HiPro-CodeGen
Automatic Programming for Parallel Numerical Simulations

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Abstract: HiPro-CodeGen is a code generation engine designed for numerical simulation development. Its central objective is to produce a parallel software framework with standard structure for an application developed on JASMIN, a domain-specific computational framework. The unique parallel part and all interfaces of the application are generated and implementation of sequential subroutines is the only part of the code left to be written manually for a programmer. The design and implementation of the code generation engine is introduced which combines numerical mathematics with component-based programming to create ontological models for parallel simulations. A hybrid programming method is proposed on the work mechanism of the engine which combines graphical and textual approaches to hide parallel programming and object-oriented programming from developers. A real application is presented to show the effectiveness and efficiency of the engine.

1 INTRODUCTION

Numerical simulation is an important method to explore the evolution of physical systems by scientists in current age (Mo, Pei, 2009). With the development of high performance computing, simulation is leading to high accuracy and high confidence in scientific study. Developing a scientific simulation covers implementing scientific methodology, algorithms, and programming models, and virtually always each advance has been accompanied by increases in the complexity of the underlying software. At the same time, the computer industry has continued to create ever larger and more complex hardware in an attempt to satisfy the increasing demand for simulation capabilities (Benjamin, 2006). These architectures tend to exacerbate the complexity of software running on these systems. Modern programmers may repeatedly rewrite applications to expose incrementally more parallelism for each next generation of hardware. It requests a programmer be knowledgeably aware of new software and hardware. Admittedly, this is a demanding task for current programmers most of which are engaged in researching on physics and mathematics, because they have been trained in sequential programming. We are facing a fact that difficulties on parallel programming embarrass the development of high performance numerical simulations.

To ease the coding issues many studies on graphical programming and automated code generation techniques have been given on developing parallel applications. Boris etc. develop an integrated development environment for visual parallel programming (Boris, 2006). It is not effective to develop complicated numerical simulations because of limitation on graphical operations. MatLab also gives some parallelism capabilities with parallel computing toolbox while the scalability and the performance of the program are limited by its parallel computing mechanism.

Experience says that programming in graphic form completely is embarrassed on solving the problems especially developing numerical simulations because of the complexities of simulations and the limitations of the graphical programming technology. Liao etc. propose a hybrid programming approach which combines graphical and textual programming to solve the problem by shielding parallel programming details and object-oriented programming languages for developing scientific applications based on JASMIN.

In this paper we present the design and implementation of the code generation engine which supply the automatic programming capabilities given in HiPro (Liao,2013), originally named with IDE-JASMIN. The content of this paper is organized as follows. Section 2 analysis the features of parallel programs developed on JASMIN. In section 3, the design of the code generation engine which utilizing the features to create topological model is presented in detail. In section 4, we show the advantages of using HiPro-CodeGen to develop a computational fluid dynamic parallel numerical simulation program in the system. Then we present our conclusion and point to directions for future work.

2 FEATURE MODEL OF A PARALLEL NUMERICAL SIMULATIONS

JASMIN abstracts a general framework from numerical simulation domain and provides large granularity software reuse in scientific high-performance computing (Mo, 2010). The framework tends to isolate the increased complexity of the software and operating environment from the programmers and utilize state of art technologies to extract the maximum possible performance. It facilitates problem solving with encapsulation of parallel computing and communication through patch-based data structures and component-based mechanism which shield data decomposition and communication from the users. Generally numerical simulations share many common features. These are utilized in JASMIN to provide a more normative architecture for developing a parallel program. We define a feature model to illustrate a numerical simulation developed based on JASMIN. It is used to direct the design of the hybrid graphical programming interface. The model includes five parts which are described in the following subsections.

Before we introduce the model, to describe the construction features of a numerical simulation, we give some key concepts:

- *Level strategy class:* strategy class which is responsible for dealing with the computation on global region. Programmers must implement some strategy procedures which are implicitly called by JASMIN.
- *Patch strategy class:* strategy class specially serves for an integrator component. It is responsible for dealing with the computation on a patch domain which is part of the global region. Programmers must implement some strategy procedures which are implicitly called by JASMIN.
- *Integrator component:* a parallel computation mode defined in JASMIN. It is invoked in a level strategy class and implicitly calls procedures defined in its registered patch strategy class.
- *Numerical kernel:* A kind of subroutine to implement part of numerical computational method. It is a sequential program.

