Learning From Generated Stencil Programs

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Abstract

Stencil computations are a well-studied field with many different implementations that utilize various types of compiler optimizations. Recent approaches in this field have used machine learning to automatize the selection of code transformations. Some autotuning techniques have shown massive improvements in execution times as they were able to significantly outperform human experts. Motivated by these improvements, we further explore the connection of these fields in the context of climate modeling and weather prediction.

In this work, we propose a novel random stencil program generator, which learns the program structure from an arbitrary set of human-written stencils and generates a set of random programs of a given size that have the learned structure. We show that the properties of the generated programs match those of the original dataset. Furthermore, we train a Gradient Boosting Trees (GBT) model on the dataset created from the replicated stencils, which can accurately predict register usage of the human-written stencils and is 50 times faster than the register allocation method of nvcc compiler. Our model's average predictions are within 10% of the actual register usage.

1 Introduction

Climate change denotes a huge threat to the entire world population. Its effects span from extreme weather such as heat waves [?] to changes in marine ecosystems [?] such as coral bleaching [?]. An accurate weather prediction cannot prevent global warming but can save lives by issuing in time warnings for incoming weather extremes like tornados or heat waves. Weather is predicted with simulations, which are powered by complex computational models predicting the physical and chemical properties of the earth's surface and atmosphere. The computations include solving partial differential equations using numerical methods. The equations capture diffusions of various substances throughout the surface, the air and the water. Earth's surface and atmosphere are modeled using grids that approximate regions on the earth. The smaller region one cell of the grid represents, the higher the resolution and the accuracy of the model. Each cell can have values for pressure, temperature, humidity, wind speed, water vapor, and more, that define the current state of the atmosphere. The grid is updated in iterations as partial differential equations cannot be solved directly but have to be approximated. Therefore, one iteration represents a change of the weather that occurred in time δ. Each iteration influences each cell of the grid with the values of adjacent cells. Correspondingly, each region on the earth impacts the weather of the neighboring locations. We call this computation a stencil computation since stencil [?] is a type of iterative kernel that accesses adjacent cells in a fixed pattern.

The growth of computational grids comes at the cost of required computational power, which introduces new challenges to the high performance computing community. For instance, a recent Alp region summer weather simulation [?] covered 30 years on the horizontal grid with 500x500x60 cells, where each cell had a resolution of 2.2 kilometers. The entire experiment took 1.5 years on the CSCS Monte Rosa supercomputer using COSMO model [?] and brought interesting results regarding the change in summer precipitation by the end of the century. Since the end of Moore's law [?] is slowly coming (due to physical limitations), manufacturers started to rely more on the multiprocessing and dedicated hardware such as GPUs or TPUs, which makes the programming model more difficult as there are more platforms to target. To simplify that, and abstract away implementation details for domain scientists, many Domain-Specific Languages (DSL) were introduced.

A recent Google initiative called MLIR [?] brought an extensible Intermediate Representation together with accompanying infrastructure, which makes building new DSLs simple and maintenance costs low. Therefore, people from the SPCL lab took the initiative to create a new DSL inside MLIR. It aims to reuse MLIR infrastructure and to provide an open-source platform for future stencil code development.

In addition to DSLs, code transformations emerged as game-changers in terms of performance. The high-quality code optimizations can improve the execution time in order of magnitude. More recently, an introduction of machine learning to compiler optimization brought some significant runtime improvements in fields of image processing [?] and deep learning computations [?]. Therefore in this work, we explore various ways of using machine learning inside compiler optimization. Since ML algorithms require extensive datasets to work well,we propose a random stencil program generator that can replicate a small dataset to a dataset of defined size. We show that such a generated dataset replicates properties of the original one precisely while introducing new, unseen programs. Moreover, we support the SPCL initiative by designing and implementing some of the fundamental pieces of the compiler, which we use in our generator as well.

In the last part of the thesis, we experiment with the training of statistical models on data collected from generated programs. We show that even basic models can be trained to

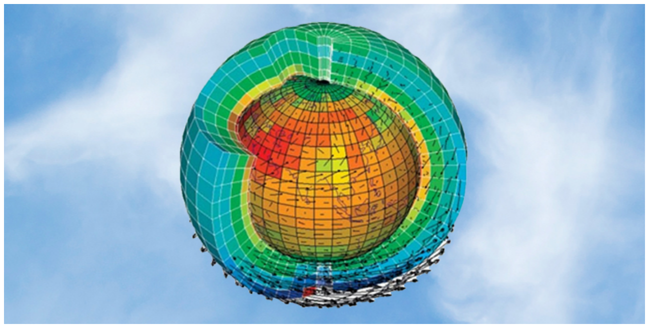


Figure 1. The world as a computational grid (Illustration: Carbones EU Project)

predict register usage accurately. Lastly, we outline promising future research directions that can build on top of our approach.

Our main contributions are as follows:

1. Implementation of the translation pass from the Standard and GPU MLIR dialects into a CUDA C code.
2. A novel, random stencil program generator that replicates any set of stencil programs written in MLIR Stencil dialect into a variable-length set of new random programs that have a structure similar to the original ones.
3. Feature extraction and optimization passes that can be used to create noise-free datasets suited for training of machine learning models.
4. An accurate register prediction model trained on the generated data and validated on the COSMO stencils. Its prediction speed is 50 times faster than obtaining register usage information via `nvcc`.

Thesis structure. In Chapter 2, we discuss the theoretical background as well as the MLIR compiler infrastructure, which is necessary for a full understanding of the program generator. Chapter 3 introduces a random stencil program generator, which is our core contribution. On the programs created by the generator, Chapter 4 shows a feature extraction, their analysis, and register usage prediction experiments together with the evaluation and future research directions.

2 MLIR & Stencil dialect

Compilers are a well-studied field in computer science with many well-known algorithms, and applications spanning throughout multiple fields. They became the "New Frameworks" since they provide full control in the optimization process, which is something that frameworks cannot do. We can particularly see these trends in web development (Angular, Babel, and TypeScript compilers), and in Domain-Specific Languages (DSL), which have their usages in mathematics, graphs, music, web, weather, and many more fields. DSLs make it easier to create programs in some specific domain. Furthermore, novel and more aggressive optimization strategies can be deployed as they take advantage of domain knowledge. Domain-specific optimization is usually followed by the code generation to one of the well-known general-purpose programming languages like `C`, `C++` or `CUDA C`. Alternatively, the code generation can target assembly language directly or use a compiler infrastructure like LLVM [**?**]. In general, DSL infrastructure creators want to avoid doing redundant work as much as they can, and thus they translate their optimized Intermediate Representation (IR) to some general-purpose IR that comes with already built infrastructure. This cuts maintenance costs and prevents reinventing the wheel. The strategy of creating only high-level IR and reusing existing infrastructure to perform well-known optimizations and lowerings to assemblies targeting different platforms is very common. Good examples are languages like Swift, Rust, Julia or Objective C that build on top of the LLVM. All of these languages have their own high-level IR which they later lower to LLVM IR. However, this pattern forces language creators to reinvent their own top-level IR together with accompanying infrastructure, which leads to a repetitive reinvention of similar technology.

To tackle this problem as well as to unify the TensorFlow graph compilation for different platforms, Lattner et al. [**?**] came with a solution called Multi-Level Intermediate Representation (MLIR). This state-of-the-art project is a novel approach to building maintainable, reusable, and extensible compiler infrastructure. It is built on top of LLVM so it takes advantage of all intermediate representation and optimization passes by providing a lowering pass from MLIR IR to LLVM IR. Furthermore, it allows users to reuse the LLVM and Clang types. In this chapter, we are going to explain the components of MLIR that we used as well as the Stencil dialect that was created using MLIR in the SPCL lab for climate modeling.

2.1 MLIR

As already mentioned, MLIR is a novel approach to building a "new generation" of compiler infrastructure. It tries to prevent reinventing of similar IRs and optimizations by introducing building blocks that standardize the building process. Furthermore, it provides infrastructure which is compatible with all constructs built with the building blocks. In this subchapter, we are going to explain the details of MLIR IR and its infrastructure, which we use in our approach.

2.1.1 MLIR Intermediate Representation. The fundamental building block is **Operation** or `Op`. Every instruction, `function` or even `module` are implemented with use of `Op`. MLIR does not come with prebuilt operations but rather encourages users to come up with their own. Since every newly defined operation inherits from `Op`, predefined compiler passes are compatible with all operations. They

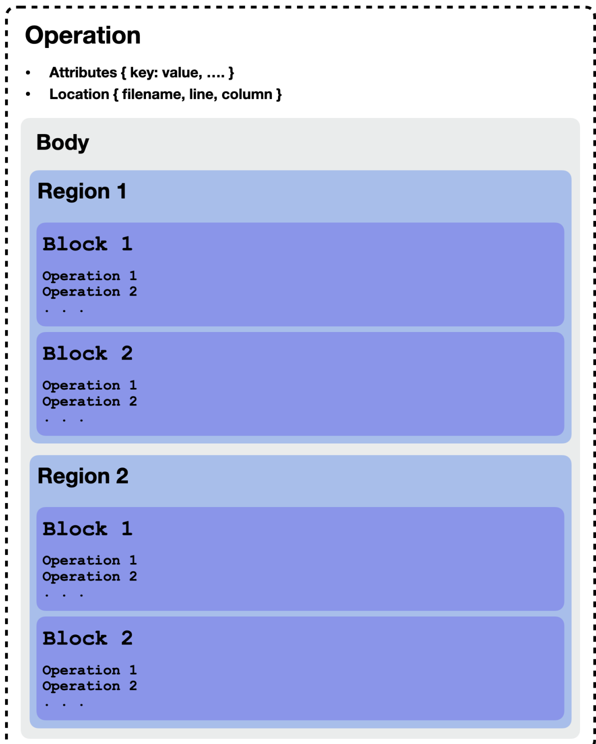


Figure 2. A structure of an MLIR `Operation`. The body consists of zero or more regions. `Region` can have zero or more blocks. `Block` groups operations that are executed sequentially one after another.

are conservative but can be instructed with help of traits, operation hooks or optimization interfaces to understand the semantics of a new operation. Each `Op` can take zero or more values, that are called *operands*, and produce zero or more values, that are called *results*. Furthermore, it can contain *Attributes*, *Block Arguments* and *Regions*. Every `Op` has a *Location* metadata, which describe its location in the source code. This object is very useful in error tracing as it helps in reversed tracking.

The next MLIR construct is an **Attribute**. It provides static, compile-time known information like constants of various types. Each operation can contain zero or more attributes. Internally, they are represented as key-value pairs. Therefore each attribute has to be uniquely identifiable within an operation. Attributes are very extendible, as some attributes have meaning only by their presence while some represent complex data structures.

Each operation inside MLIR can be uniquely identified by its **Location**. It is strongly encouraged to forward location in between lowering passes to keep track of the initial location in the source file, which speeds up debugging and error identification.

Nested structures are represented by a **Region** and a **Block**. Each operation can have a list of the attached regions. A region contains a list of blocks, and each block contains a list of operations where each operation can have a list of regions. This design enables building program structures of arbitrary depth. A region represents a Control Flow Graph (CFG) since it contains blocks that represent straight-line code sequences terminated by terminators, which can point to other blocks and thus form a graph. Since MLIR IRs are in SSA form, the authors decided to replace Φ nodes with block arguments. Each terminator can point to another block with a different argument and thus avoid a need for the Φ node.

MLIR operations are grouped in **functions** and **modules**. An MLIR function is very similar to a C function. It can take zero or more arguments, but it can also produce zero or more results. A function is thus a constrained operation since it has only one region with one block as it has only one body. The terminator of a function is return operation, which returns whatever is passed as its operands. Similarly, a module is an operation with one region containing one block, which can have an arbitrary number of other types of operations. A module is terminated by a special, dead-end module terminator which does not transfer control flow any further.

MLIR offers extensibility via **Dialects**. A dialect is a namespace that groups together attributes, types, and operations. Dialect name appears dot-separated before each operation from the dialect, which provides a visual grouping of its operations and improves a readability of the code. Dialect's main purpose is a logical grouping of operations, but it can provide some generic operation functionalities as well. Users are not forced to use some predefined patterns for dialects, but they are given freedom in their usage. However, as with namespaces, it is recommended to group the operations within the same project to a dialect not only for readability purposes but also to prevent the naming collisions. A good example would be use of `Vector`, `Load` or `Store` names for operations. These names already exist in the standard dialect and thus are always prefixed with `std`. If users want to define their operation with one of these names, they will encounter no conflicts as each operation will be prefixed with a different dialect name.

Users do not need to be reluctant in introducing more dialects due to compatibility issues, as MLIR allows mixing of dialects. Distinct dialects can coexist at any level and at any time in the IR. For instance, in our approach, we mix our custom dialect with the standard one, so we do not need to redefine all standard arithmetic operations. Furthermore, we use a `loop.if` operation from the loop dialect for branching.

