An optimizing multi-platform source-to-source compiler framework for the NEURON MODeling Language

Pramod Kumbhar
Ecole Polytechnique Fédérale de Lausanne (EPFL)

Omar Awile
Ecole Polytechnique Fédérale de Lausanne (EPFL)

Liam Keegan
Ecole Polytechnique Fédérale de Lausanne (EPFL)

Jorge Blanco Alonso
Ecole Polytechnique Fédérale de Lausanne (EPFL)

James King
Ecole Polytechnique Fédérale de Lausanne (EPFL)

Michael Hines
Yale University

Felix Schürmann
felix.schuermann@epfl.ch
Ecole Polytechnique Fédérale de Lausanne (EPFL)

ABSTRACT
Domain-specific languages (DSLs) play an increasingly important role in the generation of high performing software. They allow the user to exploit specific knowledge encoded in the constructs for the generation of code adapted to a particular hardware architecture; at the same time, they make it easier to generate optimized code for a multitude of platforms as the transformation has to be encoded only once. Here, we describe a new code generation framework (NMODL) for an existing DSL in the NEURON framework, a widely used software for massively parallel simulation of biophysically detailed brain tissue models. Existing NMODL DSL transpilers lack either essential features to generate optimized code or capability to parse the diversity of existing models in the user community. Our NMODL framework has been tested against a large number of previously published user models and offers high-level domain-specific optimizations and symbolic algebraic simplifications before target code generation. Furthermore, rich analysis tools are provided allowing the scientist to introspect models. NMODL implements multiple SIMD and SPMD targets optimized for modern hardware. Benchmarks were performed on Intel Skylake, Intel KNL and AMD Naples platforms. When comparing NMODL-generated kernels with NEURON we observe a speedup of up to 20x, resulting into overall speedups of two different production simulations by \( \approx 10x \). When compared to a previously published SIMD optimized version that heavily relied on auto-vectorization by the compiler still a speedup of up to \( \approx 2x \) is observed.

KEYWORDS
NEURON, HPC, neuroscience, DSL, compiler, code generation

1 INTRODUCTION
The use of large scale simulation in modern neuroscience is becoming increasingly important (e.g. [1–3]) and has been enabled by substantial performance progress in neurosimulation engines over the last decade and a half (e.g. [4–9]). While excellent scaling has been achieved on a variety of platforms with the conversion to Single Instruction Multiple Data (SIMD) implementations, domain specific knowledge expressed in the models is not yet optimally used. In other fields, the use of DSLs and subsequent code-to-code translation have been effective in generating high performing codes and allowing easy adaptation to novel architectures ([10–14]). This is becoming more important as the architectural diversity of computers is increasing as a reaction to mutually exclusive design trade offs forced by more evident physical and economic limitations when going to the next generation of computing systems.

Motivated by these observations, we have revisited the widely adopted NEURON simulator [15], which enables simulations of biophysically detailed neuron models on computing platforms ranging from desktop to petascale supercomputers, and which has over 2,000 reported scientific studies using it. NEURON supports networks of neurons with complex branched anatomy and biophysical properties such as multiple channel types, inhomogeneous channel distribution, ionic accumulation and diffusion-reactions. One of the key features of the NEURON simulator is extendability via a domain specific language (DSL) layer called the NEURON Model Description Language (NMODL) [16]. NMODL allows model authors to extend NEURON by incorporating a wide range of membrane and intracellular submodels such as voltage and ligand gated channels, ionic accumulation and diffusion, and synapse models. The domain scientists can easily express these channel properties in terms of algebraic and ordinary differential equations, kinetic schemes, and finite state machines in NMODL. Working at a descriptive level allows easy development of models while focusing on biological aspects rather than worrying about lower level implementation details such as solver methods, threads, memory layout, parallel execution etc.

The rate limiting aspect for performance of NEURON simulations is the execution of channels and synapses written in the NMODL DSL. The code generated from NMODL often accounts for more than 80% of overall execution time. For example, Figure 1 shows the execution profile of a Hippocampus model [17] with about 670
Figure 1: Execution profile of hippocampus CA1 model showing the percentage of time spent in various parts of the NEURON simulator. More than 90% of the execution time is spent in the kernels generated from the NMODL DSL.

There are more than six thousand NMODL files that are shared by the NEURON user community on the ModelDB platform [19]. As the type and number of mechanisms differ from model to model, hand-tuning of the generated code is not feasible. The goal of our NMODL Framework is to provide a tool that can parse all existing models, and generate optimized code from NMODL DSL code, which is responsible for more than 80% of the total simulation time.