2.1 Data Structure and Numerical Algorithm

Generally numerical simulation is solving a system of PDEs or ODEs with numerical methods on a discrete grid. JASMIN supports development of structured grid application of two types including rectilinear and deforming grid (Mo, 2009). Figure 1 shows the two-dimensional example grids often-used in numerical simulations. Data parallelism is the main form of parallelization of computing. In the kind of parallelism, as is showed in Figure 2, the region is decomposed into many domains during the process of the computation. Each domain is extended with ghost zones to satisfy the need of numerical scheme. In JASMIN, three kinds of coordinate system are available: Cartesian, cylindrical and spherical coordinates. Grid type and coordinate system determine the mesh description mode in a program.

A physical variable, which also named with field variable, is defined on the special position of the

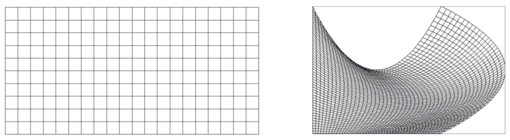


Figure 1: Rectilinear and deforming grid used in structured appliations.

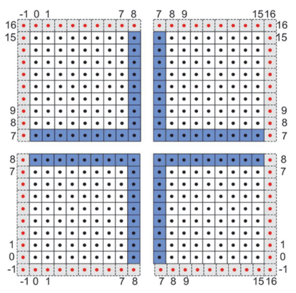


Figure 2: Domain decomposition for data parallelism.

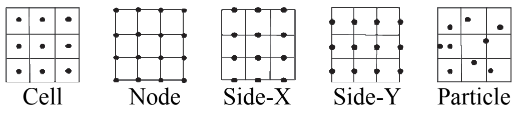


Figure 3: Discretization types of variables in a numerical simulation.

discretization grid, such as cell, node, side or face etc., as illustrated in Figure 3.

The numerical algorithm usually involves time iterations with given initial conditions, i.e. time integration algorithm. A complex algorithm is broken down into smaller and manageable parts. These parts are arranged to be executed adhering to some rules. Figure 4 shows the flowchart of a general time integration algorithm. Generally the algorithm involves four key modules which are organized in a loop and the user provides parameters to control the stop of it. All modules should be implemented according to the concrete computation.

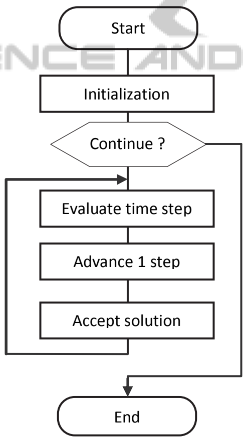


Figure 4: A general flowchart presenting time integration algorithm.

Generally developers are used to programming numerical subprograms in Fortran, which is a conventional textual, linear programming language that is familiar to programmers who engaged in the sequential numerical simulation development. Component architecture have been used for high performance scientific computing for years(Parker, 2002). Parallel integrator components are proposed to encapsulate parallel computing details on patch-based data structure (Mo, 2009). Parallelism is obtained by creating integrator components to encapsulate sequential numerical subroutines. Components encapsulate much of the complexity of parallelism inside a black box such as invoking MPI or OpenMP interfaces and utilizing multi or many-cores CPU in modern machines. We support user to implement his computational method in sequential numerical subroutines while parallelism is accomplished in integrator components. The separation makes hybrid programming of combining graphical and textual programming feasible.

