The Paraldor Project
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Paraldor is an experiment in bringing the power of categorical languages to lattice QCD computations. Our target language is Aldor, which allows the capture of the mathematical structure of physics directly in the structure of the code using the concepts of categories, domains and their inter-relationships in a way which is not otherwise possible with current popular languages such as Fortran, C, C++ or Java. By writing high level physics code portably in Aldor, and implementing switchable machine dependent high performance back-ends in C or assembler, we gain all the power of categorical languages such as modularity, portability, readability and efficiency.

1. INTRODUCTION

The main goal of the Paraldor project is to investigate to what extent we can use a high level categorical language like Aldor[1] to write programs for large scale numerical simulations, and in particular for lattice QCD, on massively parallel computers. The design constraints are that we want a code that is portable over many different architectures e.g., SMP, MPP, Cluster, Workstations, Vector, Short Vector etc. At the same time we also want efficiency on all architectures, meaning the code has to interface with assembler kernels and their data layouts. We do not wish to rely on the compiler to make clever optimizations, but merely to perform simple transformations such as inlining. We want modular code where we have abstracted away both the machine layout and the mathematical structure from the code so we know only the structure relevant for a particular algorithm. This should lead to reusability since by partitioning the problem effectively we leave clear top level code which can easily be changed without knowledge of, or alteration of low level code.

2. ALDOR STRUCTURE

The structure of Aldor is based on categories and domains. Categories contain signatures expressing only the necessary structure of the category. Domains are particular instances of a category. They implement the signatures of the category with perhaps some extra structure, however the only common structure required by different domains is that of the category. It is important to notice the difference between this model and the analogous model of base classes and derived classes in C++. This is perhaps most clearly illustrated by the relationships “domain ∈ category whereas class ⊂ base class”. Interfaces in Java use the same model as base classes, and so don’t gain anything over the C++ mechanism.

With the Aldor structure we can write physics code purely in terms of categories and their signatures. By doing this we ensure that the code can be used with any domain implementing the category. This means we can use our code on different machines or choose a different algorithm for a particular sub-task without any real change to the code. We can also build categories with more structure from a tower of simpler ones. Algorithms can then be written purely in terms of the minimum categorical structure they need.

3. COMPARISON

It is perhaps necessary at this point to justify why this approach would be useful when there are many other more popular languages in use. What deficiencies are we trying to address and what advantages are we looking to gain?

Until recently the standard practice was to write large codes in C or Fortran. For partic-
ularly time critical operations assembler kernels were added to optimize routines. This of course has the problem that we cannot write completely modular code. The codes must rely on too much global data making them very hard to maintain, and the assembler routines are completely architecture dependent. To write generic routines we must use macros/templates which have the disadvantages of lacking type safety and usually having poor error reporting.

When looking at object-oriented languages the obvious benchmarks for comparison are C++ and Java. What does Aldor have to offer over these languages?

Firstly the idea of categories has advantages over inheritance. In particular C++ cannot distinguish between things with the same structure. An example of this would be if we had classes SU(2) and SU(3) which were derived from a base class “group”. Since in C++ these would be seen as subsets of the base class with some extra structure, the binary operation defined in “group” would still be valid, so we could form nonsensical products like $x\times y$ where $x \in SU(2)$ and $y \in SU(3)$. This is avoided in the categorical approach as all that is stored is a signature of the form “each domain D implements a product which takes two elements of D and returns an element of D”, so operations are only allowed within an individual domain. Java has the same problem, it just requires a cast to convert an argument of type in domain. Java has the same problem, it just requires a cast to convert an argument of type in-domain that is stored is a signature of the form “each do- main D implements a product which takes two elements of D and returns an element of D”, so operations are only allowed within an individual domain. Java has the same problem, it just requires a cast to convert an argument of type in-domain. Java has the same problem, it just requires a cast to convert an argument of type in-domain that is stored is a signature of the form “each domain D implements a product which takes two elements of D and returns an element of D”, so operations are only allowed within an individual domain. Java has the same problem, it just requires a cast to convert an argument of type in-domain. Java has the same problem, it just requires a cast to convert an argument of type in-domain.