The last important part of MLIR is a **type system**. Every value has to have a type. MLIR comes with a predefined set of types - **Standard Types**, like floats and integers of various bit lengths, pointers or memory references. However, users can define their types inside dialects as well. Furthermore,

```
                                                        Module
func @max(%arg0 : memref<?xf32, %arg1 : i32) -> f32 {
  %0 = alloc() : memref<1xf32>                        Block
  %c0 = constant 0 : i32
  %c1 = constant 1 : i32
  store %c0, %0[%c0] : memref<1xf32>
  loop.for %i0 = %c0 to %arg1 step %c1 {
    %1 = load %0[%c0] : f32                          Block
    %2 = load %arg0[%i0] : f32
    %3 = cmpf "ugt", %2, %1 : i1
    loop.if %3 {
      store %2, %0[%c0] : memref<1xf32>           Region
                                     Block
    } else {
                . . .                Block
    }
  }
  %4 = load %0[%c0] : f32
  return %4
}
```

Figure 3. The figure shows a function returning maximal element from an array passed as an argument together with its size. The function is wrapped in the `Module` operation, which is always a top-level parent operation. A body of a function is represented as a `Block` of operations. Some `Operations` like `loop.if` can have a body and thus their attached list of regions is not empty.

types from existing systems (LLVM, Clang) can be used. They need to be prefixed with llvm or clang namespace respectively i.e. `llvm::SmallVector` or `clang::math::min`.

2.1.2 MLIR Passes and Op Definitions.

MLIR consists of two main components. An IR, which we already described and IR infrastructure, which parts we are going to describe in this subchapter.

New operations are created in MLIR with specifications, which are based on TableGen [?] and are called Operation Definition Syntax (ODS). This syntax reduces the amount of boilerplate code that needs to be written by allowing user to write only essential parts of the operation like *summary*, *description*, *arguments*, *results*, *builders* or *verification* method. Furthermore, user can specify traits which are helpful for passes to understand the semantics of an operation. For instance, `[NoSideEffect]` trait tells optimization passes that the operation is side effect free. The real C++ classes are table generated during the compilation. An example of the `FieldAccessOp` definition can be seen in figure 4.

MLIR IR is being processed with passes. A pass takes an IR as an input and produces transformed IR as an output. In theory, 2 types of transformations can be applied. The first one optimizes the given IR, and the second one lowers it. Practically, MLIR does not distinguish between these two types. It only verifies that transformations produce valid IRs. Therefore it is up to users how they want to structure passes. Furthermore, MLIR provides a pass infrastructure - pass manager, which manages the series of IR passes. MLIR provides 3 types of IR traversals.

- **ModulePass** runs on every module in an IR. The user implements a callback function, which is supposed to handle each module.
- **FunctionPass** runs on every function, users have to implement a callback function to handle each MLIR function.
- **OperationPass** Runs on every operation. Users can narrow down the type of iterating operations. However, this pass does not allow any parent or parent region to be modified, only the currently iterated operation and its children.

Users create passes to do the transformations, which require a lot of operation rewriting. MLIR has a solution for that in the form of rewriters, conversion patterns, and type converters. Conversion patterns match and rewrite operations specified by a user. An operation match consists of an operation type match and a user-provided condition. Furthermore, MLIR comes with a generic, predefined passes. These passes provide either conversion between MLIR dialects or optimizations like Common Subexpression Elimination (CSE) or

```
// A TableGen definition of the field access operation.
// The resulting name of the op would be stencil.field_access as it is inside
// stencil dialect and has name field_access. It has side effect free trait.
def Stencil_FieldAccessOp : Stencil_Op<"field_access", [NoSideEffect]> {
  // one line summary of the operation
  let summary = "field element access operation";
  // multi-line, long description of the operation
  let description = [{
      The "field_access" operation takes a stencil.field and an
      offset and returns a pointer to the field element at the
      given offset.
    }];

  // input named values, can be typed operands or attributes
  let arguments = (ins Stencil_Field:$field, I64ArrayAttr:$offset);
  // typed and named values
  let results = (outs Stencil_Pointer:$res);
  // extra function definition
  let extraClassDeclaration = [{
    static StringRef getOffsetAttrName() { return "offset"; }
  }];
}
```

Figure 4. An example of Operation Definition Syntax (ODS), which is the way of defining new operations in MLIR. This example shows a shortened definition of the `FieldAccessOp` that is a fundamental operation in the Stencil dialect.

Canonicalization. All predefined optimizations are generic enough to handle new, properly annotated operations. Annotation with traits is required for them to work well as they give semantics information.

2.2 Stencil Dialect

In this subchapter, we are going to first introduce stencil computations for weather modeling followed by the Stencil dialect [?], [?] written by Jean-Michel Gorius during his research internship at ETH Zurich, which represents them in MLIR dialect. Our coverage of these topics is far from being comprehensive as it aims to give the reader sufficient information to understand the topics that follow. For more detailed information one can follow up here [?], [?], [?], [?].

2.2.1 Stencil Computations. A stencil kernel is a type of computational kernels, which iteratively traverses a grid and updates each cell based on the adjacent cells. The pattern in which adjacent cells are accessed is called *stencil*. Such stencil can be executed on regular [?] and irregular [?] grids. A regular grid is represented as 2D or 3D array depending on the space in which a stencil is computed. In our approach, we do not consider irregular grids.

A typical usage of stencil computations is in weather simulations where grids are initialized with the current weather situation and the stencil kernel is iteratively run on the grid to simulate the change of the weather elements like temperature (heat and cold diffusion) or humidity. The iteration method is called *Jacobi method* [?], which iteratively solves a strictly diagonally dominant system [?] of linear equations [?]. For example, a following second-order partial differential equation:

$$\frac{\partial^2 F}{\partial x^2} + \frac{\partial^2 F}{\partial y^2} = 0 \tag{1}$$

is solved iteratively on grid G as:

$$G_{new}(i,j) = \frac{1}{4}(G(i-1,j) + G(i+1,j) + G(i,j-1) + G(i,j+1)) \tag{2}$$

i.e. by taking average of all 4 neighbouring cells. In another words, each cell is in each iteration equally influenced by all its neighbours. For instance, this is very useful in modelling of heat diffusion as heat spreads out through the space by heat transfer from one particle to another.

Our research area is to not come up with new stencil computations but to support the scientists working on them with high performance and user-friendly execution infrastructure.

2.2.2 Dialect Definition. In this subchapter, we are going to describe each operation inside the MLIR Stencil dialect. However, we are not its authors. Therefore we will not reason about design decisions. The goal of this subchapter is to give the reader a short reference as the next chapter builds heavily on that knowledge.

As shown in figure 6 an input to the Stencil compiler is a stencil file exported from `Dawn` [?] compiler. The authors created an intermediate dialect called IIR to model `dawn` format inside MLIR because each dialect can specify parse methods that lead the MLIR parser in parsing input files. Therefore, the sole purpose of the IIR dialect is to parse stencils exported from the `dawn`. It is always subsequently lowered into the Stencil dialect.

Stencil dialect tries to leverage existing MLIR IR by introducing types and operations that do not occur in MLIR. Thus it reuses standard arithmetic operations and types like additions, multiplications, or floats. It introduces only the following types:

- **FieldType** `!stencil<"field:f64">` represents a reference to a grid, which can be called *field* as well. In the current stage of dialect development we support only 3 dimensional grids.
- **VarType** `!stencil<"var:f64">` represents a stencil variable, that acts as a normal variable and is shared between DoMethods in the same Stage.
- **PointerType** `!stencil<"ptr:f64">` A pointer to a stencil field. Can be dereferenced to get the value and written to.

The only type used from the standard types is *f64*, which represents a value in each cell of the grid as well as the result of the comparison. The following operations form an IR structure of the stencils. Most of them are omitted in the lowering passes as they do not influence the computations:

- **IIROp** `stencil.iir(StrAttr:$stencilName)` groups multiple stencils.
- **IIREndOp** `stencil._iir_end` terminates an IIROp.
- **StencilOp** `stencil.stencil` Represents a stencil computation. It can contain various stencil kernels located in multiple stages and multi-stages. Takes zero or more fields (grids) as arguments. Stencil does not distinguish between input and output fields. All fields can be read and written.
- **StencilEndOp** `stencil._stencil_end` terminates a StencilOp.
- **MultiStageOp** `stencil.multi_stage` groups multiple Stages. Has one mandatory parameter - an order in which stages are executed. The order can take these values: *Forward*, *Backward*, *Parallel*.
- **MultiStageEndOp** `stencil._multi_stage_end` terminates a MultiStageOp.
- **StageOp** `stencil.stage` groups multiple DoMethods.
- **StageEndOp** `stencil._stage_end` terminates a StageOp.
- **DoMethodOp** `stencil.do_method` DoMethod represents a stencil kernel. It groups arithmetic, read, and write operations that do the actual computation. Takes 4 static parameters of integer type that specify lower

```
module {
  stencil.iir {
    stencil.stencil(%arg0: !stencil<"field:f64">, %arg1: !stencil<"field:f64">) {
      stencil.multi_stage "Forward" {
        stencil.stage {
          stencil.do_method [0, 0, 1048576, 0] {
            %0 = stencil.field_access %arg0 [-1, 0, 0] : !stencil<"ptr:f64">
            %1 = stencil.field_access %arg0 [1, 0, 0] : !stencil<"ptr:f64">
            %2 = stencil.field_access %arg0 [0, -1, 0] : !stencil<"ptr:f64">
            %3 = stencil.field_access %arg0 [0, 1, 0] : !stencil<"ptr:f64">
            %4 = stencil.get_value %0 : f64
            %5 = stencil.get_value %1 : f64
            %6 = stencil.get_value %2 : f64
            %7 = stencil.get_value %3 : f64
            %8 = addf %4, %5 : f64
            %9 = addf %6, %7 : f64
            %10 = addf %8, %9 : f64
            %11 = constant 4 : f64
            %12 = divf %10, %11 : f64
            %13 = stencil.field_access %arg1 [0, 0, 0] : !stencil<"ptr:f64">
            stencil.write %13, %12 : f64
          }
        }
      }
    }
  }
}
```

Figure 5. Jacobi stencil implemented in the Stencil dialect. The dashed line marks the actual stencil while the gray box highlights the body of the DoMethod.

bound, lower offset, upper bound, and upper offset on the kernel iterations.

- **DoMethodEndOp** `stencil._do_method_end` terminates a DoMethodOp.

The second group of stencil operations consists of operations that occur inside DoMethod. The only exceptions are *FieldOp* and *VarOp*, which are located outside of it. The full signature of each operation can be found in the appendix. *SqrtfOp*, *FabsOp*, *ExpOp*, *PowOp* were added as the standard dialect does not support them.

- **FieldOp** `stencil.field` Allocates memory for a local field and returns a reference to it.
- **FieldAccessOp** `stencil.field_access` Takes a field and a 3 dimensional offset as an input, produces a field pointer.
- **VarOp** `stencil.var` Creates a local variable.
- **VarAccessOp** `stencil.var_access` Takes a variable as an input and returns a pointer pointing to it.
- **GetValueOp** `stencil.get_value` Dereferences a pointer passed as an argument. Returns the scalar located at the corresponding memory address.
- **WriteOp** `stencil.write` Writes a scalar to a pointer. Both of them are passed as arguments.
- **SqrtfOp** `stencil.sqrtf` Computes the square root of a floating-point number.
- **FabsOp** `stencil.fabs` Computes the absolute value of a floating-point number.
- **ExpOp** `stencil.exp` Computes the value of the exponential of a floating-point number.
- **PowOp** `stencil.pow` Computes the floating-point power of two numbers.

An example of `Jacobi stencil` in the Stencil dialect can be seen in figure 5. The example demonstrates the usage of the operations described above. The computation itself happens inside the body of DoMethod, where all adjacent cells are read, their average is computed and stored to the output stencil.

2.2.3 Lowering Pipeline. So far, we have a working Stencil dialect and a way of transforming dawn files into it. Since our goal is to execute stencils on the GPU, the next step is to translate a program from the Stencil dialect to CUDA C. Therefore, a lowering pass to the mix of affine and standard dialect was created to reuse the existing MLIR passes for lowering affine dialect to the GPU one. This conversion automatically creates a Cuda kernel together with a launch function. The last step in the conversion is to translate the mix of GPU and standard dialect into Cuda C. Here lies our first contribution as we implemented this conversion. The stencil is run by:

1. creating a file with the main function, where all grids are initialized
2. linking generated CUDA C file
3. calling the launch function with the initialized grids
4. compiling both of them with `nvcc`
5. running generated executable.