2.2 Application Architecture and Program Organization

Domain experts develop parallel numerical applications by assembling configured parallel integrator components in a flowchart of time integrator algorithm. For each component carrying on computation task a patch strategy must be implemented and the object of it be registered to the component. Some virtual interfaces must be implemented in C++ language and in which, data of field variables is fetched via patch object and passed to a numerical kernel invoked. Therefore parallelism for a computational module is achieved by connecting the component with real numerical kernels. These components provide interfaces or ports to be invoked in level strategy. As is shown in figure 5, the application architecture model includes:

- Main program
- A level strategy class which deals with assembling components.
- Patch strategy classes. For each component some specific procedures must be implemented in a patch strategy class to invoke sequential numerical subroutines to accomplish numerical computation. The number of the patch strategy classes is determined by the number of the components created.
- Sequential numerical subroutines

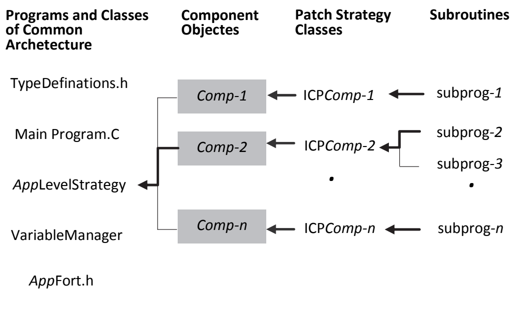


Figure 5: Architecture of an application and invoking model.

3 DESIGN OF HiPro-CodeGen

To develop a parallel program of numerical simulation the user must write program to:

- Define variables.
- Code sequential computation kernels.
- Create parallel integrator components.
- Assemble components in the time integration algorithm to construct a parallel program.
- Deal with physical model described in an input file.
- Output physical variables for visual analysis.
- Create a main procedure to organize issues listed above.

HiPro is designed to offer graphical programming capability to develop parallel numerical simulations. The system implements a graphical domain-specific programming language combined with textual editor to support parallel programming. The idea of parallel design combined with sequential coding is achieved in the visual programming environment.

According to the application model described in section 2, the programming task is classified into two types: configured on GUI and processed automatically. Upon this we shield most of them as best as we can in the programming system. Therefore to construct a numerical simulation program only the first four things of those which are mentioned at the beginning of this section left to the programmer to deal with. The other issues are handled automatically. This mechanism releases the user from complex programming. HiPro-CodeGen is the core of HiPro system which is responsible for generating codes. Next we introduce the working mechanism in HiPro-CodeGen according to the four tasks separately.

3.1 Define Variables

Variables in a scientific numerical simulation are classified into three categories according to their functionality and source, they are: grid variables, physical variables and grid independent ones. The classification is used to standardize interface definition for a procedure and build type match filtering when the procedure is called. Three variable databases are created to store the variables. They are physical variable DB, general variable DB and input parameter DB.

A grid variable gives the definition of a domain. As noticed, no database is created for grid variables. In fact, grid ones are created automatically. There are two build-in grid variables in the system. One is used to describe the patch domain and the other is used to give the information of ghost zones. This is vitally important for the system design because we use them to normalize the interface definition of numerical subroutines.

The type definition of rectilinear grid variable for a patch domain in C and C++ is

```
Typedef struct {
     int ilo[NDIM];
    int ihi[NDIM];
    double xlo[NDIM];
    double dx[NDIM];
} geom_t
```

The definition of that for deforming grid is similar with it which only needs the first two parameters. Comparative definition of them in Fortran shares the same form using derived types. We leave it out here for simplicity. The type definition for ghosts is

```
 Typedef struct {
    int ilo[NDIM];
    int ihi[NDIM];
    int btype;
    int location;
    int condition;
} ghost_t
```

For physical variables, we give a set of domain-specific data types listed in Table 1.

- *Domain-specific data type:* a kind of data type used for describing the discretization form of a physical variable specially defined in a numerical simulation.

Table 1: Domain-specific data types.

Type	Properties
Cell	Element type, Depth, Ghost width
Node	Element type, Depth, Ghost width
Side-X	Element type, Depth, Ghost width
Side-Y	Element type, Depth, Ghost width
Group Cell	Element type, Depth, Ghost width, Number of groups
Group Node	Element type, Depth, Ghost width, Number of groups

Table 2: Supplementary data type.

Type	Properties
Generic	Element type, Depth

To describe the general variables we supplement the type list with a special one, as is shown in the Table 2. Upon this we extend data types to cover all variables in JASMIN. These extensions are necessary to support full application development in scientific and engineering computing.

