Domain Specific Language for high performance computing

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Abstract

1 Introduction

1.1 Background

In astrophysics and astronomy, to numerically calculate the dynamical evolution of N particles interacting gravitationally, N-body simulations are required. Figure 1 shows the equation for interparticle interactions in N-body simulations. If the equation is naively computed, the time complexity of calculation of interparticle interactions is $O(N^2)$, where N is the number of particles. Therefore, parallelization is required to speed up numerical simulations. To write a parallelized code for a numerical simulation, a user needs to understand the architecture of computer systems in detail. If a parallelized code is automatically generated by only describing the formulas and data of the numerical simulation, the above problems are solved. To realize the parallelization, we will develop Domain Specific Language DSL), which is a programming language specialized to a domain, for example, SQL and HTML.

1.2 parallelization

SIMD is one of the categories in Flynn's taxonomy 1, related to computer arithmetic processing. Using SIMD, arithmetic operations can be applied simultaneously to multiple data. In this paper, we compute and parallelize multiple particles. For example, as shown in Figure 1, the computation of acceleration for different particles is independent of each other, allowing the process to be parallelized. As a result, for instance Assuming that the variables for particles are double-precision floating-point numbers, we can execute an operation on four elements simultaneously using the AVX2 instruction, it is possible to perform operations on four elements. Therefore, compared to non-parallelized code, there is a potential to accelerate the computation by four times. We will describe the design of a DSL in the next section to generate such parallelized code from the formulation of particle-particle interactions.

1.3 Overview of DSL

We have created a Domain Specific Language DSL)named Pyker). This language's processor can read code describing particle interaction formulas and generate code that accelerates these computations. The language allows for the definition of variables and the description of interaction formulas. In the variable definition section, it's possible to define variables such as the mass and position of particles, variables for storing results, and other necessary variables. For the formula part, we have enabled calculations including basic arithmetic operations, sqrt, power functions, and computing the norm of vectors. From this description, a kernel function is generated, which can then be called and used. We have created a Domain Specific Language DSL named Pyker. This language's processor can read code describing particle interaction formulas and generate code that accelerates these computations. The language allows for the definition of variables and the description of interaction formulas. In the variable definition section, it's possible to define variables such as the mass and position of particles, variables for storing results, and other necessary variables. For the formula part, we have enabled calculations including basic arithmetic operations, sqrt, power functions, and computing the norm of vectors. From this description, a kernel function is generated, which can then be called and used.

1.4 Aim of this paper

2 Construction

We use Sympy, a library in Python for implementing the implementation of pyker. SymPy supports various operations, and the formulas using these operations are internally treated as syntax trees. We leveraged this functionality to read formulas and generate code capable of parallel execution. For parallelization, we used an instruction set named Advanced Vector Extensions 2 (AVX2). AVX2 is one of the extended instruction sets implemented in Intel's CPUs. The next section will explain how parallelization is carried out using AVX2.

2.1 AVX2 for parallelization

To perform SIMD operations, just like with regular computations, data is first loaded from memory, computed based on that data, and the results are stored. However, in the case of SIMD, computations are performed using SIMD-specific registers, so the methods of loading, computing, and storing differ. When loading, multiple elements that will undergo the same instruction are stored in a SIMD-specific register. These are then used

to perform computations simultaneously, and the results are stored for each.

For instance, consider a calculation like C = X + Y, where elements of double-precision floating arrays x and y are computed . When using AVX2 for SIMD, since the registers are 256 bits, four elements from x and y are loaded each. These are then added simultaneously, and the results are stored in the array C. When loading into SIMD registers, if it's a 1-dimensional array, contiguous memory access is sufficient, but for data structures like Array of Structures (AoS)shown in Figure a., elements need to be loaded individually.