2 RELATED WORK

The reference implementation for the NMODL DSL specification is found in nocmodl [20], which is a component in the NEURON simulator. Over the years nocmodl underwent several iterations of development and gained support for a number of newer language constructs and a C code generator backend for the NEURON simulator. Nocmodl uses lex/flex [21] and yacc/bison [22] for its scanner and parser implementation respectively. One of the major limitations of nocmodl is its lack of flexibility. Instead of constructing an intermediate representation, such as an Abstract Syntax Tree (AST), it performs many code generation steps on the fly, while parsing input as part of the bison production rules. This leaves little flexibility for performing global analysis, optimizations, adapting code generation for different languages or targeting a different simulator altogether. The CoreNEURON library uses a modified version of nocmodl called mod2c [23]. Mod2c duplicates most of the legacy code with the modifications needed to generate code with new data structures present in CoreNEURON, different memory layouts and GPU support based on the OpenACC programming model. But, as mod2c shares most of its implementation with nocmodl, it still has some of the same limitations as nocmodl. Pynmodl [24] is a Python based parsing and post-processing tool for NMODL. The primary focus of pynmodl is to parse and translate NMODL DSL to other computational neuroscience DSLs such as LEMS [25]. Pynmodl supports a subset of the NMODL DSL specification and does not support lower level code generation for a particular simulator. The mod2c source-to-source compiler is being developed as part of the Arbor simulator [26]. It is able to generate from NMODL DSL code, optimized C++/CUDA to be used with the Arbor simulator. Its lexer and parser have been hand-implemented in C++ and generate an intermediate AST representation. However, it only implements a subset of the NMODL DSL specification and hence is only able to process a modest number of existing models available in ModelDB [19]. For a more comprehensive review of current code-generator techniques in computational neuroscience we refer the reader to Blundell et al [27]. In summary, we conclude that current tools either lack support for the full NMODL DSL specification, lack the necessary flexibility to be used as a generic code generation framework, or are unable to adequately take advantage of modern hardware architectures, and thus are missing out on available performance from modern computing architectures.

3 NMODL DSL

To understand important code generation aspects for improving performance, a simple example of a voltage-gated calcium channel written in NMODL DSL is presented in Figure 2. Due to space constraints the example is modified to highlight important language constructs.

Each named block in the NMODL DSL has the general form of KEYWORD { statements }. There are more than 90 different constructs or keywords in the language. Keywords are printed in all uppercase and marked with boldface in the example. The NEURON block specifies the name of the mechanism, ion usage, and variables used in the model. The SUFFIX keyword identifies this as a density mechanism (as opposed to POINT_PROCESS which would instead identify it as a synapse or electrode class whose instances are localized to a single point on the neuron). The USEION statement indicates the interaction of this mechanism with those other mechanisms at the same location sharing the same ion type. The RANGE keyword indicates that the encompassed variables are functions of position (i.e. each of these variables can have a different value in each compartment). LOCAL variables are block scoped variables in the block. Internal to the mod file, variables that are used as model parameters are defined in the PARAMETER block. The ASSIGNED block is used to declare variables that can appear on the left hand side of assignment statements (i.e. modifiable variables). If a model uses differential equations, algebraic equations, or kinetic reaction schemes, their
 dependent variables are listed in the STATE block. The BREAKPOINT block is used to update current and conductance at each time step. The DERIVATIVE block contains differential equations of the form \( y' = \text{expr} \) that are used to assign values to the derivatives of STATE variables. The SOLVE statement is used to specify the integration scheme (see section 5). The PROCEDURE and FUNCTION constructs are callable functions where the only difference is that the FUNCTION variation can return a value. Users can also use VERBATIM constructs to embed C code directly into the DSL. The enclosing statements will be copied to the generated code in place. This offers flexibility to implement lower level functionality not exposed by NMODL DSL, but also makes it difficult to generate portable code. More information about NMODL specification can be found in [16].

At the DSL level there is a lot of information implicitly expressed that can be used to generate efficient code and expose more parallelism. Some of the examples are:

- **USEION statement** describes the dependency of this mechanism with other ion channels (e.g. ca). This information can be used to build the runtime dependency graph to exploit micro-parallelism [28].
- **PARAMETER block** describes the variables that are constant during runtime, often with limited precision requirements and often with small range of values (e.g. gcatbar). This information can be used to improve memory access cost and reduce memory footprint.
- **ASSIGNED statement** describes modifiable variables. These variables can be allocated in fast memory to reduce access latency (e.g. minf).
- **DERIVATIVE, KINETIC and SOLVE describes ODEs which can be analyzed and solved analytically to improve the performance as well as accuracy.
- **BREAKPOINT** describes current and conductance update at each time step. If the current and voltage relation is ohmic then one can use analytical expression instead of numerical derivatives to improve the accuracy as well as performance.
- **PROCEDURE** does not allow a return value and hence often users use RANGE variables (e.g. minf, mtau). If plotting of such variables is not required, procedures can be inlined at DSL level (e.g. rates) to eliminate RANGE variables and thereby significantly reduce memory access cost as well as memory footprint.