3 Random Stencil Program Generator

The generation of meaningful random programs is a well-studied field in computer science. Random programs complement human-written ones in compiler testing as they can provide execution patterns that compiler creators were not considering. Moreover, they can act as compiler fuzzers that exhaustively test compilers for errors such as segmentation faults or floating-point errors. Lastly, they can be time-savers for the testers as they are capable of much faster program generation than humans. However, our goal is not to use the generator for compiler correctness even though it can be used for that as well. We need it for enlarging the stencil dataset as the COSMO model contains only around 30 stencils, which are not sufficient for the training of any model. Therefore the most desired properties of our generator are the quality and variety as we want to generate programs that look like they were written by a human but novel in some sense as well. In this chapter, we are going to introduce the "guts" of our random stencil generator as well as some more high-level concepts it builds on.

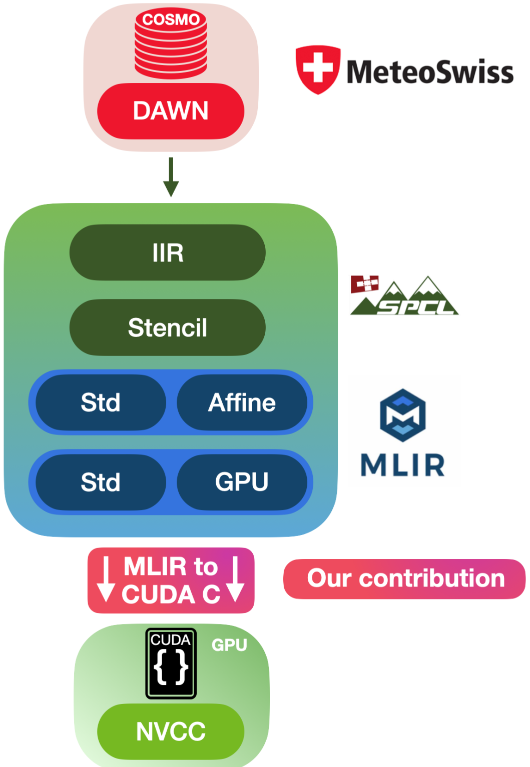


Figure 6. Current pipeline of the Stencil compiler. The input consists of COSMO stencils exported from the dawn compiler. Consequently, MLIR Stencil compiler loads and lowers them to the GPU dialect. Our contribution consists of translating the resulting mix of GPU and standard dialect into CUDA C code, which is compiled by the nvcc an executed on Nvidia GPU.

3.1 Generation Pipeline

Rather than generating a program in a single pass, we decided to make it a little bit modular and split it into two passes. The first one, which we call program chain generation, takes a set of valid stencil programs as an input and generates an operation chain without any arguments or return values. The chain defines an order in which one operation follows another in the source file. An example of such a generated chain can be:

`module` → `iir` → `stencil` → `multi_stage` → `stage` → `do_method` → `field_access` → `field_access` → `get_value` → `get_value` → `addf` → `write` → `_do_method_end` → `_stage_end` → `_multi_stage_end` → `_stencil_end` → `_iir_end` → `module_terminator`

The second phase takes the chain generated by the first phase as an input and produces an MLIR program in the Stencil dialect. One of many possible programs generated from the chain above could be:

```
module {
  stencil.iir {
    stencil.stencil(%arg0: !stencil<"field:f64">,
      %arg1: !stencil<"field:f64">) {
      stencil.multi_stage "Forward" {
        stencil.stage {
          stencil.do_method [0, 0, 1048576, 0] {
            %0 = stencil.field_access %arg0 [0, 0, 0]
              : !stencil<"ptr:f64">
            %1 = stencil.field_access %arg1 [0, 0, 0]
              : !stencil<"ptr:f64">
            %2 = stencil.get_value %0 : f64
            %3 = stencil.get_value %1 : f64
            %4 = addf %3, %2 : f64
            stencil.write %1, %4 : f64
          }
        }
      }
    }
  } attributes {stencilName = "addition"}
}
```

Listing 1. An example of the program generated from the chain

In the following subchapters, we are going to explain both phases in detail as well as the evaluation of programs generated by them.

3.2 Learning the Markov Chain

Every program generator needs to understand the program structure to generate a meaningful random program. By that, we mean, for instance, an order in which operations follow each other, counts of operation types in the program, or distribution of the program length. The understanding of the program structure can be achieved either by first studying the structure and later hard-coding it in the generator or by providing enough examples to the generator and letting it statistically learn the structure. We decided to go for the second option as we aim to make the generator generic enough in handling new program structures as well as not constraining randomness by hard coding parts of it.

We can represent a structure of any stencil program as a chain of operation types. Some of them can contain nested operations grouped in the blocks. An example of such operation type would be the `If` operation, which has two `Blocks` one that is executed when the condition is evaluated to `true` and the second one otherwise. We create chain out of nested operations by traversing them preorder. However, they introduce chain ambiguity as it is unclear to which

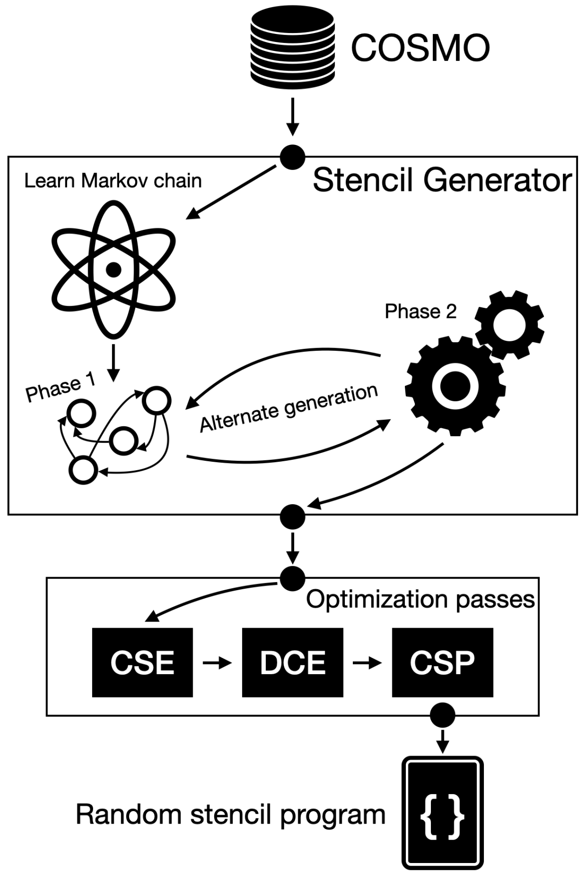


Figure 7. Diagram shows the generation pipeline. It takes COSMO stencils as an input, learns a Markov chain from them and alternates Phase 1 and Phase 2 to generate a random program. Finally, optimization passes are run on the generated program to make it look more like human-written.

parent does an operation belong. Therefore we need to explicitly mark the end of the operation's body to know that the following operations belong to the parent that is one level up. We achieved that by introducing a matching body end terminator for every operation that can have a body, as can be seen here.

In this phase, we simplified our general setting only to types of operations. We do not consider their results nor their parameters. With this setting, we can represent the structure of a general stencil program as a Markov chain where the state is a type of operation, and the edge from node A to node B is a probability with which operation B follows operation A. All outgoing edges have to sum up to 1 as they are a probability distribution of the state. The advantage of this model is its simplicity and universality. It is generic enough to express any program with such a structure yet very simple to understand and train.

On the other hand, it has some design limitations which mainly affect the quality of the generated programs but sometimes even correctness. Some chains produced by iterating Markov chain are not valid series of operations. The reason behind it lies in the fundamentals of the Markov chain, where the probability of each event depends only on the current state. However, in Stencil programs, some operations depend on more than a previous one or are entirely independent of it. Therefore there can exist incorrect chains that cannot be converted by the second phase to a valid program. The simplest incorrect chain (including operations only inside `do_method` body) would be `field_access` → `std.subf`. The chain is invalid as subtraction requires at least one value, but `field_access` produces only a pointer. Even though the probability of generating such a chain is very low (0.00374), it is still very likely to occur when generating huge datasets. Our initial solution to incorrect program chains was to ignore infeasible operations in the chain. It was working well until we started to adjust statistics of generated programs to the ones from COSMO. With this setting, it became very challenging to predict the length of the generated program as many operations were flagged infeasible, and thus not considered. Other issues were occurrences of operation pairs that never occurred in COSMO stencils. These occurrences caused some statistics of random programs to be different from the COSMO ones. Therefore we decided to change the way both phases cooperate. Rather than first generating the entire chain and then passing it to the second phase, which ignores infeasible operations, we decided for the "on the fly" chain generation. This approach enables us to use context produced by the second phase in the first one. Based on the context, we can temporarily remove outgoing edges that would lead from the current state to an infeasible state. In the new setting, it is not possible to reproduce the example from above, as this time, we would temporarily remove all outgoing edges from `field_access` that require at least one value.

The second point where program chains generated with the Markov chain need some enhancement is their quality. Our criteria for quality is to minimize the amount of generated dead or easily optimizable code. Mainly, we try to prevent the need for basic optimization passes like constant propagation, common subexpression, or dead code elimination. A great example of this problem would be a ternary operator. Since MLIR is in a static single assignment form (SSA) and we cannot inline constant values inside expressions, we need to have defined at least two values in front of it. The first value needs to have a boolean type, and it is for the condition. The second one is the return value for both cases. Ideally, we want to have a distinct value for each branch. Therefore 3 in total. In the Markov chain, a ternary operator follows a comparison operator with a very high probability, and thus it is very likely that it will succeed a comparison operator in one of the generated programs. Now let's assume that before this pair of operations, there is available only one value X. The resulting program then has to look like this:

```
%0 = cmpf %X, %X : f64
%1 = select %0, %X, %X
```

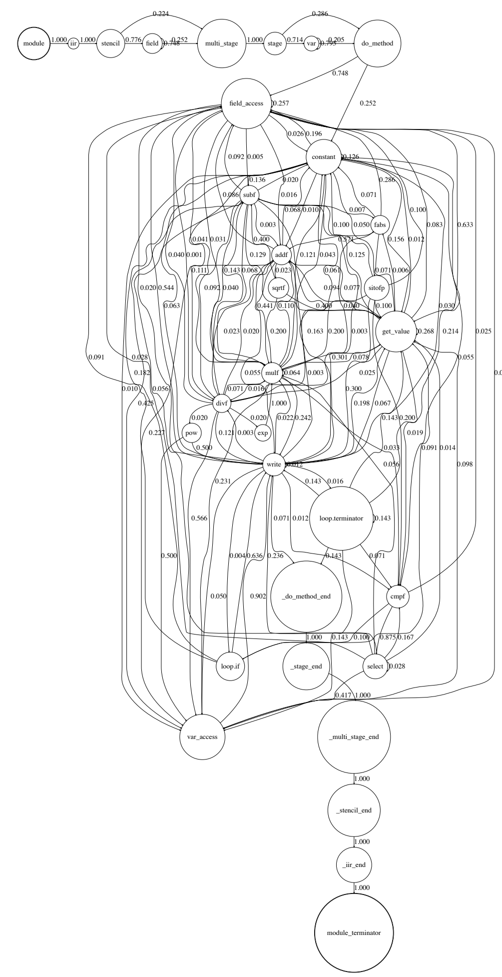
The comparison operation has to take the value X for both operands. It produces a boolean value, which will consequently be used together with X by the ternary operator. This sequence is a valid part of the program but not of high quality as it will be optimized away. To circumvent cases like this one, we had to incorporate further chain constraints. However, it is not simple to detect all code snippets that get optimized away. Therefore, we came up with the following detection strategy. First, we generated a big dataset of short programs. Second, we lowered the programs to CUDA files and obtained their register usage with the help of `nvcc` with `ptxas` flag. Finally, we detected candidates for the optimization by investigating programs using only 2 registers, which means that they became empty after the optimization. The reason why we generated short programs, was to maximize the probability of a complete program erasure and thus detection of the code snippets we should prevent in the generation. Longer programs have a higher probability of not being completely erased. With this method, we detected that the most common erasure reason was dead code, followed by a common subexpression elimination (CSE). We will explain how we partially prevented the generation of this code in the following subchapter, as it turned out that the Markov chain has very little influence on it.

We started with the Markov chain as a baseline model. Very soon, we found out that it has some limitations that more advanced models, like higher-order Markov chains, might not have, but with a small fix, we were able to solve the correctness issue as described above. The code quality problem turned out to be mostly caused by the second phase, and therefore we decided to keep building on top of it.

3.3 Generating the Operation Chain

As already mentioned, we have available around 30 stencils used in the COSMO atmospheric model. Our goal is to reproduce them in a defined quantity. We use them to learn the Markov chain as follows: First, we convert each of the input programs to a chain by iterating each program's IR preorder and appending each operation type to a list. Second, we create a graph with a node for every operation type and iterate over the program chains. For each pair of operation types (A, B), where B follows A in the chain, we increment the weight of the corresponding edge in the graph. In the last step, we compute outgoing probabilities by dividing the weight of each edge by the sum of weights of all outgoing edges. Generated Markov chain from COSMO stencils can be seen in figure 8.

Figure 8. A Markov chain generated from COSMO stencils. The nodes of the graph are operation types. The edges are annotated with probabilities.



