have identical presentation to the previous formula, and the semantics are more easily extracted (using for instance, the POM tagger). We have also developed semantic macros for sums, products, definite (or indefinite) integrals, as well as for antiderivatives, namely
\[ \text{\textbackslash Sum\{#1\}\@\{#2\}@\{#3\}@\{#4\} := } \sum_{#1=#2}^{#3} #4, \quad \text{\textbackslash Prod\{#1\}\@\{#2\}@\{#3\}@\{#4\} := } \prod_{#1=#2}^{#3} #4, \]
\[ \text{\textbackslash Int\{#1\}\@\{#2\}@\{#3\}@\{#4\} := } \int_{#1}^{#2} #4 \text{d}#3, \quad \text{\textbackslash Antider\{#1\}\@\{#2\} := } \int #2 \text{d}#1. \]

The incorporation of these semantic macros into semantic \LaTeX facilitates the translation of the mathematical \LaTeX source expression to a CAS representation. It therefore improves one’s ability to automate injection of the mathematical content into CAS.

There often exists alternate usage of mathematical notations. For example, one often writes for a sum,
\[ \sum_{n \in A} f(n), \]
where \( A \) is some subset of the integers. It is not difficult to customize the macro definitions to be capable of dealing with such notations, assuming that one has a precise description of \( A \).

3 CAS verification procedure for DLMF formulae

We translate the semantic \LaTeX for our test dataset of DLMF formulae to MAPLE CAS representation, using the tool described in [5]. We use easily configurable settings to control our verifications.

Using the configuration files, we can control and customize settings for the verification process, e.g., if one would like to perform numerical evaluations on more complicated expressions involving differences or divisions of the left-hand sides and right-hand sides of the DLMF formulae.

3.1 Symbolic Verification of DLMF formulae

Originally, we used the standalone MAPLE simplify function directly, to symbolically simplify translated formulae. See [9, 2, 8, 1] for other examples of where MAPLE and other CAS simplification procedures has been used elsewhere in the literature. Symbolic simplification is performed either on the difference or the division of the left-hand sides and the right-hand sides of extracted formulae. Thus the expected outcome should be respectively either a 0 or 1. Note that other outcomes, such as other numerical outcomes, are particularly interesting, since these may be an indication of errors in the formulae.

In MAPLE, symbolic simplifications are made using internally stored relations to other functions. If a simplification is available, then in practice it often has to be performed over multiple defined relevant relations. Often, this process fails and MAPLE is unable to simplify the said expression. We have adopted some techniques which assist MAPLE in this process. For example, forcing an expression to be converted into another specific representation, in a pre-processing step, could potentially improve the odds that MAPLE is able to recognize a possible simplification. By trial-and-error, we discovered (and implemented) the following pre-processing steps which significantly improve the simplification process:

– conversion to exponential representation;
– conversion to hypergeometric representation;
– expansion of expressions (for example \((x+y)^2\); and
– combined expansion and conversion processes.
3.2 Constraint Handling.

Correct assumptions about variable domains are essential for CAS systems, and not surprisingly lead to significant improvements in the CAS ability to simplify. The DLMF provides constraint (variable domain) metadata for formulae, and as mentioned in Section 2.1, we have extracted this formula metadata. We have incorporated these constraints as assumptions for the simplification process. Note however, that a direct translation of the constraint metadata is usually not sufficient for a CAS to be able to understand it. Furthermore, testing invalid values for numerical tests returns incorrect results.

For instance different symbols must be interpreted differently depending on the usage. One must be able to interpret correctly certain notations of this kind. For instance, one must be able to interpret the command $a,b \in A$, which indicates that both variables $a$ and $b$ are elements of the set $A$ (or more generally $a_1,\ldots,a_n \in A$). Similar conventions are often used for variables being elements of other sets such as the sets of rational, real or complex numbers, or for subsets of those sets.