To use this information and perform such optimizations, often global analysis of the NMODL DSL is required. For example, to perform inlining of a PROCEDURE one needs to find all function calls and recursively inline the function bodies. To verify if a variable can be made const, one needs to find all its usages. As nocmodl lacks the intermediate AST representation, this type of analysis is difficult to perform and these optimizations are not implemented. The NMODL code generation framework is designed to exploit all such information from DSL specification and perform optimizations.

4 **DESIGN AND IMPLEMENTATION**

The overall design of the NMODL Framework can be broken down into six components: lexer/parser implementation, AST and DSL level optimisation passes, ODE solvers, Python bindings, and finally
code generation passes. Figure 3 summarizes the overall architecture.

### 4.1 Lexer and Parser

As in any compilation process, the first two steps performed on an input NMODL DSL are **lexing** and **parsing**. The lexer implementation is based on the popular flex package and bison is used as the parser generator. To make the lexer and parser fully reentrant [29], we make use of the C++ Bison Interface parser implementation. The bison grammar is based on nocmodl, which is a reference implementation for the NMODL DSL, making our implementation fully compatible with the NMODL language specification. As parser rules are executed, appropriate C++ classes are instantiated to construct an Abstract Syntax Tree (see subsection 4.2). As opposed to nocmodl and mod2c our approach allows us to keep parsing and code generation steps completely separated and an arbitrary number of intermediate analysis and optimization steps can be interposed. The ODEs, units and inline C code (from VERBATIM blocks) need extra processing during further distinct compiler passes. To parse these constructs, we have implemented separate lexers and parsers using flex and bison.

### 4.2 Abstract Syntax Tree Representation

The goal of the NMODL Framework is to implement a general purpose parsing and code generation tool not tied to a particular simulator. For this, all language semantics need to be preserved in the Abstract Syntax Tree (AST) representation so that different higher level tools can use this information for different purposes. With more than 90 keywords, 130 different AST node types are required to represent all language semantics. Each node of the AST is implemented as a C++ class and represents a syntactic element, or a group of syntactic or semantic elements of the DSL. To avoid having to implement more than 130 C++ classes by hand, we used the declarative approach for AST design using a YAML specification [30]. Figure 4 shows an excerpt of the YAML specification of the DSL. This YAML specification is translated to C++ classes using the Python jinja2 template engine [31]. Using this approach we are able to generate most of the AST representation and AST visitor framework in a compact code base. This approach provides flexibility to extend the AST design with minimal changes and hence higher productivity.

The hierarchy in the YAML specification represents inheritance relationships with C++ AST classes. The *member* specification describes *member* variables with their types in C++ classes.

Figure 5 shows an example of the AST in-memory representation constructed by the NMODL parser for the example discussed in section 3. As the NMODL language supports block scopes, scoped symbol tables [32] are created at each block scope and attached to the corresponding AST node.

### 4.3 Optimization Passes

Modern compilers implement various passes for code analysis, code transformation, and optimized code generation. Optimizations such as constant folding [33], inlining [34], and loop unrolling [35] are commonly found in all of today’s major compilers. For example, the
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```plaintext
1  - Node:
2    description: "Base class for nodes in the AST"
3    children:
4      - Expression:
5        description: "Represents an expression"
6        children:
7          - Number:
8            description: "Represents a number"
9            children:
10             - Float:
11               description: "Represents a float number"
12                  members:
13                    - value:
14                      type: float

Figure 4: An example of YAML specification for AST base nodes like `Node`, `Expression` and child node `Float`

Figure 5: In memory AST representation of the NMODL code from Figure 2 showing different AST node types and symbol tables created.

LLVM compiler framework [36] features more than one hundred compiler passes [37].

In the context of the NMODL Framework, we focus on a few optimization passes with very specific objectives. By taking advantage of domain-specific and high-level information that is available in the DSL but later lost in the lower level C++ or CUDA code, we are able to provide additional significant improvements in code performance. For example, all NMODL `RANGE`, `ASSIGNED`, and `PARAMETER` variables are translated to `double` type variables in C++. Once this transformation is done, C/C++ compilers can no longer infer these high-level semantics from these variables. Another example is `RANGE` to `LOCAL` transformations with the help of `PROCEDURE` inlining discussed in section 3. All `RANGE` variables in the NMODL DSL are converted to array variables and are dynamically allocated in C++. Once this transformation is done, the C/C++ compiler can only do limited optimizations.

To facilitate the DSL level optimizations summarized in section 3, we have implemented the following optimization passes. As most of these optimization passes are also commonly used in compilers today, we only summarize their role in the context of NMODL DSL optimizations.