We can see that the Markov chain has one starting state, which has no incoming edges as well as a dead-end stage, which has no outgoing edges. Starting state is the operation of type `module` as it is the parent operation for any MLIR program. Since the module is an operation with a body, it needs to have a matching terminator op. Its name is `module_terminator`, and it is the "dead-end" state in our Markov chain. It indicates the end of the only top-level operations body because no other operation is allowed to reside on the same level as the module. The generation algorithm of random program chains is as follows:

"On the fly" generation starts in the initial state of the Markov chain. First, we temporarily remove all outgoing edges that lead to invalid states based on the context, which

Algorithm 1 Pseudocode for sampling a chain from the Markov chain.

```
1: function CREATERANDOMPROGRAMCHAIN(programs, min, max)
2:     context ← createContext()
3:     chain ← createMarkovChain(programs)
4:     curr_op ← "module"
5:     end ← "_do_method_end"
6:     curr_length ← 0
7:     while curr_op ≠ "module_terminator" do
8:         view ← (s) => isValid(s, context) ∧ i ≥ min ∧ s ≠ end
9:         curr_op ← chain.getNextOp(curr_op, view)
10:        if i = max then
11:            curr_op ← end
12:        end if
13:        secondPhase(curr_op, context)
14:        curr_length ← curr_length + 1
15:    end while
16: end function
```

is updated by the second phase after processing the current state. Second, we update the probabilities of the outgoing edges such that they still form a probability distribution and sample a new state from it. We add back all temporarily removed edges and recompute original probability distribution. Finally, we set the sampled state to the current state, run the second phase on top of it, and repeat the same procedure with the updated context again. A Markov process can generate infinitely long program chains but very short ones as well. Therefore, we had to implement other measures that keep program length in the interval defined by us.

To prevent the generation of very short programs, we always temporarily remove `_do_method_end` from the outgoing edges if the current chain length is shorter than the minimum required length. This removal prevents the Markov process from entering the stage from which exists only one way, and it leads to the dead-end stage. To avoid infinite chains, we set the next stage to `_do_method_end` if the current chain length exceeds the maximum allowed length. This rule allows us to control the upper bound of the program chain, and thus we can adjust the length of generated programs to our needs.

3.4 Operation Chain Conversion

The second step in the Stencil program generation is to convert the operation chain generated by the first phase to a program in the Stencil MLIR dialect. As already mentioned in the previous chapter, we decided to change the generation pipeline. Instead of separating both phases, we decided to let them interleave on every operation. Therefore the second phase needs to be modular so it can handle the conversion of a single operation type to a concrete instantiation of it in the Stencil dialect. Furthermore, it needs to attach the instantiation to the program IR as well as to update the current context of the generation. Therefore we have to make this phase stateful as we need a state for inter-stage information sharing.

As can be seen in algorithm 1 on line 2, we first create a context. Context is a data structure that is being used by the generator for sharing generated values and pointers in between operations. In the second phase, we receive a chain of operation types together with their program order produced by the first phase. To generate a valid MLIR program, we need to create new instances from the operation types and attach them to the program IR. If we want to create a new operation instance, we need to ensure that we give it valid as well as meaningful arguments. Furthermore, we need to share the result of every operation with the following operations so that they can use it as an argument. Context provides both of these functionalities, and its structure is as follows:

- **fields** : `UniformDistribution` of the input `Fields`
- **vars** : `UniformDistribution` of the variables defined before `DoMethod`
- **read_pointers** : `ExponentialDistribution` of the pointers that can be read
- **write_pointers** : `ExponentialDistribution` of the pointer that can be written
- **values** : `ExponentialDistribution` of the `double` values that can be used in the computation or can be written to a pointer
- **bool_values** : `ExponentialDistribution` of the `boolean` values that can be used in `If` conditions or `Select` operations

We are using two types of distributions for two different scenarios. Fields and variables are always bulk inserted into the context as they are defined only at one place each. All fields come as arguments of the `Stencil` operation. Similarly, all variables definitions are in a row before the `DoMethod`. Therefore, we give every field as well as every variable equal chance to be sampled and thus be used by some operation.

On the other hand, we give the exponential distribution to all other context fields because they are no longer defined at the same place, but their definitions are spread throughout the entire body of the `DoMethod`. If we had used the uniform distribution, it would have made it unfair for the recently defined values as the older ones already had more chances to be sampled. Furthermore, in a human-written code, most recently defined values have much higher chances of being used in the current expression than the older ones. Therefore we decided to model this distribution as the exponential one. In other words, the most recently defined value has the same chance of being sampled as all older values combined. Another advantage of this distribution is the contribution to the reduction of the need for dead code elimination as it maximizes the usage of the distinct values. If we had used the uniform distribution, the values defined at the beginning of the program would have had a much higher chance of being used in some expression. Moreover, they would be sampled multiple times while values defined at the end of the program would not be sampled at all, and thus their definitions would become dead code.

We split the fields in the context into two groups: read and write ones. Initially, we had only one group for all pointers, but later we observed that this approach is responsible for the generation of redundant operations that are erased by the CSE optimization pass.

In our setting, we always ensure the generation of unique field accesses. Therefore pointer aliasing is not possible as all pointers always point to distinct parts of the memory. This fact allows us to optimize pointer reads and writes more drastically with two optimizations. The first one removes the second of the two consecutive reads and replaces all its usages with the value from the first read as it would read the same value. The second optimization removes the first of the two consecutive writes to the same pointer as the first write gets always rewritten by the second write.

These two optimizations are the reason why we decided to split all pointers into the read and write group and introduced the following rules for the insertion and removal. Every time a field is accessed, and thus a new pointer is produced, we insert it to both groups as field entry can be either read or written. On the other hand, when a variable is accessed, we insert the produced pointer only into the writing group as read of an uninitialized variable causes undefined behavior. Furthermore, two more operations consume pointers. The write operation writes to a pointer, and thus it first samples from the write pointers, then it removes the sampled element, and finally, it inserts the element to read pointers, as we don't want to have two writes to the same pointer in a row. Similarly, read operation samples from the read pointers, removes the sampled operation, and inserts it into the write pointers.

Another relevant line in algorithm 1 is the definition of a view. View is a lambda function applied to every outgoing edge from the current state. If the function returns false for some edge, we do not consider it for sampling. We use this view for temporal edge removal by applying it in each stage on top of the Markov chain.

The view function consists of three conditions joined by a conjunction. The second part: $i \geq min \wedge s \neq$ "_do_method_end" controls the minimal program length by prohibiting the Markov chain to sample the next method state because it leads to an end state. The first part is more critical as it ensures both correctness and quality by filtering out states that either cannot be processed with the current context or would result in dead code. The algorithm 2 shows the rules that filter invalid stages based on the current context.

In the following list, we are going to explain the logic behind every rule and show how it improves both quality and correctness. We numbered the rules as they appear in the code and state line number for each rule as well.

Algorithm 2 Rules of the `isValid` *view* function.

1: **function** isValid(op, context)
2:   **if** op = "$stencil.field\_access$" $\wedge$ $context.fields.empty()$ **then**
3:     **return** $false$
4:   **else if** op = "$stencil.var\_access$" $\wedge$ $context.vars.empty()$ **then**
5:     **return** $false$
6:   **else if** op = "$stencil.get\_value$" $\wedge$ $context.read\_pointers.empty()$ **then**
7:     **return** $false$
8:   **else if** op = "$stencil.write$"$\wedge$
9: $(context.write\_pointers.empty()$ $\vee$ $context.values.empty())$ **then**
10:     **return** $false$
11:   **else if** op = "$std.select$"$\wedge$
12: $(context.values.size() < 2$ $\vee$ $context.bool\_values.empty())$ **then**
13:     **return** $false$
14:   **else if** op = "$loop.if$" $\wedge$ $(context.bool\_values.empty())$ **then**
15:     **return** $false$
16:   **else if** op in $unOps$ $\wedge$ $context.values.empty()$ **then**
17:     **return** $false$
18:   **else if** op in $binOps$ $\wedge$ $context.values.size() < 2$ **then**
19:     **return** $false$
20:   **end if**
21: **end function**

- **Rule 1** (line 2) `FieldAccess` operation requires one field as an argument. Therefore we need to have at least one in the context. This rule ensures correctness as it prohibits to enter the invalid state.
- **Rule 2** (line 4) `VarAccess` operation requires a variable as an argument. Therefore we cannot enter this state without having at least one in the context.
- **Rule 3** (line 6) `GetValue` operation dereferences a read pointer, and thus it needs to have some available.
- **Rule 4** (line 8) `Write` operation requires a pointer and a value that is written to it. Therefore we need to have both them available.
- **Rule 5** (line 11) `Select`, in other words, ternary operator, requires one boolean value for the condition and 2 values for both branches.
- **Rule 6** (line 14) `If` operation requires only one boolean value for the condition.

- **Rule 7** (line 16) `Unary` operation requires one value as an argument.
- **Rule 8** (line 18) `Binary` operation requires at least one value. However, the only meaningful binary operation with both operators the same is multiplication `x * x` and addition `x + x`. Since multiplication can be replaced with `pow(x, 2)`, and addition with multiplication `2 * x`, we decided to increase the quota to 2 to prevent the generation of easily optimizable operations.

3.4.1 Accumulators.

To successfully create a Stencil operation in MLIR, we need to know three things: type of the operation, location in the IR, and its arguments. We can further divide arguments into two groups. The first one consists of the ones that are results of the other operations, and thus we call them dependent arguments. The second group contains arguments that are independent of any previous operations as they depend only on their type. Therefore we will call them independent arguments.

So far, we have available all elements needed for the construction of operation except for the independent arguments. Type of the operation and its location can be inferred from the operation chain, while dependent arguments can be sampled from the context. Furthermore, when creating an operation, we can always assume that it is constructible. The last missing piece in our puzzle is to create independent arguments.

As already mentioned, a large part of the operation types has independent arguments. Since they are independent, we can isolate their learning and sampling processes per operation type. For that purpose, we created an accumulator for each operation containing independent arguments. In the following list, we are going to explain each accumulator, which arguments it accumulates, and how they are later sampled.

- **Field Access Accumulator** `FieldAccess` operation takes as an argument a field and an offset. A field is sampled from the context since it is a dependent argument. An offset needs to be generated. This accumulator extracts all field accesses from all learning programs and forms a distribution where the probability of sampling an offset increases with the number of its occurrences in the learning programs. Therefore, the generated offset is never unique but rather one of the offsets occurring in the learning programs.
- **Constant Accumulator** `Constant` operation is one of the operations that does not contain dependent arguments, and therefore can be placed in the program anywhere from the beginning till its first usage. The only parameter it takes is the actual number. In this case, we first started with collecting maximal and minimal constant occurring in the learning programs. However, it turned out to not be working well as constants in the COSMO model have their meaning, while constants in our stencils were just random numbers generated in the large range. Therefore we adopted the same approach as in the case of `FieldAccess` - we stopped to introduce unseen constants. Instead, we sampled from values seen in the learning programs with probabilities adjusted for counts.
- **MultiStage Accumulator** `MultiStage` operation does not contain any dependent arguments, only one independent - an order in which it evaluates the child stages. Since it can take only a very restricted list of values, we compute cardinality for each of them and adjust probabilities accordingly.
- **DoMethod Accumulator** `DoMethod` operation has four independent arguments, which are lower bound, lower offset, upper bound, and upper offset. Our initial approach was to collect ranges for each of these four values. It worked well, but we decided to not generate novel ranges since they were not useful for us. Furthermore, the experiments we do in the next chapter required a low variance across these values. Therefore we decided to sample from the accumulated values with probabilities computed according to cardinalities.
- **Access Pattern Accumulator (experimental)** We implemented one more accumulator, which is not meant for a single operation but rather for a group of operations that we decided to call the access pattern. It consists of one or more `FieldAccess`, `VarAccess`, and `GetValue` operations. We observed in the COSMO stencils that fields tend to be accessed in groups together with variables. Furthermore, a couple of `GetValue` operations follow to obtain values from the pointers. Therefore we decided to model this behavior with access patterns. First, we extract all access patterns from the learning programs. We do extraction by searching for subsequences containing only one of the three types mentioned above. From the subsequences, we extract offsets, fields, variable IDs, and store them to a list. Later, we create a new access pattern by first filtering the list of accumulated patterns based on the number of fields and variables it requires. We need to filter out patterns that require more fields or variables than we have available in the context. In the second step, we sample from this filtered uniform distribution by sampling the required number of fields and variables from the context and creating needed operations with the help of the other accumulators.

We tried to generate programs with this new setting by replacing the direct generation of field and variable accesses with access patterns. However, resulting programs did not significantly differ from the ones generated without access patterns. Therefore we decided to keep the old version as the default one. We decided to keep the code for the access patterns for further experimenting.