Also, one must be able to interpret the constraints as variables in sets defined using an equals notation such as $n=0,1,2,\ldots$, indicating that the variable $n$ is a integer greater than or equal to zero, or together $n,m=0,1,2,\ldots$, both the variables $n$ and $m$ are elements of this set. Since mathematicians who write $\LaTeX$ are often casual about expressions such as these, one should know that $0,1,2,\ldots$ is the same as $0,1,\ldots$. Consistently, one must also be able to correctly interpret infinite sets (represented as strings) such as $=1,2,\ldots$, $=0,2,4,\ldots$, or even $=3,7,11,\ldots$, or $=5,9,13,\ldots$. One must be able to interpret finite sets such as $=1,2$, $=1,2,3$, or $=1,2,\ldots,N$.

An entire language of translation of mathematical notation must be understood in order for CAS to be able to understand constraints. In mathematics, the syntax of constraints is often very compact and contains textual explanations. Translating constraints from $\LaTeX$ to CAS is a compact task because CAS only allow precise and strict syntax formats. For example, the typical constraint $0 < x < 1$ is invalid if directly translated to MAPLE, because it would need to be translated to two separate constraints, namely $x > 0$ and $x < 1$.

We have improved the handling and translation of variable constraints/assumptions for simplification and numerical evaluation. Adding assumptions about the constrained variables improves the effectiveness of MAPLE’s simplify function. Our previous approach for constraint handling for numerical tests was to extract a pre-defined set of test values and to filter invalid values according to the constraints. Because of this strategy, there often was no longer any valid values remaining after the filtering. To overcome this issue, instead, we chose a single numerical value for a variable that appears in a pre-defined constraint. For example, if a test case contains the constraint $0 < x < 1$, we chose $x = \frac{1}{2}$.

A naive approach for this strategy, is to apply regular expressions to identify a match between a constraint and a rule. However, we believed that this approach does not scale well when it comes to more and more pre-defined rules and more complex constraints. Hence, we used the POM-tagger to create blueprints of the parse trees for pre-defined rules. For the example $\LaTeX$ constraint $x,y \in \Real$, rendered as $x,y \in \mathbb{R}$, is given by $\text{var1, var2} \in \text{\Real}$. A constraint will match one of the blueprints if the number, the ordering, and the type of the tokens are equal. Allowed matching tokens for the variable placeholders are Latin or Greek letters and alphanumerical tokens.

3.3 Numerical Verification of DLMF formulae

Due to the fact that CAS simplification verification is not extremely effective, we also used our CAS translation to perform numerical testing as well. To perform automated numerical evaluations, we extracted all variables from the expression. Variables are extracted by identifying all names.
from an expression. This will also extract constants which need to be deleted from the list first. Afterwards, we set each variable to a specific numerical value and numerically evaluate the expression. One is given the capability to choose the numerical values of the given variables as either complex numbers, real numbers, or even as integers. Given this typing of variables, we also check the values to ensure that they are subject to the the constraints (see Section 3.2 above). We allow for the definition of a set of numerical values for variables that we want to verify, and for multiple variable choices, the power-set of these choices is looped over (we evaluate all combinations of variable-value pairs). We consider an evaluation to be successful if the outcome is below a given threshold (currently set at 0.001) compared with a certain precision (currently set at 10).

4 Summary

We have created a test dataset\(^8\) of 4,078 semantic \LaTeX\ formulae, extracted from the DLMF. We translated each test case to a representation in MAPLE and used MAPLE’s simplify function on the formula difference to verify that the translated formulae remain valid. Our forward translation tool (Section 2) was able to translate 2,405 (approx. 59\%) test cases. Most likely, a translation failed because it encountered a DLMF/DRMF semantic macro without a known translation to MAPLE (1,021 of non-translated cases, approx. 61\%). An example of such a non-supported macros is the (basic) \(q\)-hypergeometric function \([7, (17.4.1)]\). In other cases, translation of expressions failed because they contained insufficient semantic information, such as when the prime and superscript notations for derivatives are used (Section 2.3), or encountered assorted errors in the translation engine. Such assorted errors include unimplemented grammar mappings from the POM tagger such as handling subsuperscript outputs or overlining expressions for complex conjugations.