- **Inlining**: To facilitate optimizations such as `RANGE` to `LOCAL` conversion and facilitate other code transformations, the `Inlining` pass performs code inlining of `PROCEDURE` and `FUNCTION` blocks at their call sites.
- **Variable Usage Analysis**: Different variable types such as `RANGE`, `GLOBAL`, `ASSIGNED` can be analysed to check where and how often they are used. The `Variable Usage Analysis` pass implements `Definition-Use (DU)` chains [38] to perform data flow analysis.
- **Localiser**: Once function inlining is performed, `DU` chains can be used to decide which `RANGE` variables can be converted to `LOCAL` variables. The `Localiser` pass is responsible for this optimization.
- **Constant Folding and Loop Unrolling**: The `KINETIC` and `DERIVATIVE` blocks can contain coupled ODEs in `WHILE` or `FOR` loop statements. In order to analyse these ODEs with SymPy (see section 5), first we need to perform constant folding to know the iteration space of the loop and then perform `loop unrolling` to make all ODE statements explicit.

All above-described optimization passes operate on the `AST` and are implemented using the `Visitor Pattern`.

### 4.4 Code Generation

Once DSL and symbolic optimizations (see section 5) are performed on the AST, the NMODL Framework is ready to proceed to the code generation step (cf. Figure 3). Table 1 summarizes the various target languages supported for different hardware platforms. The C++ code generator plays a special role, since it constitutes the base code generator extended by all other implementations. This allows easy implementation of a new target by overriding only necessary constructs of the base code generator.

While our initial code generation target was C++, allowing us to validate the code against the original implementation, our primary target is the Intel SPMD Program Compiler (ISPC) [39]. ISPC is built on top of the LLVM compiler framework, leveraging its modular architecture and powerful code generation backend supporting a multitude of hardware platforms. We chose ISPC for its performance portability and support for all major vector extensions on x86 (SSE4.2, AVX, AVX2, AVX-512), ARM NEON and NVIDIA GPUs (using NVPTX) giving us the ability to generate optimized SIMD code for all major computing platforms. Since the standard library of ISPC is lacking double precision implementations for several transcendental functions such as `exp`, we provide our own implementations based on VDT [40]. Measurements of our ISPC implementation of `exp` show on-par performance with state-of-the-art mathematical libraries such as Intel’s SVML.
Table 1: Summary of supported target platforms by NMODL framework. In addition to the standard C++ target, ISPC is used to target various hardware platforms with optimal SIMD performance.

| Target Language | Hardware Platform | Features |
|-----------------|-------------------|----------|
| C++             | CPUs              | x86 SIMD using ivdep |
| C++ + OpenMP    | CPUs              | multithreading |
| C++ + OpenACC   | CPUs, GPUs        | accelerators |
| ISPC            | x86, ARM          | native SIMD |
| CUDA            | NVIDIA GPGPUs     | native SPMD |

We have, furthermore, extended the C++ target with an OpenMP and an OpenACC. These two code generators emit code that is largely identical to the C++ code generator but add appropriate pragma annotations to support OpenMP shared-memory parallelism and OpenACC GPU acceleration. Finally, our code-generation framework supports CUDA as a main backend to target NVIDIA GPUs. We were able to integrate NMODL as a code generation backend for CoreNEURON with only a few minor modifications to the build system. The CoreNEURON build process calls NMODL to generate C++/ISPC/OpenACC/CUDA files, which are subsequently compiled and linked to the simulator binary using the appropriate compilers. We can thus use NMODL as a drop-in replacement for the current mod2c transpiler, allowing us to easily perform numerical validation and performance benchmarking. The OpenACC and CUDA backend targeting GPUs require changes in CoreNEURON and this is an ongoing effort.

4.5 AST to NMODL Transformation

Various optimization passes discussed in subsection 4.3 are performed at the DSL level by keeping the language semantics intact as part of the AST. We have implemented a AST-to-NMODL transformation compiler pass to convert optimized AST back to the NMODL DSL form. This is not only useful to track the AST transformations during development/debugging but also to generate optimized NMODL DSL that can be consumed by existing transpilers like nocmodl and mod2c which lack such optimization capabilities.

5 ODE SOLVERS

5.1 Overview

NMODL allows the user to specify the equations that define the system to be simulated in a variety of ways.

- The KINETIC block describes the system using a mass action kinetic scheme of reaction equations.
- The DERIVATIVE block specifies a system of coupled ODEs (note that any kinetic scheme can also be written as an equivalent system of ODEs.)
- Users can also specify systems of algebraic equations to be solved. The LINEAR and NONLINEAR blocks respectively specify systems of linear and nonlinear algebraic equations (applying a numerical integration scheme to a system of ODEs typically also results in a system of algebraic equations to solve.)