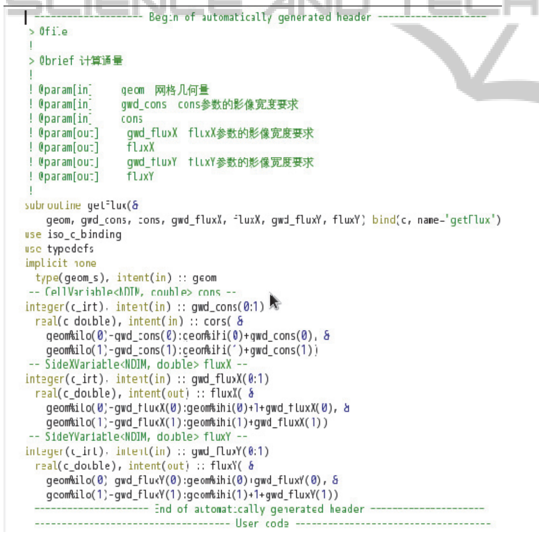
Programmer defines a variable through graphical user interfaces interactively while the system will invisibly generates the corresponding source code of it. For instance, the code of a physical variable of Cell type for a two dimensional application is given as below:

```
integer :: gw_varName(0:1)
ElementType [,IntentType]:: varName
 (geom%ilo(0)-gw_varName(0)  :
geom%ihi(0)+gw_varName(0),
geom%ilo(1)-gw_varName(1)   :
geom%ihi(1)+gw_varName(1))
```

3.2 Program Sequential Numerical Subroutines

In the system numerical subroutines are classified into three categories:

- (Sub I) Execute computation on a domain.
- (Sub II) Fill physical boundary.
- (Sub III) Process grid independent variables



```
! ------------------- Begin of automatically generated header -------------------
! > @file
!
! > @brief 计算通量
!
! @param[in]    geom  网格几何量
! @param[in]    gwd_cons  cons参数的影像宽度要求
! @param[in]    cons
! @param[out]    gwd_fluxX  fluxX参数的影像宽度要求
! @param[out]    fluxX
! @param[out]    gwd_fluxY  fluxY参数的影像宽度要求
! @param[out]    fluxY
!
subroutine getFlux(&
    geom, gwd_cons, cons, gwd_fluxX, fluxX, gwd_fluxY, fluxY) bind(c, name='getFlux')
use iso_c_binding
use typedefs
implicit none
  type(geom_s), intent(in) :: geom
 -- CellVariable<NDIM, double> cons --
integer(c_int), intent(in) :: gwd_cons(0:1)
  real(c_double), intent(in) :: cons( &
    geom%ilo(0)-gwd_cons(0):geom%ihi(0)+gwd_cons(0), &
    geom%ilo(1)-gwd_cons(1):geom%ihi(1)+gwd_cons(1))
 -- SideXVariable<NDIM, double> fluxX --
integer(c_int), intent(in) :: gwd_fluxX(0:1)
  real(c_double), intent(out) :: fluxX( &
    geom%ilo(0)-gwd_fluxX(0):geom%ihi(0)+1+gwd_fluxX(0), &
    geom%ilo(1)-gwd_fluxX(1):geom%ihi(1)+gwd_fluxX(1))
 -- SideYVariable<NDIM, double> fluxY --
integer(c_int), intent(in) :: gwd_fluxY(0:1)
  real(c_double), intent(out) :: fluxY( &
    geom%ilo(0)-gwd_fluxY(0):geom%ihi(0)+gwd_fluxY(0), &
    geom%ilo(1)-gwd_fluxY(1):geom%ihi(1)+1+gwd_fluxY(1))
  -------------------- End of automatically generated header --------------------
  ---------------------------------- User code ----------------------------------
```

Figure 6: Generated code for a numerical kernel interface in Fortran 90.

Requirements of dummy parameters are different according to the classification. For example, no dummy parameter of physical variable type is permitted in the third category. A parameter of *geom_t* is absolutely necessary in the first and second category and *ghost_t* is mandatory in the second one. There must be one and only one parameter of such type. The classification is used to build interface requirement match for integrator component definition.