We applied our symbolic verification techniques to the 2,405 translated expressions. The proposed simplification was able to verify 481 of these expressions (20\%). Pre-conversion improved the effectiveness of simplify and was used to convert the translated expression to a different form before simplification of the formula difference. We used conversions to exponential and hypergeometric form and expanded the translated expression. Those pre-processed manipulations increased the number of formulae verified from 481 to 660 (approx. 27.4\%). The remaining 1,745 test cases were translated but not verified. Note that verification should also fail because either expression would not contain a logical relation and therefore are unverifiable (Section 2.2), but these are filtered out in a pre-processing step, or that the CAS is not yet sophisticated enough to verify (such as in the case of asymptotic representations).

We have also applied several numerical tests to these remaining test cases (Section 3.3). The results of the numerical tests strongly depend on the tested values. Besides the defined numerical values for general tests, we applied special values for certain constraints. This was realized by our new approach of applying rules for blueprints of common constraints (Section 3.2). In automated evaluations, we performed numerical tests by setting variables in test expressions to values contained in the set \([-0.5, 0.5, 1.5]\). In the cases where the tested expression is an equation, we tested the difference between the left- and the right-hand sides of the equations. For other relations, we tested if the relation still remains for the calculated numerical values. With this set of the three values and the set of special values depending on additional constraints, 418 of the remaining unverified test cases return a valid output (approx. 24\%). 14 numerical tests stopped, because they exceeded our pre-defined time-limit of 300 seconds. In 892 cases (approx. 51.1\%), the calculated values were above our given threshold of 0.001. Note that numerical verifications may fail because of one of four reasons:

1. the numerical engine tests invalid combinations of values;
2. the translation is incorrect;
3. there may be an error in the DLMF source; or
4. there may be an error in MAPLE.

Typical origins for reason 1 are errors produced in the translations of constraints (Section 3.2), and may prevent the numerical test engine from using valid numerical values for evaluation. Another typical problem is missing information from context, such as if a variable was pre-defined by substitution, but the test case misses this information. For example, \([7, (9.6.1)]\) defines \(\zeta = \frac{2}{3} \cdot 3^{3/2}\).

\(^7\) A name in MAPLE is a sequence of one or more characters that uniquely identifies a command, file, variable, or other entity.

\(^8\) This dataset is available on request to the authors.
Table 2. Overview of symbolic and numerical testing for each DLMF chapter with the corresponding DLMF chapter 2-letter codes (2C), chapters numbers (C#), number of extracted expressions of the second extraction scan (F2), number of translated expressions (T) with approximated percentages, number of translated and symbolically verified cases (TVn) with approximated percentages, and number of translated cases where the numerical evaluations returned valid outputs for the set of test values \{-0.5, 0.5, 1.5\} (TVs) with approximated percentages (excluding the number of symbolically verified translations). The best results of each technique are highlighted in bold.

| 2C | C# | F2  | T        | TVs | TVn |
|----|----|-----|----------|-----|-----|
| AL | 1  | 85  | 44 (51.8%) | 4 (4.7%) | 8 (9.9%) |
| AS | 2  | 56  | 27 (48.2%) | 2 (3.6%) | 0 (0%) |
| NM | 3  | 41  | 34 (82.9%) | 1 (2.4%) | 1 (2.5%) |
| EF | 4  | 466 | 406 (87.1%) | 182 (39.1%) | 61 (21.5%) |
| GA | 5  | 56  | 39 (69.6%) | 10 (17.9%) | 15 (32.6%) |
| EX | 6  | 44  | 13 (29.5%) | 0 (0%) | 1 (2.3%) |
| ER | 7  | 80  | 60 (75.0%) | 21 (30%) | 11 (19.6%) |
| IG | 8  | 120 | 89 (74.2%) | 24 (20%) | 13 (13.5%) |
| AE | 9  | 160 | 71 (44.4%) | 8 (5%) | 19 (12.5%) |
| BS | 10 | 355 | 174 (49.0%) | 44 (12.4%) | 47 (11.9%) |
| ST | 11 | 83  | 71 (85.5%) | 20 (24.1%) | 11 (17.5%) |
| PC | 12 | 100 | 71 (71.0%) | 14 (14%) | 12 (14%) |
| CH | 13 | 174 | 168 (96.6%) | 61 (35.1%) | 24 (21.2%) |
| LE | 14 | 173 | 163 (94.2%) | 31 (17.9%) | 37 (26.1%) |
| HY | 15 | 174 | 170 (97.7%) | 39 (22.4%) | 34 (25.2%) |
| GH | 16 | 32  | 18 (56.3%) | 3 (9.4%) | 0 (0%) |
| QH | 17 | 96  | 0 (0%) | — | — |
| OP | 18 | 253 | 141 (55.7%) | 58 (22.9%) | 23 (11.8%) |
| Σ  |  |  |  |  |  |
| 60 |  |  |  |  |  |