For example, when considering the 3-dimensional coordinates of particles as double-precision floats in pos[n][3](where n is the total number of particles, and pos[i][0], pos[i][1], pos[i][2]represent the x, y, z coordinates of the i-th particle, respectively), and calculating the difference in x coordinates between particles i and j, it becomes dx = pos[i][0]- pos[j][0]. However, for parallelization with SIMD, desiring dx0 = pos[i][0]- pos[j][0], dx1 = pos[i+1][0]- pos[j][0], dx2 = pos[i+2][0]- pos[j][0], dx3 = pos[i+3][0]- pos[j][0], the data are packed as (pos[i][0], pos[i+1][0], pos[i+2][0], pos[i+3][0]), (pos[j][0], pos[j][0], pos[j][0], pos[j][0), (dx0, dx1, dx2, dx3)and subtraction is performed simultaneously. However, since data needs to be loaded onto SIMD registers all at once, the gather instruction is used to load data for particle i. The gather instruction is used to read non-contiguous data elements from memory addresses by specifying addresses. An explanation of the gather instruction is shown in Figure x. Data loaded in this way are computed simultaneously using SIMD instructions.

```
dx0 = pos[i][0] - pos[j][0]
dx1 = pos[i + 1][0] - pos[j][0]
dx2 = pos[i + 2][0] - pos[j][0]
dx3 = pos[i + 3][0] - pos[j][0]
```

```
(x1, x2, x3, x4) + (y1, y2, y3, y)
```

When storing computation results, addresses may not be contiguous. In such cases, there is an instruction called scatter, which is the counterpart to gather, but it is not supported in AVX2, so data are stored using pointers individually. In this way, parallelization is achieved with SIMD. Moreover, these instructions can be explicitly handled in high-level programming languages like C and C++ using intrinsic functions. To handle intrinsic functions in C and C++, include the file immintrin.h, which is available as a standard in the language. An example of C++ code that calculates the difference in x coordinates, simd_tmp.cpp, is shown. Pyker generates C++ code capable of executing SIMD instructions like simd_tmp.cpp from the described formulas. The next section will explain the Pyker.

2.2 Pyker

In this DSL, code is generated by writing and compiling two definitions: the definition of variables and the definition of interaction formulas. First, let us explain the variable definition.

In this DSL, variables are classified into classes: EPI, EPJ, FORCE, and others. EPI represents particles that receive interactions, while EPJ represents particles that provide interactions. FORCE holds the results of the interaction calculations, and other variables include softening parameters and the like. To perform calculations using these variables, in C++, it would be similar to 2.

Listing 1: skeleton code

```
int kernel(double xi[][3], double xj
    [][3], double ai[][3], double eps2
    , int n){
  // (1).preprocess
  for(int i = 0;i < n;i += 4) { //
      (2)Increment the number of
      parallels
    // (3).load EPI
    // (4).Initialization of tmporary
        force
    for(int j = 0;j < n;j += 1) {
        // (5) load EPJ
        // (6) calculate interparticle
            interactions
    }
    // (7). Store calculation result in
        the FORCE
  }
}
```

(1) involves preparatory steps such as defining variables necessary for the calculation. (2) involves loading the variables of EPI. (3) is about initializing variables that temporarily hold the results of the interaction calculation. (4) involves performing the interaction calculation and saving the results in the primary variable of force. (5) involves storing the results in the FORCE variables. To generate this code, in variable definition, information about the class of the variable, its type, and its dimension is necessary. Therefore, in pyker, variable definitions are written as follows. . The first column, if it is a class, writes the name of the class and its member variable name. The second column explicitly writes the dimensions of the vector if there are any, specifying 3 or 4 dimensions, and the type is either 32-bit or 64-bit floating-point. The third column becomes the name of the variable handled on pykg. For example, "EPI.pos vec3<F64> xi" would be a member variable of EPI named pos, a 3-dimensional 64-bit floating-point variable named xi. The definition of interaction formu-

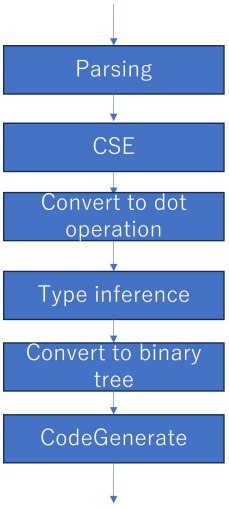
las is written to accumulate the results in the FORCE variable using the defined variables. Primary variables necessary for the mathematical description can be newly defined using previously defined variables. Available operations include basic arithmetic, sqrt, and the power symbol "**". The result is stored in the FORCE variable using '='.For instance, to generate code that c alculates the gravitational interaction formula shown in Figure 1, it would be written in this DSL as figure1.pyker.