3.4.2 Building the IR.

Now we have all components ready for joining them together. As already mentioned, we are alternating both phases for the optimal results. The reason for the alternation is the context that is being updated by the second phase and read by both phases. As can be seen in algorithm 1 line 13, we designed the second phase to handle conversion from operation type and context to a new instance. So far, we explained how we create or sample arguments, but we did not explain how we attach the new operation to the IR.

The second phase function is a mapping between operation type and a function that handles its construction. All construction functions have a unified signature. They take a context as the only argument. Furthermore, they internally share an instance of the `Builder` class, which is an MLIR construct for creating new operations. The `Builder` not only creates new instances but also attaches them to the IR as it keeps track of the current insertion point. Therefore, it simplifies the entire process as we don't need to modify the IR ourselves.

For every new instance, except for the `Module`, we assume that the `Builder` has the insertion point set correctly. The `Module` is a very specific operation. Since it has no parent, there is no insertion point possible during its construction. Therefore we have to create the module without a builder and set the insertion point to its body once we create it. For all operation types that have a body, we need to set the insertion point to the beginning of the body after we create their instance. The `Builder` will create all the following operations inside the operations body. For all terminators, we need to update the insertion point again as they end the parent operations body. Therefore we move it one level up, right behind the parent operation.

3.4.3 DCE, CSE and CSP Passes.

Even though we tried our best, we were not able to completely prevent the generation of the code that can be optimized or erased. Furthermore, we detected that COSMO stencils have some space for optimization as well. Therefore we decided to use the optimization passes to get rid of the unnecessary code. We wrote some passes ourselves as well as we used the Common Subexpression Elimination (CSE) pass from the MLIR toolkit. We run these passes on the generated programs at the very end of our pipeline. In this subchapter, we are going to describe each of the passes.

Dead-code elimination (DCE). pass is responsible for recursive removal of the dead code. An operation in Stencil dialect is considered dead if there are no usages of its result or if all operations using its result are considered dead. Therefore, in dead code removal, we have to start the analysis from the back of the basic block. We don't need a recursive lookup when iterating a block backward because we already checked all its usages.

Another optimization, DCE pass performs, is flattening of `If` operation. If we can evaluate the value inside the condition during compilation time, we flatten the corresponding body of the `If` operation. The second body is erased as it will never be executed. If both bodies are found empty, we completely erase the `If` operation.

```
1  %0 = stencil.field_access %arg0 [0, 0, 0]
2         : !stencil<"ptr:f64">
3  %1 = stencil.field_access %arg1 [0, 0, 0]
4         : !stencil<"ptr:f64">
5  %2 = stencil.get_value %0 : f64
6  %3 = stencil.get_value %1 : f64
7  %4 = addf %3, %2 : f64
8  stencil.write %1, %2 : f64
9  stencil.write %1, %4 : f64
10 %5 = stencil.get_value %1 : f64
11 stencil.write %0, %5 : f64
```

Listing 2. A code sequence before DCE pass

The last optimization, this pass does, is a field and a variable propagation. We know that memory accesses are expensive operations, and thus it is always beneficial to minimize them. Furthermore, any unnecessary operation confuses machine learning models more in their predictions as they lack deep program understanding. In listing 2, is an example of a program before the DCE pass. This program performs one unnecessary read and write. The write at line 8 is redundant as the write at line 9 will rewrite it. Therefore we can safely remove this operation. The read at line 10 can be removed as we know the value that will be read. The resulting program sequence can be seen in listing 3.

```
%0 = stencil.field_access %arg0 [0, 0, 0]
       : !stencil<"ptr:f64">
%1 = stencil.field_access %arg1 [0, 0, 0]
       : !stencil<"ptr:f64">
%2 = stencil.get_value %0 : f64
%3 = stencil.get_value %1 : f64
%4 = addf %3, %2 : f64
stencil.write %1, %4 : f64
stencil.write %0, %4 : f64
```

Listing 3. A code sequence after DCE pass

We can generalize this example to two optimization rules.

1. Every time, we encounter two write operations to the same pointer in a row, i.e., they are not interleaved by the read operation, we safely remove the first one.
2. Every time we encounter a pointer that is first written and then read within the same basic block, we remove the read operation and replace all its usages with a value that is written to the pointer.

Common subexpression elimination (CSE). pass is an MLIR pass that reduces program length by searching for duplicate common subexpressions and removes all but one. It performs some limited dead code elimination as well. However, the CSE pass is not able to propagate fields and variables, and thus DCE and CSE pass form a powerful optimization pipeline. This pass comes as a part of the MLIR.

Constant propagation (CSP). pass is a well-known optimization that we implemented because we observed many binary expressions that had constants as both operands.

To sum the entire generation process up, we first create the Markov chain, which is a directed graph with nodes being states and edges transitions between them. In our case, nodes are operation types. We learn the probabilities in the Markov chain from the COSMO stencils as we want to replicate them. However, our approach is general enough to replicate other datasets.

Second, we introduced the context as a way of sharing state between stages. In the first stage, we need the context for filtering invalid stages while in the second stage, we use it for sharing of values and pointers between operations.

Third, we introduced the second phase together with accumulators. The second phase creates new instances from operation types and context. It does it by having a mapping between operation type and a handler function. Each handler function is responsible for creating an instance of a different operation type by using the context and particular accumulator. Accumulators are classes that are responsible for the accumulation and sampling of independent arguments. We divide arguments into two groups. Dependent arguments are values or pointers that are produced by other operations. We call them dependent because they depend on the other operations. The second group is independent arguments. The group consists of arguments that are independent of other operations. A good example would be a field offset.

Lastly, we explained how we used the MLIR `Builder` class for building program IR. The builder uses an insertion point as the location for new instances it creates. We change the insertion point when we encounter an operation with a body or a terminator. The result of this process is a valid program in MLIR Stencil dialect.

3.5 Evaluation

In the previous subchapters, we introduced a method of replicating some dataset into a much larger one by learning its structure. Furthermore, we described the problems we encountered along the way, the enhancements we did to increase the similarity of generated programs to the learning ones. In this subchapter, we are going to evaluate the dataset of stencil programs generated by us with the COSMO one.

We can define the objectives of our entire approach in two words: correctness and quality. We further split correctness into two types. The first one is the correctness of the generator. Here we had to ensure that we never generate a state which cannot be constructed. While it is hard to prove the correctness mathematically, we generated a sufficiently large amount of random programs without entering the invalid state. Therefore we gained confidence that the generator works at least for the COSMO stencils very well. The second type concerns the correctness of generated programs. The mathematical proof for this type of correctness is even harder as we would need to prove that every generated program is a correct program. Furthermore, we found it equally challenging to come up with a testing infrastructure for random programs because the correct result is not known to us either. Therefore, we left this task for future research.

The second objective of our approach is the quality of the generated programs. We came up with two measures to assess it. The first one is an internal one. We measure how many lines of code get erased by DCE, CSE, and CSP pass. This measure indicates how much unnecessary code we generate. As already discussed in the previous subchapter, we cannot entirely prevent the generation of dead-code. However, it is still interesting to observe how some measures influence this number. In the case of the CSE pass, we could have prevented the duplicate generation of subexpressions. However, we decided to prevent only the generation of duplicate variable accesses, field accesses, and pointer dereferences. We did not prevent the generation of the common subexpressions because we would just duplicate the functionality of the CSE pass. The final versions of the generated programs have all of these passes applied. Therefore the final effect would have been the same.

3.5.1 Evaluation of the Optimization Passes.

As already mentioned, one of the measures for the stencil program generator is the amount of easily optimizable code it generates. For some program generators, easily optimizable code is the desired property because their goal is to test the optimization passes in the compiler. However, we use our random programs for training machine learning models that are not capable of deep program understanding. For instance, we cannot train a statistical model on a program with dead code as the model would treat it as a normal code, and thus it would introduce an inconsistency between the program features and the ones to be predicted.

Our first approach in dealing with dead code was to remove it during the code generation. Later, we decided to move it into a separate optimization pass as we needed it for optimizing COSMO stencils as well. This move made our generation pipeline more modular, and we were able to trace the bugs more efficiently.

On top of figure 9, we can see the optimization pipeline. First, we generate "raw" programs, which are later polished by our optimization passes. The pipeline order is very important as the DCE pass makes some assumptions that are fulfilled only by the CSE pass. Below the pipeline, are confidence intervals that display a percentage of a program that is removed from the previous stage. On average, passes remove more than half of the "raw" program. In most cases, the CSP pass removes zero lines because constant propagation can rarely be applied. On the other hand, generated programs contain a high percentage of dead code and common expressions.

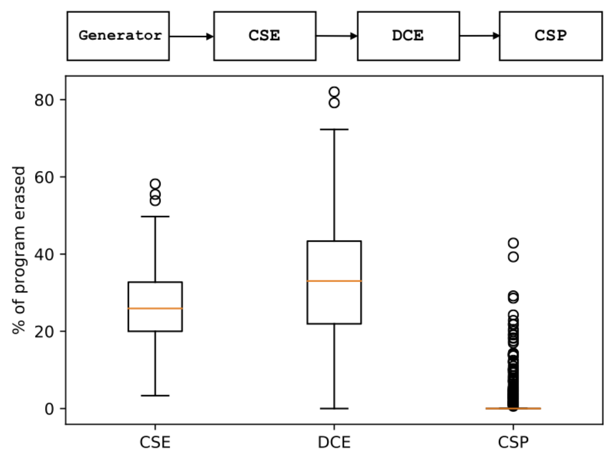


Figure 9. Optimization pipeline. The plot below shows how many percent of a program are being erased by the optimization stage in the pipeline. The evaluation dataset consists of 1000 random Stencil programs generated by our generator.

3.5.2 Evaluation of the Generated Stencil Programs.

Complete prevention from dead code generation would mean that every result of every non-void operation needs to be used. To achieve that, we would need to write all unused results to distinct field pointers at the end of the program. For that, we would most likely have to create new pointers. This would result in programs not similar to the COSMO ones as they would all have many write operations at the end of their `DoMethods`. Therefore, we adopted the opposite approach, where we generate longer operation chains, which result in larger stencils. Consequently, optimization passes shorten them, so they end up having, on average, the same length as COSMO stencils. Figure 10 shows a comparison between lengths of generated and optimized stencils, while figure 11 displays a comparison between optimized and validation (COSMO) stencils. We can see that only around 60% of the generated stencils are shorter than 100 lines, while in the case of optimized stencils, it rises to 90%. The same applies to the number of unique SSA values where this number increases from 76% to 96% because arithmetic expressions are the most frequently marked as dead. On the other hand, maximal expression depth is not affected, which indicates that deeper expressions are less likely to be eliminated, and they have

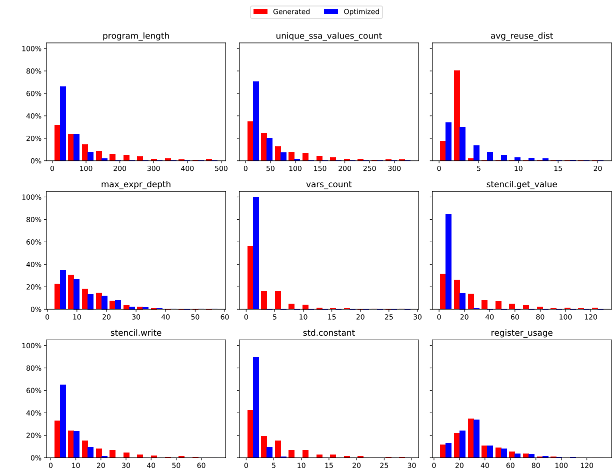


Figure 10. A comparison between random programs before and after optimization passes. Each of the plots shows a distribution of one program feature. We can observe a shift toward lower values in most plots as optimized stencils are much shorter. Register usage changes slightly because optimized stencils are semantically equivalent.

a higher chance of being written to a field. Furthermore, average reuse distance increases as dense expressions which reduce it are removed.

The plot in the middle shows that optimization passes remove all variables. As we were writing optimization passes, we realized that in our setting, there is no need for variables. The only exception is a variable which is written in both branches of an `If` operation and subsequently read. The reasons why we can replace variables inside `DoMethod` are summarized in the following points:

- Values in variables cannot be shared between `DoMethod` iterations, as they do not have default values, and therefore first read in the first iteration is undefined unless it is a write operation, in which case value from the previous iteration is always rewritten.
- We can propagate variable writes to their subsequent reads, remove first of the two writes in a row and remove the last write as it will never be read.
- The only case when we cannot remove variable is, as already mentioned, a variable that is written in both branches of `If` operation because we cannot do the value propagation in this case.