Aldor is a very strongly typed language. It allows operator overloading which is forbidden in Java. It has parameterized types and allows overloading on return types, neither of which are permitted in Java or C++. These features allow us to write generic code once for all types that are being used with the types being checked at compile time. The alternative in say C++ is to either write separate routines for different types, or to write the routines as macros/templates which again have the disadvantages of no compile time type checking and are hard to debug.

4. PERFORMANCE

We set up a toy model to test the performance of the code in comparison to a baseline C code. Consider inverting an $N \times N$ Hermitian positive definite matrix by the Conjugate Gradients (CG) algorithm. We have implemented the CG algorithm in C, and have implemented several Aldor variations of the algorithm for comparison. All the Aldor variations share the same categorical structure (see Figure 1), only the back end domains, which implement matrix-vector and vector-vector operations differ.

Figure 1. Aldor Categorical CG code

We will denote the various code versions as follows:

C – Our baseline C Code
A1 – Aldor Categories, Aldor Back End, Aldor Garbage Collection (GC)
A2 – Aldor Categories, Aldor Back End, Manual Memory Management
Our results are shown in Figure 2, where we plot the ratio of the test run time to the baseline C code runtime for a problem of the same size. The results from the C code are also plotted.

The Aldor back end test results (A1, A2 - top graph) appear to be over 100 times slower than baseline code and the Aldor mark and sweep garbage collector is clearly not effective and leads to thrashing. The C Back End Test Results (A3, A4 - bottom graph) are seen to be of the same order of magnitude as C Code (until thrashing for A3). For A4 the ratio of timings is tending towards 1 with increasing problem size. A3 starts to thrash due to memory leak, as the Aldor garbage collector cannot see memory allocated by the C routines.

From these results a few things become immediately obvious. Firstly using C-back-ends and memory management, Aldor code performs nearly as fast as the corresponding C code. Also the overhead decreases with problem size (and should already be negligible for lattice of $V = 2^4$ sites where the fermion matrix has dimension $N = 2^4 \times 4 \times 3 = 192$). This demonstrates that the complexity of categories etc, is quite successfully optimised away by the Aldor compiler and that one can write efficient code using Aldor. It is also clear that memory management is an important issue. We need ways to manage memory better than the compiler currently does either by using other garbage collection schemes or by performing some kind of manual memory management.

5. MEMORY MANAGEMENT

A by-product of writing code in a totally modular way, as was apparent in the performance results, is that the memory management becomes highly non-trivial. One major problem that arises is that individual program elements which interact may have no way of knowing when data is no longer required and hence that memory can be freed. This forces us to have a more automated memory management scheme. We also have different types of data to handle. To maintain efficiency we must have a modular memory management system as well. This leads to the idea of memory spaces.

With memory spaces we store different types of data in different areas of memory, each with its own memory management scheme. For large objects (such as an entire pseudofermion field) a reference counting method may be preferred as it will free these objects as soon as they go out of scope with only a small relative overhead in terms of storage and keeping the reference count. For smaller objects such as closures it is not as critical that they are cleaned up immediately and so a mark and sweep process is preferable.

6. SUMMARY & FUTURE WORK

By writing top level physics code in Aldor and implementing switchable machine dependent back ends in C we have shown in principle that we can write portable, modular, readable and reusable code without sacrificing efficiency. The next step is to categorise Krylov space methods to implement a wide variety of efficient inverters and
eigenvalue solvers. We also have to begin building the physical objects such as gauge fields and to categorise Monte Carlo algorithms and other relevant structures with a long term view of a full QCD code.

7. ACKNOWLEDGEMENTS

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REFERENCES

1. www.aldor.org