The following equations are only valid considering the pre-defined numerical value for \( \zeta \). Furthermore, this equation is a definition of \( \zeta \). If we test this equation by simplifications or numerical evaluations, we get invalid results. We call such failed numerical evaluations by reason 1, false positives, since they were marked as particularly interesting cases (for reasons 2-4) but they were caused by missing semantic information originating from the source. It seems that the number of false positive results is very high and plan to reduce this in the future. Table 2 gives an overview of the symbolic and numerical testing for each DLMF chapter. The overview of translations (T) per chapter reveals the weakness of our translation engine especially in the Chapters 17 (QH) and 34 (TJ). A high ratio of symbolically verified and translated formulae indicates a large success rate for translating macros into MAPLE functions. This is one explanation for the fact that our best result comes from Chapter 4 EF.

Originally, the verification rules were developed to identify errors in the translation engine, see reason 2. However, further investigations of the 892 cases reveals a sign error in the DLMF (reason 3), and this corresponded to [7, (14.5.14)], namely

\[
Q_n^{-1/2}(\cos \theta) = \left( \frac{\pi}{2 \sin \theta} \right)^{1/2} \cos \left( \frac{\nu + \frac{1}{2}}{\nu} \theta \right),
\]

where \( Q_n \) is the Ferrers function of the second kind. This error can be found on [12, p. 359], and was reported in DLMF Version 1.0.16 on September 18, 2017. Other cases where formulae seem to be unverified by numerical tests are for DLMF formulas which are valid on Riemann surfaces, but fail because MAPLE functions. This is one explanation for the fact that our best result comes from Chapter 4 EF.
Acknowledgements. We are indebted to Bruce Miller and Abdou Youssef for valuable discussions and for the development of the custom macro set of semantic mathematical \LaTeX macros used in the DLMF, and for the development of the POM tagger, respectively. We also thank the DLMF editors for their assistance and support.

References

[1] D. H. Bailey, J. M. Borwein, and A. D. Kaiser. “Automated simplification of large symbolic expressions”. In: J. Symbolic Comput. 60 (2014), pp. 120–136. ISSN: 0747-7171. DOI: 10.1016/j.jsc.2013.09.001. URL: https://doi.org/10.1016/j.jsc.2013.09.001.

[2] C. Ballarin, K. Homann, and J. Calmet. “Theorems and Algorithms: An Interface Between Isabelle and Maple”. In: Proceedings of the 1995 International Symposium on Symbolic and Algebraic Computation. ISSAC ’95. Montreal, Quebec, Canada: ACM, 1995, pp. 150–157. ISBN: 0-89791-699-9. DOI: 10.1145/220346.220366. URL: http://doi.acm.org/10.1145/220346.220366.

[3] L. Bernardin et al. Maple Programming Guide. Waterloo ON, Canada: Maplesoft, a division of Waterloo Maple Inc., 2016.

[4] H. S. Cohl et al. “Growing the Digital Repository of Mathematical Formulae with Generic \LaTeX Sources”. In: Intelligent Computer Mathematics, Lecture Notes in Artificial Intelligence 9150. Springer, 2015, pp. 280–287.