To reduce duplication of functionality for dealing with these related systems of equations, we implemented a hierarchy of transformations as shown in Figure 6. First, any KINETIC blocks of mass action kinetic reaction statements are translated to DERIVATIVE blocks of the equivalent ODE system. Linear and independent ODEs are solved analytically. Otherwise a numerical integration scheme such as implicit Euler is used which results in a system of algebraic equations equivalent to a LINEAR or NONLINEAR block. If the system is linear and small, it is solved analytically at compile time using symbolic Gaussian elimination. Optionally, Common Subexpression Elimination (CSE) [41] can then be applied.

If the system is linear and large, it is solved (at run time) using a lower–upper (LU) matrix decomposition. Non-linear systems of equations are solved at run time by Newton iteration, which makes use of the analytic Jacobian calculated at compile time.

The use of external library solvers for analytic and numerical ODEs offers far superior efficiency, precision, and simplicity compared to the legacy implementation. The analytic ODE solver uses SymPy [42], a Python library for symbolic calculations, which can simplify, differentiate and integrate symbolic mathematical expressions. Our analytical solver replaces the purely numerical approach used in other NMODL source-to-source compilers and simulators. It allows us to perform some computations analytically at compile time that were previously carried out at run time at each time step using approximate numerical differentiation. This increases both the numerical accuracy and performance of simulations. The numerical ODE solver uses the Eigen [43] numerical linear algebra C++ template library, which produces highly optimized and vectorized routines for solving systems of linear equations.

5.2 SymPy

We use the SymPy library to perform algebraic simplifications, differentiate and integrate expressions, and identify common subexpressions. Performing these operations analytically and exactly at compile time removes a source of numerical errors and increases the overall run time performance.

Linear and independent ODEs have been typically replaced by an analytic solution that treats the coefficients as constant over a time step. NMODL increases the runtime performance by performing algebraic simplification and optionally replacing computationally expensive exponential calculations with the (1, 1) Padé approximant [44], consistent with the overall second order correct simulation accuracy (as suggested in [45], and implemented in [26]).

For coupled ODEs, the implicit Euler numerical integration scheme is applied which results in a set of simultaneous algebraic equations. For a linear systems of equations, such as those that arise from a set of linear reaction equations in a KINETIC block, the sparse solver method is used. For non-linear systems, the derivimplicit solver method is used.

The sparse solver chooses from two solution methods, depending on the size of the system to be solved. For small systems (three or less equations), the system is solved by symbolic Gaussian elimination at compile time. Additionally the solver will also optionally...
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**Figure 6**: On the left, unified ODE solver workflow showing ODEs from different NMODL constructs either produces compile-time analytical solutions, or run-time numerical solutions. On the right, example of KINETIC block and its transformation to SymPy based solution.

perform CSE. Figure 6 contains a simple example of this process. For larger systems, performing Gaussian elimination at compile time may not result in a numerically stable solution. Instead we construct a linear system of equations, which can be solved numerically using Eigen.

The derivable implicit solver constructs a system of non-linear equations, which we solve using Newton’s method at run time. We therefore compute the system’s Jacobian, which is then used in the iterative solver. The existing solver in NEURON calculates the Jacobian by numerical approximation at run time. Using Sympy, Newton’s method, which is an iterative solver that requires a linear derivative. Since the AST can be analyzed to determine that a conductance, which is the derivative with respect to voltage of a current. By default in NEURON these derivatives are numerically approximated at run time. This introduces an additional numerical error and generally doubles the computation time. To avoid this issue, the CONDUCTANCE keyword was previously introduced in NMODL [46], which allows the user to manually indicate the presence of an ASSIGNED variable that represents the current derivative. Since the AST can be analyzed to determine that a conductance calculation needs to be performed, our implementation automatically generate an appropriate local conductance variable and CONDUCTANCE statement to further reduce unnecessary run time computation.

### 5.3 Eigen

To solve linear systems of equations we use the Eigen PartialPivLU() routine [47], which performs LU decomposition with partial pivoting, a fast and stable algorithm for square invertible matrices.

For non-linear systems, we offer a simple implementation of Newton’s method, which is an iterative solver that requires a linear system to be solved at each iteration. For large system matrices this linear solve also uses PartialPivLU(). For 4x4 or smaller matrices, however, we directly invert the matrix using the invert() routine. For such small matrices this is numerically safe. Additionally this method does not involve any pivoting and hence does not incur any branching, which leads to significantly faster code than LU decompositions.

In general, using Eigen routines in favor of our own implementations provides two main benefits. First, the code becomes more maintainable: often a long and complex routine can be replaced with a single Eigen call, which renders the code easier to read and maintain. Second, the code performance is improved: Eigen offers highly tuned and parameterized routines and specialized implementations for different matrix sizes through generic programming. Replicating or beating the performance offered by a specialized numerical library is hardly practical and beyond the aim of this work.

