Challenges of applying an embedded domain specific language for performance portability to Earth system models

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Abstract

Weather and climate modeling, reliant on substantial computational resources, faces challenges of escalating resource demands and energy consumption as problem sizes and model complexity increase. Leveraging Graphics Processing Units (GPUs) for accelerated simulations demands performance portability across diverse High Performance Computing (HPC) architectures. The concept of embedded Domain Specific Language (eDSL) emerges as a lightweight solution, aiming to streamline GPU utilization without extensive code rewrites and to enhance code portability across HPC architectures. This study explores the practical implementation of an eDSL within the Icosahedral Nonhydrostatic (ICON) weather and climate model, primarily written in Fortran. Our evaluation contrasts eDSL utilization within ICON against other Earth system models, with particular emphasis on three-dimensional mass transport, or advection. Through assessing the eDSL's efficectiveness in various models, especially its application in the ParFlow and EULAG models, insights into its potential for ICON emerge. While the eDSL presents a promising avenue for performance portability, challenges in adapting Fortran-based codes, GPU support, and resource allocation underscore the need for necessity for thorough planning and resource allocation in model development endeavors. Overall, the eDSL offers a viable pathway for harnessing GPU acceleration while mitigating the complexities of code portability across diverse HPC architectures, essential for advancing weather and climate modeling capabilities.

1 Introduction

Weather and climate models rely heavily on computational resources and share a significant part of the compute resources available on today's high performance computing (HPC) systems. The finite difference or finite volume methods applied in these models require frequent communication between the compute devices (e.g., CPUs and GPUs) and also require a large amount of memory to save the variables within the problem domain. As the problem size increases, the need for computational resources, along with energy consumption, will increase non-linearly [1]. Therefore, exploiting the increased parallel capabilities offered by GPUs to accelerate simulations requires performance portability for high resolution simulations on different HPC architectures [2]. With the introduction of complex model codes to new computing architectures, changing programming paradigms as well as compiler specifics emerge as new issues.

The concept of the embedded Domain Specific Language (eDSL) is a proposed as a lightweight solution to use GPUs without largely rewriting scientific codes, and to improve the portability of the codes on different HPC architectures. The eDSL method usually uses an abstraction layer to, for example, encapsulate compute loops and lambda functions to reduce code complexity. In general, with the concept of eDSL, researchers can put more effort in scientific coding instead of having to solve the difficulties related to dealing with different types of computational software and hardware. The eDSL approach therefore relates to the concept of "separation of concerns". However, the eDSL is more of a bottom-up solution for developers of existing codes, as it embeds a macro layer for well-developed applications for performance portability without without having to rewrite the entire code for a different programming model or hardware.

In the German preWarmWorld project, we focused on the Icosahedral Nonhydrostatic (ICON) weather and climate model [3], which is mainly written in Fortran, to evaluate the possibility of implementing the eDSL approach in the code. ICON comprises a complex code design and structure and a large part of legacy code to support different applications in climate simulation and weather forecasting. In the preWarmWorld project, we evaluated how the eDSL approach could be practically applied to ICON, by contrasting it also with applications of the eDSL in other Earth system models. Particular focus was given to three-dimensional mass transport, also referred to as advection.

2 The DSL approach

A Domain Specific Language (DSL) is a programming language dedicated to a specific problem domain. DSLs are designed to be expressive and concise to provide some specialized constructs or abstractions to fit into a specific task or application. A good example of a DSL is the Hypertext Markup Language (HTML), which can be seen as a language for the web application domain.

The main characteristics of DSL are: i) narrow focus, ii) expressiveness, iii) abstraction, and iv) productivity. A DSL will focus on the specific problems, and thus it is not as general as e.g. C/C++ and Python. And thus, a DSL can express the context of the specific domain and allow developers to express the concepts to that domain problems, e.g. the computational fluid dynamics, or the computation for grid cell-based model, e.g. GT4PY [4].