CSE and DCE pass cause a massive reduction of `GetValue` and `Write` operations, as shown in the middle right and bottom left plots, respectively. We attribute `GetValue` reduction mainly to the elimination of common field accesses and consequent elimination of `GetValue` operations. The second reason is the write to read propagation mentioned a few times already. It partially causes `Write` operation removal as

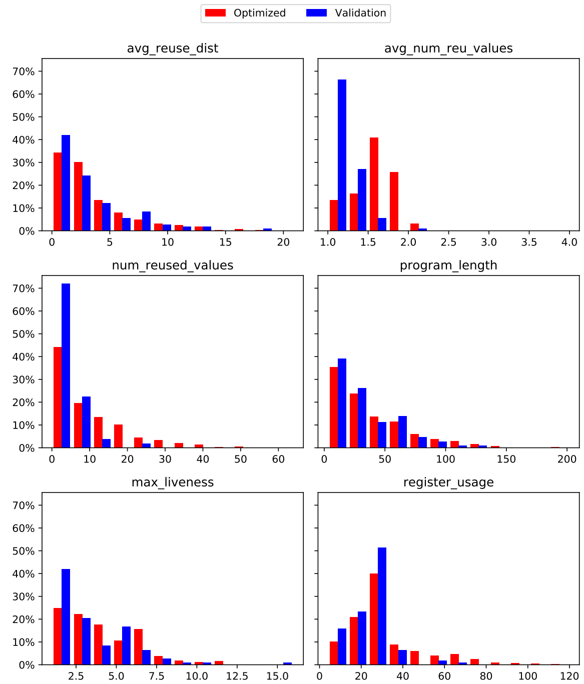


Figure 11. A comparison between random stencils generated by us and validation stencils from the COSMO model. Each of the plots compares a distribution of one program feature. Our stencils match all features of validation ones except for the average number of reused values where we reuse one value on average slightly more.

well. The second contributor to `Write` operation elimination is the removal of the first of two `Write` operations in a row. Lastly, dead code elimination removes some of the `GetValue` operations as well, while the `Write` operation is never dead.

Figure 11 shows a comparison between the optimized version of our random stencil programs and validation stencils, which we obtained from the COSMO model. This comparison was the main objective for our generator as it shows how close our stencils are to the real ones. This figure has only six but the most important subplots. We attached the full comparison of all features for both figures in the appendix.

All selected features compared in figure 11 are not related to any concrete operation, as this would be easy to replicate. For instance, generating a dataset where we set the objective to match the quantity of each operation type would be much easier to generate as the one where we would compare maximal expression depth. Therefore we decided to select the "deep" features as our objective because they express the information about the program's structure. For instance, register usage cannot be tricked with dead code as the underlying `nvcc` compiler would optimize it away and allocate fewer registers.

In the following list, we are going to explain each subplot in the more details starting from the top left:

- **avg_reuse_dist:** Average reuse distance is the number of distinct values accesses between two consecutive usages of the same value. Therefore, this statistic includes only values that are used more than once. As can be seen, we are replicating this feature accurately by not producing too long reuse distances. This feature is mainly influenced by the distribution we use for value and pointer sampling. The exponential distribution is thus modeling the value usage correctly.
- **avg_num_reu_values:** This feature denotes the average number of times a value is reused. Here we can see that the validation stencils tend to reuse values less. Furthermore, this subplot shows where our generator can be improved. Real stencils tend to read the fields in a group, compute a new value from them, and write it back to some field. Our stencils differ in one point. They share intermediate values between various computations, which causes higher value reuse.
- **num_reused_values:** This subplot compares the number of values that are used more than once. Again, it shows that our stencils reuse values more than COSMO ones, but this time the difference is smaller because the quantity is not taken into account.
- **program_length:** We are capable of replicating program length accurately because we can control the upper and lower bound on the Markov chain. We aim for the generation of longer sequences, as we know that a big portion of the program will be removed by the optimization passes. Therefore we set the lower bound to 20 and upper bound to 500, so most of the optimized stencils are in the range [20,150].
- **max_liveness:** Another important feature is the maximum number of live variables at any point in the program. Here we tend to have slightly more live variables than COSMO stencils due to average higher usage of a single value.
- **register_usage:** This feature is obtained by running `nvcc` with all optimizations, except for loop unrolling, turned on. Therefore we cannot fake other features by generating code that can be optimized away. Our stencils use approximately the same amount of registers as the validation ones. Few high register pressure stencils occur in random stencils while not in the validation ones, but we do not treat it as an issue.

In this subchapter, we evaluated the optimization passes by comparing features of stencils before and after their application. Figures 9 and 10 demonstrate that passes were able to remove great parts of the programs while maintaining roughly the same amount of registers. Moreover, integration tests were created to assess their correctness.

Furthermore, we evaluated the random stencil generator by comparing random stencils with COSMO ones. We did it by plotting distributions of the most important features next to each other. The main objective was to get each distribution of the generated programs as close to the COSMO one as possible. The comparison shown in figure 11 demonstrates that the random stencil generator can reliably reproduce the COSMO dataset and thus generate stencils that are suitable for further compiler research.

4 Experiments

The motivation behind the random stencil generator is to enlarge the existing COSMO dataset with new, meaningful stencils that can be used for training machine learning models predicting either other program features or optimization strategies. Machine learning models work best when provided with a noise-free and feature-rich dataset. Furthermore, a dataset has to fully cover parts of the input space we are interested in. In this chapter, we are going to explain how we created datasets suitable for machine learning, how dataset features were selected and collected, and which experiments we tried with these datasets together with their evaluation and future research directions.

4.1 Datasets

Since machine learning algorithms work with floating-point numbers but not with a text directly, we had to find a way of representing a stencil program as a feature vector of fixed size. To do it, we had to identify a set of features precisely representing a program. The optimal set of features never represents two different programs with the same feature vector. Furthermore, each feature vector variable called independent variable should correlate with at least one predicting variable also called dependant variable. In other words, if we want to predict some property y of the program λ, then at least one feature from the feature vector X of program λ has to have some relationship with property y. The most critical element weakening the relationship is noise. Therefore, our primary goal before actual feature definition and collection was to clean the generated stencils off the noise. Initially, we identified dead code as the main source of the noise, followed by an easily optimizable code. However, this is not a problem anymore as the optimization passes remove most of it.

4.1.1 Featurization. Featurization or feature engineering is the process of using domain knowledge for feature definition and later extraction. In our case, this was the most crucial step in the entire experiment as choosing the right features makes machine learning algorithms work. After some trial and error, the resulting set of the features looks like this:

loop_order An order in which a loop is executed. Can take 3 values: *forward*, *backward* and *parallel* which we map to 1, 2 and 3 respectively.

loop_size The number of iterations computed as the difference between the upper and lower bound. Offsets are not considered.

avg_reuse_dist An average reuse distance of all values that have more than one usage.

avg_num_reu_values An average number of times a value is reused. Here are included all values.

num_reused_values Number of values that are reused i.e. used more than once.

fields_count Number of total fields. This is the sum of the locally defined fields and fields passed as parameters.

unique_ssa_values_count Sum of all values used in a stencil.

max_expr_depth Maximal expression depth. Starts in the read of some field or constant and ends in a write of the computed value.

bin_ops_count Number of arithmetic operations that have two operands.

un_ops_count Number of arithmetic operations that have one operand.

unique_offsets Number of unique offsets across all field accesses. We do not take the accessed field into consideration, only its offset.

program_length Length of the body of the `DoMethod`. We do not consider other operations as they are boilerplate code, which is not directly translated into CUDA C.

max_liveness The maximal amount of variables that are live at any point in a stencil computed with standard live variable analysis.

stencil.field_access The number of field accesses. Since it is computed on the optimized stencils, it is the number of unique field accesses as well.

stencil.get_value Number of pointer dereferencings.

stencil.write Number of writes to a pointer.

std.addf Number of additions.

std.cmpf Number of comparisons.

std.divf Number of divisions.

std.mulf Number of multiplications.

std.subf Number of substractions.

std.select Number of ternary operators.

stencil.sqrtf Number of square roots.

stencil.pow Number of "raise to power" operations.

stencil.fabs Number of absolute value operations.

stencil.exp Number of "compute exponential function" operators.

std.constant Number of floating-point constants.

register_usage Number of registers used by a program.

4.1.2 Data Collection. Features are extracted from programs in two ways. The first one is by using custom feature extraction MLIR pass that extracts features from programs written in the Stencil dialect. The pass iterates Stencil IR, collects statistics about operation types, reuse distances, etc. and outputs a feature vector of direct stencil features.

After running the direct feature extraction pass, we have to collect the remaining feature that cannot be extracted from the source code directly. It is register usage. In order to extract it, we have to use the following passes (chained in the listed order) to lower a stencil program to CUDA C:

1. Passes from `mlir-opt`:
   - `--convert-stencil-to-affine` (Written by J.M. Gorius) Lowers stencil dialect to the affine one.
   - `--lower-affine` (Written by MLIR authors) Lowers affine constructs to the standard Dialect.
   - `--cse` (Written by MLIR authors.) Well known Common Sub-expression Elimination.
   - `--convert-loops-to-gpu` (Written by MLIR authors) Creates kernel and launch function out of two outer loops while keeping the inner most inside the kernel function.
   - `--gpu-kernel-outlining` (Written by MLIR authors) Outlines kernel out of launch function into a separate function.
   - `--cse`
2. Passes from `mlir-translate`:
   - `--mlir-to-cudac` (Written by us) Converts the mix of GPU and standard dialect into `CUDA C` file.

Once a stencil program is lowered to `CUDA C`, we run `nvcc` with `ptxas` flag to get the number of allocated registers, which is appended to the list of features obtained directly. The feature extraction process is visualized in figure 12.

A dataset is generated by running the process described above on top of all generated programs, accumulating features of all programs into a 2-dimensional array, and storing it into a CSV file. In the end, we defined 4 types of datasets we are interested in:

- Random stencil programs
- Optimized random stencil programs
- Validation stencil programs
- Optimized validation stencil programs

By *optimized*, we mean a dataset cleaned by optimization passes. The *validation stencils* are stencils taken from the COSMO model, which we later use as validation data.

4.1.3 Data Analysis. In this subchapter, we are going to analyze the following properties of the generated datasets:

- **Input space coverage** The input space is a set of all possible inputs that feature vector can take. Theoretically, most of our features can take an infinite number of input values, but practically neither programs have unlimited lengths nor variables. Furthermore, we do not take variable values into account as they are irrelevant to register usage, and all features except for the `loop_size` and `loop_order` are dependant on the program length. Here we are going analyze which values can some of the most relevant features take and how well we cover the input space compared to the validation data.
- **Dataset size** Since our generator is flexible in terms of generated dataset size, we will examine different dataset sizes and reason about the optimal size based on the achieved accuracy as well as the input space coverage.
- **Dimensionality** Here our goal is to analyze the correlation between features and understand the dataset by reducing its dimensionality and visualizing it.

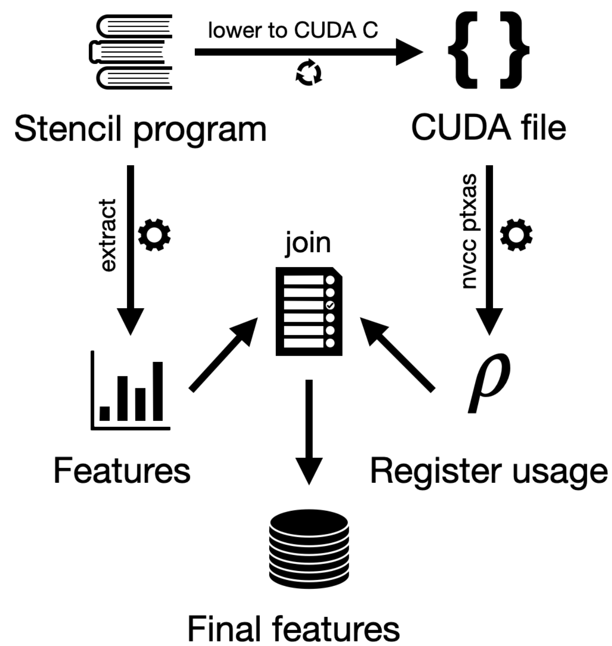


Figure 12. Diagram shows the feature extraction process from a program written in the Stencil dialect. All features, except for the register usage, are extracted from the source code directly using feature extraction pass. In the case of register usage, the program is first lowered to CUDA C, compiled using `nvcc`, and register usage is extracted using `ptxas` flag. Finally, all features are joined and appended to the final dataset.

Input space coverage. As already shown in figure 11, we are able to replicate the properties of validation dataset quite accurately. Here we are going to analyze the input space for each of the most relevant features and a way of influencing it.

By experimenting with stencils of various lengths, we identified **120** as the maximal and **2** as the minimal number of registers that `nvcc` allocates. Furthermore, we observed,

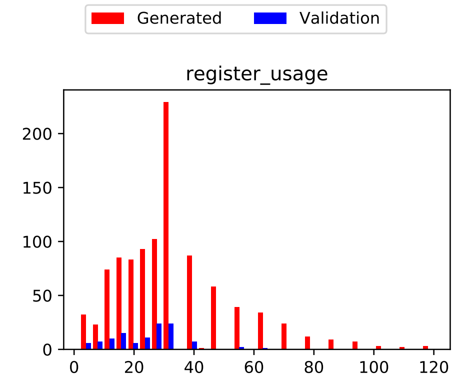


Figure 13. A comparison between register usage in generated and validation stencils expressed in absolute numbers. The generated dataset contains 1200 samples while validation one 113.