### 6 ANALYSIS CAPABILITIES

An important goal of the NMODL Framework is to not only generate fast code but to also provide the computational neuroscientist with a versatile and easy-to-use tool for introspecting and programatically modifying models written in NMODL DSL. Currently, the NEURON NMODL database counts over 6,300 mechanism descriptions contributed by a worldwide community of researchers. Until now, any meta-analysis of these NMODL files had to be done either manually or using home-made tools. The problem with such tools is that their parsing capabilities are often fragile since they rely only on regular expressions or simple manually implemented parsers. In contrast, the NMODL Framework features a robust parser along with a complete intermediate representation and a powerful visitor framework. Using the AST and visitor classes, a programmer can do any analysis or modification they wish. The downside is that using the framework requires knowledge of modern C++ and ideally some experience with compiler frameworks. We therefore provide
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Figure 7: Performance characterization of different mechanisms using high level AST analysis from NMODL Framework: A) and B) shows global view of different operations performed by State Update and Current Update kernels respectively and in C) for AMMPANMDA one can zoom into a specific mechanism to understand detailed performance characteristics.

```python
import nmodl.dsl as nmodl
from nmodl import ast, visitor

class OpVisitor(visitor.AstVisitor):
    def __init__(self):
        self.ops = {'+':0, '-': 0, '*': 0, '/': 0}
        super().__init__()

    def visit_binary_operator(self, node):
        op = node.eval()
        if op in self.ops:
            self.ops[op] += 1

    def analyze(nmodl_string):
        driver = nmodl.NmodlDriver()
        nmodl_ast = driver.parse_string(nmodl_string)
        return OpVisitor().visit_program(nmodl_ast).ops
```

Figure 8: A simple example of a user-defined AST visitor to count FLOPs showing how C++ visitors can be extended using Python API

Python bindings to all AST classes and the visitor framework using the pybind11 library [48]. Additionally, we expose the ODE solver tools described in section 5 in the Python API. This gives the user access to all the ODE solving and simplification functionality available within the framework. When combined with SymPy, this yields a comprehensive analysis framework for mechanism dynamics described in the NMODL DSL.

7 BENCHMARKS

To evaluate the achieved performance gains through NMODL, we have performed comprehensive benchmarks on three major production hardware platforms summarised in Table 2. Since in this work we are primarily interested in the on-node performance increase from the generated code, we focus on single node benchmarks. We utilize all cores by pinning one MPI process on each core. From
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previous work on the parallel scalability of NEURON and CoreNEURON, those single node improvements will translate directly into equivalent improvements for parallel execution.

Benchmarks performed on the Intel platforms were compiled with Intel Parallel Studio 2018.1, while those on the AMD platform were compiled with GCC 7.3.0. All benchmarks have been compiled with -O2 -xHost flags respectively. Note that these benchmarks are not meant to compare one platform with other and hence we did not investigate the full spectrum of hardware capabilities on each platform (e.g. hyperthreading).

We selected two brain tissue models: a somatosensory microcircuit and a hippocampus region model. The first, a somatosensory cortex microcircuit of a young rat published by the Blue Brain Project has 55 layer-specific morphological types and 207 morpho-electrical types [1]. The second, a model of a rat hippocampus CA1 [17] is built as part of the European Human Brain Project and has 13 morphological types and 17 morpho-electrical types. These models are selected because they are computationally expensive and have a large number of mechanisms which allow us to assess performance benefits for different types of kernels used in production simulations. Based on these two models, we presented results for two benchmarks:

Channel Benchmark: This benchmark consists of 21 different morpho-electrical types selected to include all the unique mechanisms from somatosensory cortex and hippocampus CA1 models. A total of 2,304 cells are created without network connectivity as this benchmark is designed to measure performance of code generation for individual mechanisms.

Simulation Benchmark: This benchmark measures the overall performance improvement for production simulations. We used subcircuits of 1,000 cells from the two models above simulating one second of biological time using a timestep of 0.025 ms.

8 RESULTS

In order to understand the impact of the various optimizations and performance of generated code, we implemented a first draft of code generation backend for the CoreNEURON library. The same code generation backend can be adapted for the original NEURON simulator in the future. As the CoreNEURON library is a compute engine executed under the NEURON simulator producing binary identical results, the performance results can be directly compared between NEURON and CoreNEURON. More details about CoreNEURON library can be found in Kumbhar et al., 2010 [6].

We have performed benchmarks for a representative set of NMODL mechanisms as described in section 7.