Listing 2: hoge

```
EPI.pos vec3<F64> xi
EPJ.pos vec3<F64> xj
EPJ.m F64 mass
FORCE.acc vec3<F64> ai
F64 eps2
F64 g
dr = xj - xi
ai = g * mass * dr / sqrt(dr ** 2 +
    eps2) ** 3
```

2.3 Implementation

The process of generating code is illustrated in the following flowchart. In Parsing, the information of the variables defined in the DSL code is converted into a hash with the variable names as keys. Formulas are converted into syntax trees using the sympify() method of Sympy, and a list of these trees is obtained. Next, Common Subexpression Elimination (CSE) is performed on the syntax trees of the converted formulas. CSE is the process of reducing the number of operations by pre-calculating common subexpressions in formulas and using their results in subsequent calculations. In type inference, the types of the primary variables in the formulas are inferred. Afterward, all syntax trees are converted into binary trees to align them with SIMD operations. Finally, the code for calculating interactions is generated by traversing the processed syntax trees. The following sections describe how the implementation was carried out in the order of Parsing, CSE, type inference, conversion to binary trees, and Code generation.



2.3.1 Parsing

In Parsing, the process is divided between variable definition and formula handling. In variable definition, objects with class, vector, type, and variable name are created respectively. A hash with the variable name as the key is then made (name_variable_map). Formulas use the sympify() method from the Sympy library to convert the code read as a string into a syntax tree of formulas, obtaining a list of these syntax trees (expr_list). Next, Common Subexpression Elimination (CSE) is performed.

2.3.2 CSE

2.3.3 type inference

2.3.4 convert to binary trees

2.3.5 code generatation of non SIMD

Listing 3: hoge

```

#include<math>
int kernel( (1) double xi[][3], double
     xj[][3], double eps2, double ai
    [][3], ...) {
  //(2)
  int i;
  int j;
  double dr_v0;
  double dr_v1;
  double dr_v2;
  // ...
  // ...
  // ...

  for(i = 0;i < n;i += 1) {
    for(j = 0;j < n;j += 1) {
      //(3)
      dr_v0 = -xi[i][0] + xj[j][0];
      dr_v1 = -xi[i][1] + xj[j][1];
      dr_v2 = -xi[i][2] + xj[j][2];
```

```
      // ...
      // ...
      // ...
    }
  }
}
```

2.3.6 code generatation of SIMD

Listing 4: hoge

```
//(1) include part
#include<math>
#include<immintrin.h>
int kernel( (2) double xi[][3], double
     xj[][3], double eps2, double ai
    [][3], ...) {
  //(3) decleare tmp variable
  int i;
  int j;
  __m256d xi_tmp_v0;
  __m256d xi_tmp_v1;
  __m256d xi_tmp_v2;
  __m256d eps2_tmp;
  // ...
  // ...
  // ...
  //(4) def not class variables
  eps2_tmp = _mm256_set1_pd(eps2);
  // ...
  // ...
  // ...

  // (5) loop increment
  for(i = 0;i < n;i += 4) {
    // (6) Load EPI variable part
    int index_gather_0[4] = {0, 3, 6,
        9};
    __m128i vindex_gather_0 =
        _mm_load_si128((const __m128i*)
        index_gather_0);
    // ...
    // ...
    // ...

    // (7) initialize result temporary
        variable
    ai_tmp_v0 = _mm256_set1_pd(0.0);
    ai_tmp_v1 = _mm256_set1_pd(0.0);
    ai_tmp_v2 = _mm256_set1_pd(0.0);


    for(j = 0;j < n;j += 1) {
      // (8) Load EPJ variable part
        xj_tmp_v0 = _mm256_set1_pd(xj[j
            ][0]);
        xj_tmp_v1 = _mm256_set1_pd(xj[j
            ][1]);
        xj_tmp_v2 = _mm256_set1_pd(xj[j
            ][2]);
       // ...
       // ...
       // ...

      // (9) calculate interparticle
        dr_tmp_v0 = _mm256_sub_pd(
            xj_tmp_v0, xi_tmp_v0);
        dr_tmp_v1 = _mm256_sub_pd(
            xj_tmp_v1, xi_tmp_v1);
        dr_tmp_v2 = _mm256_sub_pd(
            xj_tmp_v2, xi_tmp_v2);
        ai_tmp_v0 += _mm256_div_pd(
            _mm256_mul_pd(//.....));
        ai_tmp_v1 += _mm256_div_pd(
            _mm256_mul_pd(//.....));
        ai_tmp_v2 += _mm256_div_pd(
            _mm256_mul_pd(//.....));

    }

    // (10) Store result part

  }
  return 0;
}
```

3 Experiments

4 Conclusion

5 Acknowledgement