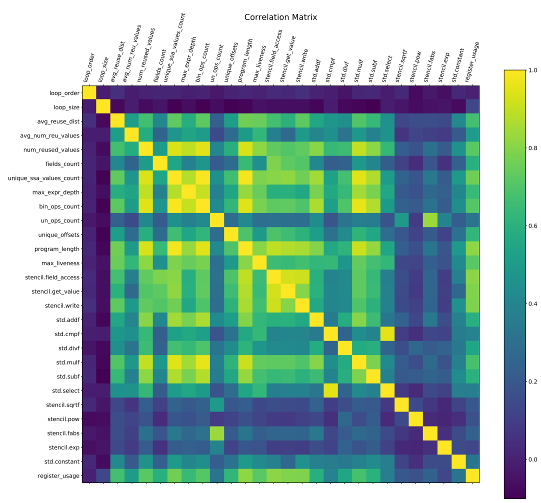


Figure 14. A correlation matrix of the generated dataset showing how strong relationships between the features are. Especially relevant is the correlation of the register usage with other features as we are going to train models predicting it.

that in the interval [4,32] any number of registers can be allocated while in [33,120] range most of the numbers are never picked. Figure 13 shows the comparison of register usage between generated and validation data in absolute terms. The most common number of allocated registers is 32 (157 times), followed by 30 (67 times).

As already mentioned, we can influence other features to some degree by changing the interval of desired program length. We can see that correlation in figure 14 shows very strong dependencies between program length and all other features except for: (1) the loop size and order, which are completely independent of program length as they don't represent operation quantities, (2) unary operations which occur rarely in the programs, and (3) the average number of reused values, which is influenced by distribution for value selection. The relationship of program length with other features shows that our generator can reproduce properties of any input dataset by searching for the optimal interval of program length.

Size	MSE_f	Mean_f	Med_f	STD_f	MSE	Mean	Med	STD
100	22.868	3.254	2.391	3.504	40.251	4.099	1.881	4.842
200	25.102	3.345	2.361	3.73	55.601	4.962	3.183	5.566
500	18.093	2.598	1.572	3.368	62.255	4.765	1.728	6.288
750	19.591	2.55	1.266	3.618	73.716	5.146	1.892	6.873
1000	16.293	2.351	1.363	3.281	69.439	5.046	1.65	6.631
1200	16.173	2.384	**1.153**	3.238	58.374	4.671	**1.486**	6.045
1500	16.518	2.509	1.29	3.197	75.666	5.385	1.743	6.831
1750	16.702	2.422	1.209	3.291	64.288	4.975	1.656	6.288
2000	17.2	2.507	1.229	3.304	65.617	5.075	2.226	6.313
5000	17.335	2.584	1.714	3.265	58.809	4.929	2.031	5.874
10000	17.001	2.454	1.469	3.313	53.169	4.67	2.262	5.6
12000	17.14	2.617	1.782	3.208	58.25	4.74	2.311	5.981
15000	16.062	2.477	1.663	3.15	54.76	4.565	2.167	5.824
20000	15.335	2.418	1.693	3.08	47.115	4.227	2.1	5.408
25000	16.914	2.555	1.736	3.223	46.543	4.244	2.066	5.342
30000	16.146	2.433	1.606	3.197	49.523	4.393	2.355	5.497

Table 1. An accuracy of focused (f) and fully trained GBT model for different dataset sizes. We measured the accuracy always on the same dataset of validation (COSMO) stencils that have 113 samples.

Dataset size. The second property and from our perspective, the most important one is dataset size. With dataset size, we can influence input space coverage as a bigger dataset has a higher chance of covering the properties of validation one. Furthermore, more data can improve model training as they cover the input and output space better. However, they can cause overfitting as well, which is something we want to avoid. Therefore, we generated a huge dataset containing 30K stencil programs and searched for the optimal size by training the best performing model - Gradient Boosting Trees (GBT) on the subsampled data of various sizes. The results of the search are summarized in table 1. We rerun the experiment five times for each size with always newly uniformly subsampled data and took an average. It turned out that five reruns are enough as we observed only a small variance between runs. Furthermore, we did the focused training where we trained the model only on data having register usage smaller or equal to 45. The reason behind that is an observation that in this range model can fit the data better than it would in the full range while covering 98%

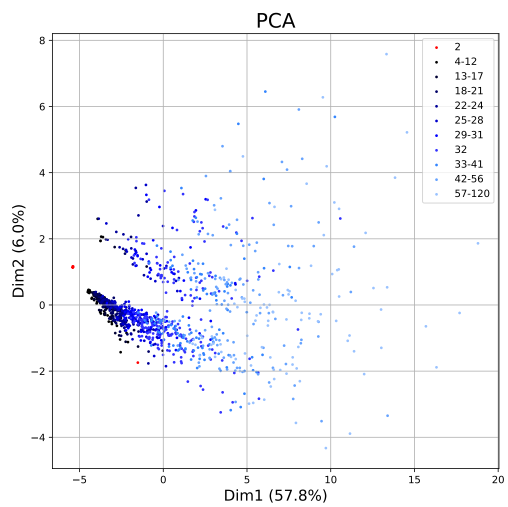


Figure 15. Datapoints of the generated dataset projected to a 2D plane by using 2 most dominant principal components. The first two components maximize variance and thus capture almost 64% of all variance.

of the register usage space of validation data. We validated both models on the same validation data. The results for the focused model are shown as well in table 1 with subscript f. From now on, we will show all results for the focused models, which are more accurate. The results for the "full models" are in the appendix.

Dimensionality. Figure 15 shows a projection of the high-dimensional, optimized random stencil dataset to a 2D plane. To do the projection, we had to reduce dataset dimensions from 26 to 2. We used PCA for dimensionality reduction and selected 2 most dominant principal components. The color of each data point depends on its register usage. Since the range of possible register usages is extensive, we decided for the split into smaller intervals with evenly distributed data points

It is interesting to observe how data points in figure 15 are getting sparser together with the increase in register usage, which implies that they have higher dimensionality as well as the reconstruction error. It is logical as these programs tend to be longer and have more difficult structures, which require more features to express. Therefore high register usage programs make training more challenging to converge as models have to distribute weights among more dimensions. Furthermore, they enlarge output space, which makes data fitting more complex.

The red dots in figure 15 represent stencils using only 2 registers. These stencils got eliminated either by our optimization passes or by nvcc. Even though they are all empty and thus have all essential features the same, PCA projects

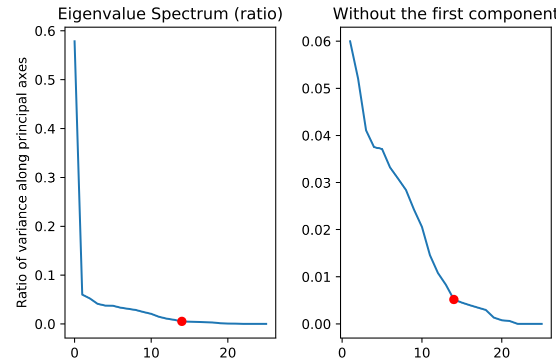


Figure 16. Eigenvalue Spectrum ratio shows how much variance is across principal components. The most dominant one takes more than a half (57.8%) of it, followed by the significant drop until it stops in the 14th eigenvalue (red dot), which is the "knee" in the eigenspectrum, i.e., the first of components that we do not keep among the set of reduced dimensions. The first 13 components contain ≈ 98% of all variance, and thus the reconstruction error is ≈ 2%, which means that the dataset has low to medium dimensionality.

one data point among nonempty stencils. The reason behind it is that our optimization passes did not eliminate this stencil's body away, but nvcc managed to. Therefore the feature vector of this stencil contains a lot of noise as dead code regions influence most of the features, which nvcc eliminates. After a small investigation of this case, we found that our constant propagation pass had some space for improvement, but we decided to keep it as a demonstration of PCA usefulness in dataset visualization and investigation.

Figure 16 displays an eigenvalue spectrum. Since PCA tries to maximize variance for every principal component, given that they have to be orthogonal to each other, we can see a massive drop of variance starting from the second component. The drop is no surprise as the first component has to have the largest possible variance. Therefore, we can simultaneously maximize variance and minimize the number of dimensions by identifying a "knee" in the Eigenvalue spectrum and keeping all components in front of it. In the case of this spectrum, the "knee" lies in the 14th component, and thus we can express ≈ 98% of all variance in only 13 dimensions, which is half of the original dimensions.

Based on all of the points discussed above, we concluded that the dataset of 1200 optimized random stencil programs is the most suited one for the register usage prediction. Figures evaluating some of the other datasets are in the appendix.

4.2 Predicting Register Usage

Register usage provides a piece of essential information for compiler optimization. If we could obtain a register usage of any stencil program in order of milliseconds, we would be able to try multiple optimization strategies and pick the one using the smallest amount of registers and thus eliminate high register pressure. However, the time it takes `nvcc` to produce register usage information does not allow a broad search for the best optimization. Therefore, we decided to circumvent `nvcc` by training machine learning models that can predict register usage much faster.

Since our datasets have low dimensionality and small input space, we decided to use simple statistical models, which are easy and fast to train and work well with small training datasets. In particular, we decided to use *Ridge Regression* as a baseline model and *Gradient Boosting Trees* as the second model. In the following subchapters, we are going to explain how both models work and the results we achieved using them.

We identified register usage prediction as a regression [**?**] problem. In regression analysis, we try to estimate the relationship between dependant variables (in our case only one - register usage) or **y**, and independent variables called input variables or **X**, which are in our case collected features. In other words, we want to automatically find how stencil features influence the number of allocated registers. Furthermore, we want to leverage this knowledge in predicting new, unseen data.

In the linear regression, we are searching for the line that best fits the data according to the given error function. In other words, we want the line that minimizes the distance between the predicted values and the actual values. More formally this optimization problem can be defined as:

$$\min \frac{1}{n} \sum_i (\hat{y}_i - y_i)^2 \tag{3}$$

where

$\hat{y}_i$ is the predicted value
y_i is the actual value
n is the number of samples

and we try to minimize the *mean squared error* (MSE) - that is, the average squared difference between predicted and actual values.

4.2.1 Ridge Regression.

Tikhonov regularization or ridge regression is a well-known regularization method of ill-posed problems. It solves a regression problem where the loss function is linear least squares, and it uses l2-norm as a regularization. Therefore the objective function is:

$$||y - Xw||_2^2 + \alpha||w||_2^2 \tag{4}$$

which has only one hyperparameter α - a regularization strength (must be a positive number). X denotes the input data (independent variables) and y the independent variables. The model tries to find the optimal vector of weights w, whose product with X minimizes the least squares [**?**] loss function. α reduces the variance of the predicting values as well as improves conditioning.

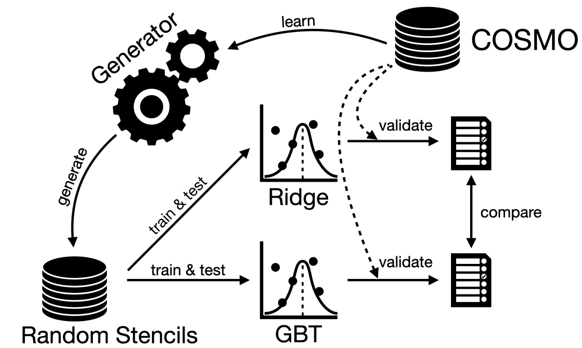


Figure 17. Diagram shows a high-level overview of the register prediction pipeline. The important note is that we never train on COSMO data directly. They are always used only for validation.

We run the model with different α values and results are summarized in table 4.2.1.

In our experiment, we used the scikit learn implementation of the algorithm, which one can find here [**?**]. For more information about the regression itself, we recommend to follow up here [**?**].

Mean	Std	α
-14.305176	2.757947	0.25
-14.298890	2.749494	0.5
-14.287009	2.733225	1.0
-14.265767	2.702987	2.0
-14.231775	2.650073	4.0
-14.188361	2.565548	8.0
-14.156424	2.444302	16.0

Table 2. Grid search for the optimal α value. Table shows MSE, the mean and standard deviation for different α values with 10-fold cross-validation of the Ridge regression model.

Figure 18 shows the prediction accuracy. The closer a point is to the red dashed line, the more accurately it was predicted. We can see that accuracy is dropping as the number of registers increases. We think that it is caused by the higher dimensionality of the programs with high register usage, as shown in figure 15. However, few exceptions were predicted accurately despite their high register usage. The median prediction error is 2.7656, the average 3.539, and the standard deviation 3.475. These numbers are our baseline, even if we already consider them accurate enough.