For calculating the speedup, we compare the runtimes of the mechanisms translated using NMODL Framework with ISPC backend and simulated using CoreNEURON with the same mechanisms compiled with the NEURON simulator using nocmodl. The results of these benchmarks are shown in Figure 9. We restrict ourselves

![Figure 9: Speedup of different channels selected from neocortex and hippocampus circuits on Intel Skylake, Intel KNL and AMD Naples platform](image-url)

| Benchmark | Mechanisms | Description |
|-----------|------------|-------------|
| Channel Benchmark | cur-ca | Code generation for individual mechanisms. |
| Simulation Benchmark | cur-Ih | Overall performance improvement for production simulations. |

Table 2: Details of Benchmarking Systems

| System | Processor | Cores | Memory |
|--------|-----------|-------|--------|
| Intel Skylake | Xeon 6140, 36 cores @2.3GHz, 384GB DRAM | 36 | |
| Intel KNL | Xeon Phi (7230), 64 cores @1.3GHz, 16GB MCDRAM, 96GB DRAM | 64 | |
| AMD Naples | AMD EPYC 7451, 24 cores @2.3GHz, 128GB DRAM | 24 | |

![Table](image-url)
v = v+12.3;

double m[n], h[n], mInf, mAlpha, mBeta, hInf, hTau, hAlpha, hBeta;

void nrn_state(.....) {
  for (int id = start; id < end; id++)  {
    m[id] = m[id]-1.0*exp(dt*(1.0-(1.0)))*
           (-((m[id])/hTau[id])/(1.0+(1.0)))+(1-m[id])
           (-((mInf[id])/hInf[id])/(1.0)-(1-mInf[id]))
    h[id] = h[id]+(1.0-exp(dt*((((-1.0))/hTau[id])))*
           (-((mInf[id])/hInf[id])/(1.0)-(1-mInf[id])))
    (1-m[id]))
  }
}

tabs(.....) {
  foreach (id = start ... end)  {
    mAlpha[id] = 0.0055*(-27.0-0.0)/((exp((-27.0-0.0)/3.8)-1.0));
    mBeta[id] = (0.00665/0.00665)*exp((-15.0-28.0)-1.0));
    hAlpha[id] = (0.000047+exp((-13.0-0.0)+50.0));
    hBeta[id] = (0.00457*exp((-13.0-0.0)/50.0));
    hTau[id] = 1.0/(hAlpha[id]+hBeta[id]);
    v = v+12.3;
  }
}

tabs(.....) {
  foreach (id = start ... end)  {
    mAlpha[id] = 0.0055*(-27.0-0.0)/((exp((-27.0-0.0)/3.8)-1.0));
    mBeta[id] = (0.00665/0.00665)*exp((-15.0-28.0)-1.0));
    hAlpha[id] = (0.000047+exp((-13.0-0.0)+50.0));
    hBeta[id] = (0.00457*exp((-13.0-0.0)/50.0));
    hTau[id] = 1.0/(hAlpha[id]+hBeta[id]);
    v = v+12.3;
  }
}

tabs(.....) {
  foreach (id = start ... end)  {
    mAlpha[id] = 0.0055*(-27.0-0.0)/((exp((-27.0-0.0)/3.8)-1.0));
    mBeta[id] = (0.00665/0.00665)*exp((-15.0-28.0)-1.0));
    hAlpha[id] = (0.000047+exp((-13.0-0.0)+50.0));
    hBeta[id] = (0.00457*exp((-13.0-0.0)/50.0));
    hTau[id] = 1.0/(hAlpha[id]+hBeta[id]);
    v = v+12.3;
  }
}

Figure 10: Comparison of unoptimized and optimized code (from calcium mechanism, simplified): On the left, nrn_state kernel generated from DERIVATIVE block calling rates function as generated by nocmodl and mod2c. On the right, corresponding ISPC code generated by the NMODL Framework after the DSL optimizations and SymPy transformations described in subsection 4.3 and section 5.
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| Simulation   | Component      | Intel Skylake | Intel KNL |
|--------------|----------------|---------------|-----------|
|              | NRN-NOCMODL    | CN-MOD2C      | CN-NMODL  | NRN-NOCMODL | CN-MOD2C | CN-NMODL |
| Hippocampus  | SRU             | 1298.83       | 316.11    | 138.15      | 4786.48  | 713.7    | 233.64 |
|              | CU              | 1102.56       | 239.84    | 165.53      | 2732.88  | 181.94   | 348.72 |
|              | Other           | 154.13        | 44.08     | 40.78       | 828.94   | 236.11   | 203.24 |
|              | Total           | 2555.52       | 600.04    | 344.46      | 8348.29  | 1131.74  | 785.6  |
| Speedup wrt NEURON | 1   | 4.26         | 7.42      | 1           | 7.38     | 10.63    |
| Plasticity   | SRU             | 199.8         | 33.17     | 25.41       | 846.5    | 63.77    | 43.86  |
|              | CU              | 179.89        | 36.2      | 21.58       | 422.39   | 38.43    | 61.73  |
|              | Other           | 47.71         | 19.1      | 17.12       | 310.93   | 89.43    | 78.49  |
|              | Total           | 427.44        | 88.46     | 64.11       | 1579.82  | 191.63   | 184.08 |
| Speedup wrt NEURON | 1   | 4.83         | 6.67      | 1           | 8.24     | 8.58     |