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To further illustrate the concept, we provide pseudo code examples. In Pseudo code 1, an application uses a loop and the intrusion of gpu-related pragmas (e.g. OpenACC) to build the application to compute the variable. In the DSL approach, a variable can simply be computed using a more plain language, as shown in Pseudo code 2. However, in Pseudo code 2 the subroutine (as "define") can also deal with the specific details of the loops, for example, how to deal with grid cells at the boundaries.

Pseudo codes 1: a non-DSL example

```
#pragma acc parallel loop
for (i=0;i<N;i++)
{
    y[i] = a * x[i] + b
}
```

Pseudo codes 2: a DSL example

```
y = Boxloop( a * x + b)

...

#define Boxloop(loop_body)
{
  #pragma acc parallel loop
  for (i=0;i<N;i++)
  {
    loop_body;
  }
}
```

Therefore, to address the problem of a specific domain, DSLs often provide a higher-level abstraction instead of writing the whole set of codes for each application or solution. For example, a DSL that deals with grid cells with loops will have abstraction codes to perform the solution.

An embedded domain specific language is designed to use macros to represent parts of the code to accelerate the code development by intermediate level programmers. This allows domain scientists to focus on the development of the scientific part rather than the computational part of the problem. In Earth system modeling, the simulations are often based on finite difference or finite volume methods, and thus looping through grid cells to compute the variables is an essential part of the codes. Therefore, using a domain specific language to create template functions helps reducing development time and costs, especially when porting to GPUs [4, 5].

For example, the weather forecasting model Consortium for Small-Scale Modeling (COSMO) applies two different methods of DSLs, STELLA DSL [5] and GridTools [4], to port the dynamical core of the model and to evaluate the efficiency of DSLs for weather simulation using C++. By taking advantage of the C++ features, both tools can run the COSMO dynamical core on NVIDIA GPUs.

3 THE eDSL APPROACH IN PRACTICE

3.1 *Application in the ParFlow model*

ParFlow is a three-dimensional finite difference physical groundwater model written in C/C++. The submodule CLM (Common Land Model) that is coupled with ParFlow is based on the Fortran programming language [6, 7, 8]. After decades of development of ParFlow, which originally supported only the Multiple Processing Interface (MPI), ParFlow now supports utilization of GPUs via the eDSL approach[9, 10].

The details of applying the eDSL approach to ParFlow are outlined by Piotrowski et al. [10]. The key points of the eDSL approach for ParFlow can be summarized as follows:

- enable use of the Kokkos library to write portable applications with high performance
- use Kokkos as the backend and a macro layer of boxloop macros for the stencils for advection computation
- refactoring of the ParFlow code to use the stencils

The code should recognize the use of the GPU device but Parflow adapts Kokkos to recognize GPU device for code and data management. ParFlow now only supports NVIDIA GPUs and thus CUDA and OpenMP are supported. So ParFlow started out working with CUDA and therefore use Kokkos as memory management backend when porting to GPU. To manage the memory allocation and data transfers from/to CPU and GPU, Kokkos, the low level library for performance portable applications, is used as a backend.

The code has large parts with loops applying the finite differencing method. And therefore a number of backends is used to do the loops with the stencil codes. This can reduce the complexity of the codes and provide a redundancy for writing the codes. The device-dependent codes (e.g. allocating the memory or defines for the different language) can be handled outside the main codes within these backend codes.

Looking at the code, out of more than 200 source file in `parflow_lib`, only six source files take care of interfacing with the CUDA library (like `solver.c` or `vector.c`), and thus, the domain science developers can indeed focus on the scientific aspects. The computational loops and related backends are developed in backend files (e.g. `pf_cudaloops.c` and `pf_omploops.c`), and the architecture of the loops can be selected by the backend files `backend_mapping.c`). Therefore, the domain scientific work can continue with very few exchange steps through the computational structure or methods.

However, Kokkos mainly supports C/C++ codes, which is relatively easier to implement as a general backend for ParFlow, in contrast to Fortran-based Earth system model codes. For ICON, the implementation of an eDSL approach would be more likely to follow the approach of the EULAG model.