Figure 19 shows weights that Ridge regression assigns to the features. The model makes pointer dereferencing - `stencil.get_value` the most valuable feature, followed by a `max_liveness` and a `loop_size`. It is quite logical as pointer dereferencing produces a value that resides in a register, and `max_liveness` determines the maximum amount

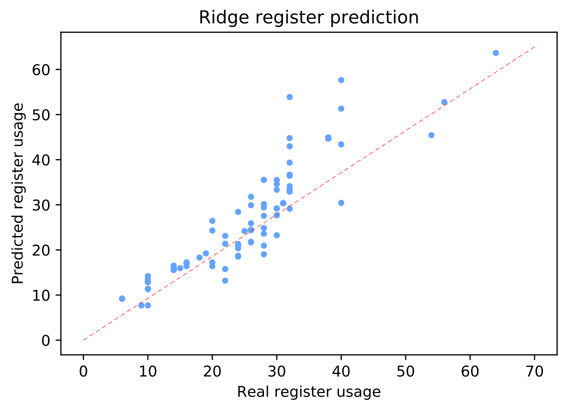


Figure 18. Scatter plot target vs predicted values. Prediction results are very accurate for programs with low register usage. However, the accuracy is dropping as the number of registers increases.

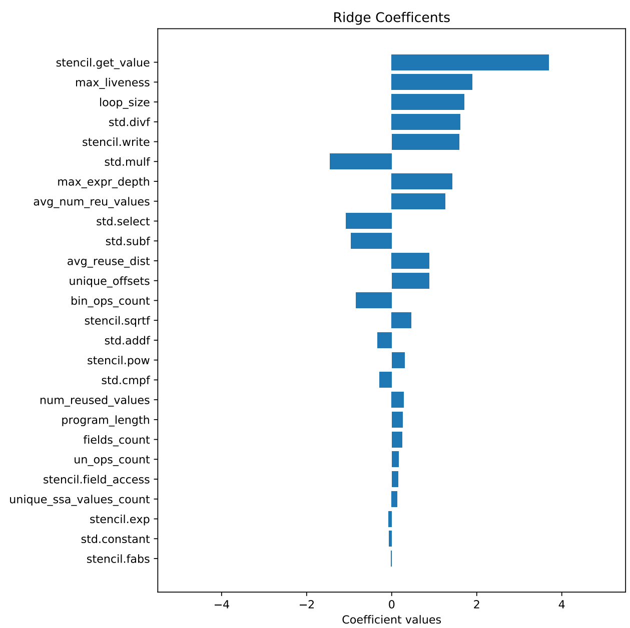


Figure 19. The ridge weight vector with coefficients. Their absolute values indicate variable importance to Ridge regression because higher value influences the resulting number more.

of values that need to be live at the same time and thus should ideally be put in registers as well. However, `loop_size` makes a little sense since we prohibited loop unrolling optimization inside the `nvcc`, and thus only the body of the for loop matters in terms of register usage. The following features - a division and a write, are logical as well. A division requires more registers than any other binary operation, and a write computes the index, loads the value, and stores it, which is

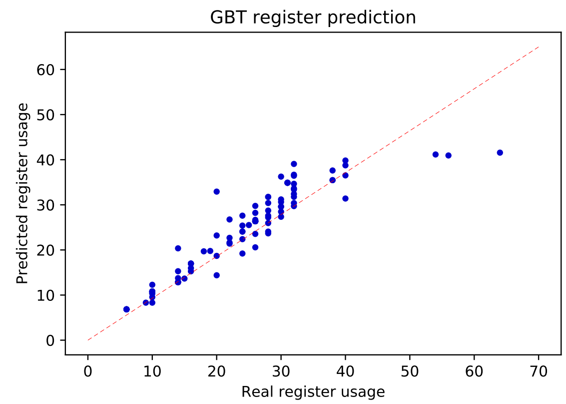


Figure 20. Scatter plot target vs predicted values. GBT model produces more accurate prediction results than Ridge regression. Furthermore, GBT is not only accurate for programs with low register usage, but it produces reliable results for stencils with medium register usage as well. However, prediction for the three stencils with the highest register usage is still inaccurate due to focused learning.

demanding on the number of registers as well. The unique offsets feature indicates the actual number of offsets that compiler computes as it eliminates the computation of redundant offsets. Furthermore, features related to reuse distance express how many values operations reuse and thus should be kept in registers. The `avg_reuse_dist` indicates that values with long reuse distances kept in registers are good candidates for register spilling. The `avg_num_reu_values` and `num_reused_values` represent values that should ideally reside in registers to prevent duplicate loading. Most of the other features have lower importance either because they have lower occurrence rates in learning programs or because the model was not able to find a strong connection between them and register usage.

4.2.2 Gradient Boosting Trees. The second model we tried is Gradient Boosting Trees (GBT). We picked this algorithm as it often produces the best predictive performance by connecting fixed size decision trees with gradient boosting. This way, it combines many usually weak learners into a single strong one. The gradient boosting is iterative functional gradient descent, which optimizes a given loss function by iteratively choosing the negative direction of the gradient. It is very easy to train as default hyperparameter values usually work well. In our approach, we used the implementation from scikit learn [?] and more information about the algorithm can be found here [?], [?].

The average accuracy on the validation data is 2.384, median 1.153, and a standard deviation of 3.238. All of these values are better than the ones of Ridge regression. Furthermore, median accuracy improved 2.4 times. We expected

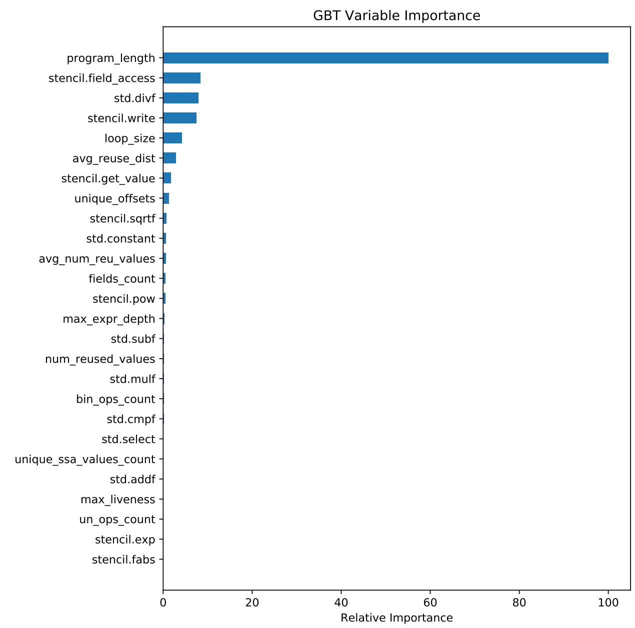


Figure 21. Figure shows how the `program_length` dominates in GBT weights by wide margin.

this improvement as GBT has one of the best prediction accuracies in this field of machine learning. Figure 20 shows a scatter plot with prediction accuracy for the individual validation stencils. The model is, unlike Ridge regression, accurate for both low and high register usage stencils. The only exceptions are three stencils with the highest register usage that GBT predicted inaccurately as its training focused on low and medium register usage stencils. However, unfocused training can predict those accurately as well but overall is slightly less accurate, as can be seen in table 1.

Figure 21 shows variable importance inside GBT. We can see that the model has chosen a completely different approach as the Ridge regression since it put most of the weight on `program_length` while Ridge regression treated it as an unimportant feature. The reason behind that might be that we focused the training on stencils with lower and medium register usage where dependency between program length and register usage is stronger than in high register usage stencils. Furthermore, register usage has the highest correlation with program length, which influences GBT as well. Division and write operations were selected as important features in this model as well, which is logical. Unfortunately, the GBT model does not tell us anything about the relationship between these features nor signs of their impact or magnitude. Therefore it is hard to infer more information about model decisions.

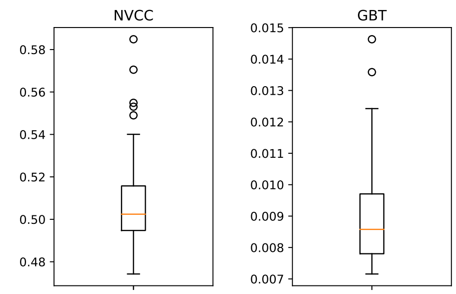


Figure 22. Runtime comparison of `nvcc` with the GBT model that is, on average more than 50 times fasters. We measured runtimes of both methods 20 times for each validation stencil and took the average. The figure shows confidence intervals of the resulting measurements.

4.3 Speed Comparison

Figure 22 shows a speed comparison between GBT and `nvcc`. As expected, GBT is a clear winner. It is more than 50 times faster than `nvcc` because it just multiplies learned weights with a feature vector, whereas `nvcc` has to perform all kinds of analyses. Therefore we conclude that register prediction should have its place in stencil optimization as it outperforms traditional analyses, and its accuracy is acceptable.

In this chapter, we presented the experiments we performed with generated stencils. The first stage was data collection, which consists of a feature vector definition and feature extraction. In the second stage, we analyzed the collected data to understand them. Lastly, we trained two models on the generated data and validated them on the COSMO stencils. The results show that register prediction is more than 50 times faster than register allocation done by `nvcc` and reliable enough to be used in future research.

5 Related Work

Stencils computations have been studied extensively in the last decade. They are used heavily in many fields, including weather simulations [?], machine learning [?], physical simulation and modeling [?], deep learning [?], computer vision, and image processing [?]. Following current trends, stencil computations try to exploit parallelism by proposing autotuning solutions for parallel stencil computations [?], [?], [?], [?], that come either in the form of frameworks [?] that extend existing programming languages or compilers that introduce their own DSLs. [?]

Since our work focuses more on learning which optimizations to perform rather than optimization improvement or parallelism, the more related papers are from Ashouri et al. [?] and Wang et al. [?], which both took an extensive survey on machine learning applications in compilers. They split recent advances into two major categories: (1) Choosing the best optimization, and (2) An order of optimization passes. Ashouri et al. introduced COBAYN [?], which uses Bayesian networks to predict the optimal order of optimization passes and thus falls into the second category. While from the long term perspective, our thesis builds a foundation for the search of the best optimization (1st category), the short term goal was to predict program properties like runtime or register usage, which does not fall into these categories. Therefore, our approach is closer to the one of Raychev et al. [?] that predicts syntactic and semantic properties inside the program. In particular, it focuses on deobfuscation by learning the associations between variable names and their locations inside the program structure.

Probably the closest approaches to ours are Autotvm from Chen et al. [?] and Halide Autoscheduler from Adams et al. [?]. Both of them aim to find the optimal loop fusion and tiling by searching the optimization space. They perform the search by employing different search strategies (Halide - tree search, Autotvm - simulated annealing), but both are using a ranking function, which is a pre-trained machine learning model predicting relative runtime for each schedule based on its features. An alternative approach is Absinthe [?] from Gysi et al., which solves the problem of optimal parameters for loop fusion and tiling as a linear optimization problem.

6 Future Work

As the future research direction, we propose to experiment more with high register usage stencils, which require more advanced machine learning techniques because of their higher dimensionality. Another research direction could be to use our existing infrastructure to collect runtime of our random stencils and train a machine learning model that predicts it. Having predictors for both register usage and runtime would enable their usage in search of the best optimization strategy. For example, one can decide whether to inline 2 stencils by predicting both register usage and runtime before and after inlining. If both numbers are better for inlined stencils, then the compiler keeps the stencil inlined. Otherwise, it undoes the inlining. Similarly, we can use it for stage fusion and other optimizations requiring a search for the optimal strategy.

7 Conclusion

Global warming starts to threaten the entire world population. The need for fast and accurate weather prediction systems is growing together with a need for saving human lives by providing in time weather warnings. Recent approaches in improving prediction systems usability and efficiency led to the invention of stencil domain-specific languages that abstracted away unnecessary implementation details, gave software developers more space for optimization, and enabled domain scientists to focus solely on their research domain. A very recent Google introduction of MLIR enabled compiler developers to rapidly develop new DSLs by providing extensible Intermediate Representation together with accompanying infrastructure. This technology attracted scientists from the SPCL lab at ETH Zurich to create a new MLIR Stencil dialect, which would create a new platform bringing all Stencil computations and languages under one roof.

This thesis brings many contributions to the dialect infrastructure. Firstly, we implemented a translation of GPU and Standard Dialect into a CUDA C code, which enabled us to run Stencil programs on the GPU. However, the main contribution is the random stencil generator that replicates existing stencil programs by learning their structure. Furthermore, we extended IR infrastructure for feature extraction and collection passes that one can utilize in the creation of new datasets. In addition to that, we implemented two optimization passes that are cleaning programs off the noise, i.e., dead and easily optimizable code. Lastly, we showed that datasets created by the generator and cleaned with optimization passes are suitable for further compiler optimization research by training simple statistical models that can predict stencil register usage accurately. Their prediction speed is more than 50 times faster than retrieving register usage information via `nvcc`, which enables a search for optimal optimization parameters in a much bigger space or various optimization decisions used in stencil fusion or inlining.

A Appendix

Text of appendix …