Table 3: Absolute time(s) and speedup of the hippocampus and somatosensory cortex simulations on Intel Skylake and Intel KNL platform using NEURON with noemodl (NRN-NOCMODL), CoreNEURON with MOD2C (CN-MOD2C) and CoreNEURON with NMODL Framework (CN-NMODL)

generation backend. The third configuration (CN-NMODL) uses the CoreNEURON library with the here-presented NMODL Framework as a code generation backend.

The NMODL Framework shows up to $7 \times$ speedup on Skylake and up to $11 \times$ speedup on the KNL platform. The hippocampus model shows a larger speedup compared to the somatosensory cortex model because it uses cacum, cacumb and kca mechanisms with the derivimplicit integration scheme. The Eigen based solver implementation in NMODL brings additional performance improvements. When compared with CN-MOD2C, CN-NMODL shows up to $2 \times$ performance improvement. Note that the CN-MOD2C is heavily dependent on auto-vectorization capabilities of the compiler. For example, if the GCC compiler is used instead of Intel, CN-NMODL becomes 5x faster compared to CN-MOD2C. The breakdown of the execution times is shown in Table 3. As discussed before, State Update and Current Update represent the time spent in the execution of code generated from NMODL DSL and the rest of the time is shown as Other. On the Intel KNL platform the Current Update kernel is ~2x slower in CN-NMODL compared to CN-MOD2C. This is due to a performance issue found with ISPC when atomic reductions are used in the kernel. This performance issue will be addressed in a future release of NMODL Framework.

9 CONCLUSIONS

Having real-world scientific applications make efficient use of modern computer architectures' performance features is an involved task and heavily relies on the successful combination of using optimized libraries, auto-vectorizing compilers, and exposure of parallelism and hints by the programmer. Good performance on one architecture does not imply automatically good performance on the next architecture. In times of increasing architectural diversity this poses real challenges.

Additionally, many scientific applications do not encode only a single mathematical problem, but the scientific users provide the mathematical equations that need to be integrated by the solvers on a case by case basis. In the worst case, this can severely impact the success of auto-vectorization. In the best case, the way the users express their specific equations, e.g. through DSLs may help in producing optimized code.

In this paper we presented a novel NMODL Code Generation Framework for the DSL of the widely used NEURON simulator. The DSL constructs are translated into an AST that lends itself to specific optimization passes before it is handed off to different backends for generation of optimized code for the target platform.

We have implemented optimization passes that relate to straightforward transformation of the DSL code, but also more advanced optimization passes that intercept ODE statements for which an analytical solution can be used instead of having to resort to numerical integration. This functionality is built on top of the SymPy and Eigen libraries.

For code generation we have developed backends for C++ and OpenMP targeting CPUs and ISPC to target a wide variety of CPU architectures providing optimal SIMD performance and reducing the dependency on auto-vectorization capabilities of the compiler. Furthermore, we have developed both a CUDA backend specifically with NVidia GPUs in mind as well as a more generic OpenACC. Both GPU backends will, however, require more integration work with the simulators and benchmarking.

We have benchmarked kernels from production simulations of two different large-scale brain tissue models on Intel SKL, Intel KNL and AMD EPYC platforms. On those individual kernels, we saw performance improvements from $5 \times$ to $20 \times$. In order to test how those kernel improvements translate into speedup of the entire simulations (which use the kernels in different ratios or not at all), we benchmarked production simulations on Intel KNL and Intel SKL platforms. Compared to the regular NEURON simulation environment, a speedup of $6 \sim 10 \times$ has been observed. Compared to an optimized version of the NEURON simulator, CoreNEURON, which heavily relies on auto-vectorization of the compiler, the work presented here nonetheless resulted in a speedup of up to $2 \times$.

Beyond the absolute performance, a central goal of our effort was the ability to parse all previously published models. By using the grammar specification from the original NEURON NMODL language, we were able to demonstrate compatibility with 6,370
channels from the public model repository ModelDB. We furthermore took care to maintain the language semantics of the DSL in the AST, allowing retranslating of the AST optimization into the DSL constructs, thus making the optimizations available to the regular NEURON simulator without having to rely on our code generation backends (albeit with reduced overall speedup). Lastly, our framework is exposed through a Python interface, providing great flexibility to use NMODL as a generic NMODL parsing framework and build new tools on top of it.

Availability
NMODL Framework is open source and available on GitHub [50].

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