3.2 *Application in the EULAG model*

EULAG [11, 12, 13] is a dynamical core for convective-scale numerical weather prediction written in Fortran. The EULAG dynamical core is implemented in the Consortium for Small-Scale Modeling (COSMO) model for regional climate modelling.

In EULAG, the backend only supports the use of CUDA for offloading to the GPU devices (i.e. NVIDIA hardware), and thus the model codes are utilizing the CUDA macro for the eDSL approach. The EULAG eDSL first predefines the macros for the compute loops and memory management within a customized interface layer, and then the domain science code is modified to use the loop stencils defined in the interface layer.

It is important to note that not only the loops in the algorithms need to be modified, but also the data structure need to be mapped with CUDA macros (`MANAGED` or `DEVICE`) in the main source code to achieve a sufficient level of abstraction.

However, due to the nature of Fortran codes, the loop stencil can only be written in a "one-line code" style, which means that the loop body (i.e. the parameterization or calculation of the physics) should be done without an operator, that is, the code needs to be written without being broken by conditional statements or logical blocks (e.g. if-statements). The conditional statements can only exist outside the loops, not inside.

4 Evaluation of the eDSL approach for ICON

The eDSL approach, especially for the loop stencils, is considered as a practical method for performance portability of ICON [4]. The embedded kernels and stencils for looping can be used to tackle the large redundancy in the code. We found two main loops used in the advection kernel to implement the stencil. The ICON model uses the finite volume method, so the body of the loop is generally not as complex as for the finite differencing method, i.e. as for ParFlow and EULAG. In ICON, the loops of cells and edges are a good place to start, which is shown in the codes of Codebox 3 as an example for edge looping.

Pseudo codes 3: ICON loop stemcil for edge looping

```
DO jb = i_startblk, i_endblk
  CALL get_indices_e__adv(p_patch, ... ){
  #ifdef __LOOP_EXCHANGE
    DO je = i_startidx, i_endidx
      DO jk = slev, elev
  #else
    DO jk = slev, elev
      DO je = i_startidx, i_endidx
  #endif
        loop_body
      END DO
    END DO
END DO
}
\label{code:icon_adv_edge|
```

However, the only existing ICON granule with GPU support that was available for testing the approach was based on the microphysics of graupel. This code relies heavily on conditional statements, so the structure of the code will need to be modified first to use the eDSL approach for Fortran. Therefore, the second best candidate for testing the eDSL approach would be the advection scheme, which was not implemented with GPU support at the time of this assessment. Further work should focus on implementing the eDSL approach for the advection kernel of ICON.

Also, the backend for ICON needs to be decided upon with the main developers of the model. The current ICON GPU support is based on OpenACC and OpenMP. Therefore, a new eDSL implementation should focus on using the existing software architecture instead of creating a new customized layer for eDSL support with different backends.

The manpower and development time for implementing the eDSL approach should also be considered. At least one year of development time was required to implement the eDSL approach into other codes [9, 10]. The development of more advanced DSL approaches for ICON took multiple years [4]. Therefore, even with support from experienced developers of ICON, the implementation of an eDSL approach is too demanding within the given time constraints.

5 Summary and conclusions

The DSL approach is considered a rescue for effectively exploiting modern HPC architectures as GPU computation is becoming mainstream. Large geoscience-related codes are composed of millions of lines of codes and thus a portable performance of GPU support implementation is required for the codes.

The ICON model contains on the order of one million of lines of code. In order to further develop and improve ICON for future applications, it would be highly beneficial to overcome the challenge of applying it to new hardware or software environments.It would be advantageous to use different compilers or different GPU hardware and to avoid paradigm programming by using stencil codes or a so-called macro layer to include the choice of different compilers without increasing the complexity of the codes.

While GPU porting may be more feasible using the eDSL approach for the C/C++ language [14], the codes (especially legacy codes) written in Fortran are less supported when using hardware from other vendors than NVIDIA, e.g. GPUs from AMD. Therefore, it is important to carefully plan and decide the approach for porting codes to GPUs. A wrong coding direction will cost time and manpower with few applicable results.

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