We use Fortran 2003 as the programming language for coding numerical subroutines. The code of interface definition is generated and inserted into the beginning of the program file automatically. This approach frees users from error-prone and tedious type definitions and variable declarations.

Figure 6 shows an example code generated for a subroutine. The code will be updated and replace the older one when the user modify the definition through GUI.

3.3 Create Parallel Integrator Components

A type library of component is provided in the system. Each type of components performs some kind of well defined task and has specially designed GUI. Available types of integrator components and their functional properties are listed in Table 3. The property specifies acceptable categories of subroutines and whether this kind of component needs to register patch data to accomplish memory management or data communication.

Table 3: Integrator component types and functional properties.

Type	Properties
Initialize	Sub I, RegisterPDI
Numerical	Sub I+II, RegisterPDI
Dt	Sub I, RegisterPDI
Reduce	Sub I, RegisterPDI
Memory	RegisterPDI
Copy	RegisterPDI
ParticleComm	RegisterPDI

In fact, creating and using a parallel integrator component in HiPro needs only three simple steps:

- Create a component from an appropriate component model;
- Configure necessary properties of it;
- If necessary, select a proper numerical subroutine and pass actual arguments to it.

3.4 Assembling Components in Computational Flow Charts

Main concern of writing a program is how to compose these components together to form applications. A flow chart is the graphical representation of control flow of an algorithm (Tia, 2004).

- *Predefined flowchart*: expressing the general numerical computation execution process of a time integration algorithm.

A predefined flowchart, as is shown in figure 7 representing the time integrator algorithm is used to fit the need of rapid numerical integration algorithm implementation. The main flowchart is composed of some semi-predefined flowcharts which includes *initalizeLevelData*, *getLevelDt, advanceLeve*l and *acceptTimeDependentSolution.* They are actually the member procedures of the level strategy class. A flowchart is semi-predefined means that the interface of it is built-in defined and the body of it need to be implemented by the user. In HiPro, components are inserted into the flowchart to define the implementation of the procedure. Loops, conditional branches and other control structures can be used to configure the execution logic of the components. On the right of the Figure 7, part of *advanceLevel* is illustrated, where some integrator components are created and used to organize the actual computation.

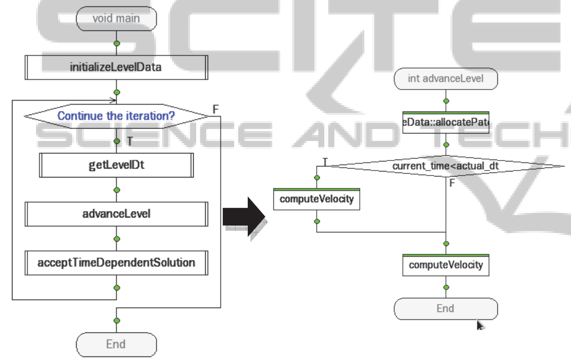


Figure 7: Assembling integrator components to implement a procedure for the level strategy class.

Flowcharts and kernels as well as other data from graphical input are stored into a database, which are then feed into code generation engine to accomplish automatic code generation using predefined code templates.

4 APPLICATION

We give a test on developing a simulation program for solving linear advection equation:

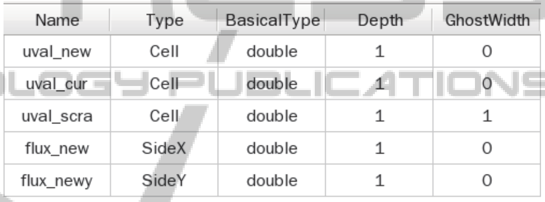
$$\frac{\partial u}{\partial t} + \nabla(a \bullet u) = 0$$

The initial value is given by $u(x,0) = u_0(x)$ and the boundary condition is set as $u(x,t) = u_\Gamma(t)$.

The computation is decoupled into six numerical subroutines. Six components are created to implement parallel computing and communication. The subroutines with category specification and components are listed in Table 4. Generally there is a one-to-one relationship between the subroutines and the components. One exception is that a subroutine of category Sub II must be assigned to a component together with a subroutine of category Sub I. The other exception is that a component of Memory type must be created to allocate or deallocate memory for physical variables.