[5] H. S. Cohl et al. “Semantic Preserving Bijective Mappings of Mathematical Formulae Between Document Preparation Systems and Computer Algebra Systems”. In: Lecture Notes in Computer Science 10383, Intelligent Computer Mathematics: 10th International Conference, CICM 2017, Edinburgh, UK, July 17-21, 2017. Ed. by H. Geuvers et al. Springer International Publishing, 2017, pp. 115–131. ISBN: 978-3-319-62075-6. DOI: 10.1007/978-3-319-62075-6_9. URL: https://doi.org/10.1007/978-3-319-62075-6_9.

[7] NIST Digital Library of Mathematical Functions. http://dlmf.nist.gov/, Release 1.0.18 of 2018-03-27. F. W. J. Olver, A. B. Olde Daalhuis, D. W. Lozier, B. I. Schneider, R. F. Boisvert, C. W. Clark, B. R. Miller and B. V. Saunders, editors. URL: %5Curl%7Bhttp://dlmf.nist.gov/%7D.

[9] J. Harrison and L. Théry. “A Skeptic’s Approach to Combining HOL and Maple”. In: Journal of Automated Reasoning 21.3 (Dec. 1998), pp. 279–294. ISSN: 1573-0670. DOI: 10.1023/A:1006023127567. URL: https://doi.org/10.1023/A:1006023127567.

[9] W. Koepf. “On two conjectures of M. S. Robertson”. In: Complex Variables. Theory and Application. An International Journal 16.2-3 (1991), pp. 127–130. ISSN: 0278-1077. DOI: 10.1080/17476939108814474. URL: https://doi.org/10.1080/17476939108814474.

[10] B. R. Miller. \LaTeX to XML/HTML/MathML Converter. http://dlmf.nist.gov/LaTeXML/. June 2018. URL: http://dlmf.nist.gov/LaTeXML/.

[11] B. R. Miller and A. Youssef. “Technical Aspects of the Digital Library of Mathematical Functions”. In: Annals of Mathematics and Artificial Intelligence 38.1-3 (2003), pp. 121–136.

[12] F. W. J. Olver et al., eds. NIST handbook of mathematical functions. With 1 CD-ROM (Windows, Macintosh and UNIX). U.S. Department of Commerce, National Institute of Standards and Technology, Washington, DC; Cambridge University Press, Cambridge, 2010, pp. xvi+951. ISBN: 978-0-521-14063-8.

[13] M. Schubotz et al. “Improving the Representation and Conversion of Mathematical Formulae by Considering their Textual Context”. In: Joint Conference on Digital Libraries 2018, June 2018, Fort Worth, TX (2018).

[14] M. Schubotz et al. “VMEXT: A Visualization Tool for Mathematical Expression Trees”. In: Lecture Notes in Computer Science 10383, Intelligent Computer Mathematics: 10th International Conference, CICM 2017, Edinburgh, UK, July 17-21, 2017. Ed. by H. Geuvers et al. Springer International Publishing, 2017, pp. 340–355. ISBN: 978-3-319-62075-6. DOI: 10.1007/978-3-319-62075-6_24.

[15] A. Youssef. “Part-of-Math Tagging and Applications”. In: Lecture Notes in Computer Science 10383, Intelligent Computer Mathematics: 10th International Conference, CICM 2017, Edinburgh, UK, July 17-21, 2017. Ed. by H. Geuvers et al. Springer International Publishing, 2017, pp. 356–374. ISBN: 978-3-319-62075-6. DOI: 10.1007/978-3-319-62075-6_25. URL: https://doi.org/10.1007/978-3-319-62075-6_25.
Listing 1.1. Use the following BibTeX code to cite this article

```bibtex
@inproceedings{CohlGS18,
    author = {Cohl, Howard S. and Greiner-Petter, Andr	extquoteleft{e} and Schubotz, Moritz},
    title = {Automated Symbolic and Numerical Testing of DLMF Formulae using Computer Algebra Systems},
    booktitle = {Proceedings of the 11th International Conference on Intelligent Computer Mathematics (CICM)},
    series = {Lecture Notes in Computer Science},
    volume = {11006},
    pages = {39--52},
    publisher = {Springer},
    doi = {10.1007/978-3-319-96812-4_4},
    year = {2018}
}
```