Table 4: Subroutines and integrator components created for the simulation.

Sequential Subroutines(Category)	Component(Type)
initset(Sub I)	initComp(Initialize)
getdt(Sub I)	dtComp(Dt)
setphy(Sub II)	fluxComp(Numerical)
getflux(Sub I)	
updateconser(Sub I)	connComp(Numerical)
acceptsolution(Sub I)	updateComp(Copy)
	allocComp(Memory)



Name	Type	BasicalType	Depth	GhostWidth
uval_new	Cell	double	1	0
uval_cur	Cell	double	1	0
uval_scra	Cell	double	1	1
flux_new	SideX	double	1	0
flux_newy	SideY	double	1	0

Figure 8: Screenshot of physical variables created in HiPro for solving the linear advection equation.

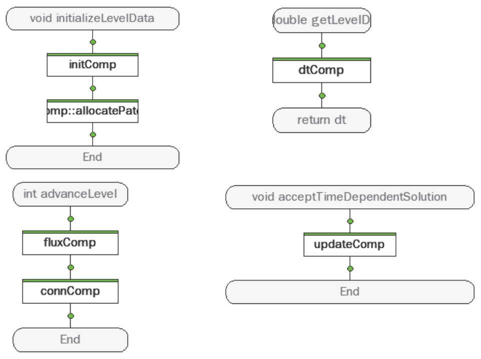


Figure 9: The four implemented semi-predefined flowcharts.

Figure 8 shows the screenshot of physical variables created in HiPro for the simulation. Four semi-predefined flowcharts with components inserted are shown in figure 9. As is presented in Table 5, in this application it consists of 17 C++ program files, 2 files coded in C language, 7 Fortran files and 1 CMake file. Among 1947 lines of source code about 6 percent of them are coded by hand.

Table 5: Program files and ratio of auto-generated for the simulation of solving linear advection equation.

Program files	Language	Lines	Ratio of auto-generated
Main.C	C++	237	100%
VariableManager.h	C++	59	100%
VariableManager.C	C++	152	100%
LinAdvLevelStrategy.h	C++	92	100%
LinAdvLevelStrategy.C	C++	99	100%
ICPInitComp.h	C++	33	100%
ICPInitComp.C	C++	58	100%
ICPDtComp.h	C++	42	100%
ICPDtComp.C	C++	90	100%
ICPFluxComp.h	C++	40	100%
ICPFluxComp.C	C++	106	100%
ICPConnComp.h	C++	40	100%
ICPConnComp.C	C++	90	100%
ICPUpdateComp.h	C++	40	100%
ICPUpdateComp.C	C++	86	100%
ICPAllocComp.h	C++	26	100%
ICPAllocComp.C	C++	35	100%
LinAdvFort.h	C	33	100%
TypeDefs.h	C	26	100%
typedef.f90	Fortran	29	100%
initset.f90	Fortran	42	50%
getdt.f90	Fortran	23	70%
setphy.f90	Fortran	59	50%
getflux.f90	Fortran	64	50%
updateconser.f90	Fortran	60	60%
acceptsolution.f90	Fortran	40	70%
CMakeLists.txt	CMake	246	100%

5 CONCLUSIONS

Parallel programming usually involves tedious amount of coding and often error-prone for domain experts. HiPro-CodeGen, a powerful automatic code generation engine, is developed to generate major and tedious part of a JASMIN application. Plenty of knowledge and technologies are shielded from the programmers, including:

- Object-oriented programming
- C++ language
- Hybrid programming with C++ and Fortran
- Component-based programming

It frees users from unnecessary exposure to complex features of programming issues of languages and JASMIN interfaces together with the application code organization. Users only need to write body code for numerical kernels with well-defined interface through GUI in Fortran which has been used for scientific computing program development for tens of years and is quite familiar to them.

Practice demonstrates that non-programmers can create fairly complex programs with little training. It greatly reduces programming complexities and make numerical application development easy and fast. Real world applications show that HiPro-CodeGen ensures high-performance and high-quality for scientific numerical simulation.

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