PROGRAPE-1: A Programmable, Multi-Purpose Computer for Many-Body Simulations

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Abstract

We have developed PROGRAPE-1 (PROgrammable GRAPE-1), a programmable multi-purpose computer for many-body simulations. The main difference between PROGRAPE-1 and "traditional" GRAPE systems is that the former uses FPGA (Field Programmable Gate Array) chips as the processing elements, while the latter rely on the hardwired pipeline processor specialized to gravitational interactions. Since the logic implemented in FPGA chips can be reconfigured, we can use PROGRAPE-1 to calculate not only gravitational interactions but also other forms of interactions such as van der Waals force, hydrodynamical interactions in SPH calculation and so on. PROGRAPE-1 comprises two Altera EPF10K100 FPGA chips, each of which contains nominally 100,000 gates. To evaluate the programmability and performance of PROGRAPE-1, we implemented a pipeline for gravitational interaction similar to that of GRAPE-3. One pipeline fitted into a single FPGA chip, which operated at 16 MHz clock. Thus, for gravitational interaction, PROGRAPE-1 provided the speed of 0.96 Gflops-equivalent. PROGRAPE will prove to be useful for wide-range of particle-based simulations in which the calculation cost of interactions other than gravity is high, such as the evaluation of SPH interactions.

1 Introduction

GRAPE ("GRAvity piPE"; [4][5]) is a special-purpose computer for the calculation of the gravity in the astronomical many-body simulations. It has hardware specialized for
the calculation of the gravity, which is the most expensive parts in the astronomical many-body simulations. Its only function is to calculate the gravitational interactions between particles. All other calculations, such as I/O, time integration and diagnostics, are handled by a general-purpose computer (the “host computer”) connected to GRAPE. This hybrid architecture has proved itself quite useful, because the special-purpose nature of GRAPE hardware made it possible to achieve very high performance with relatively low cost, while the programmability of the host computer made it possible to apply the same GRAPE hardware to wide variety of astrophysical problems, from formation of Moon [3] to the formation of galaxies using N-body approach [4] or SPH approach (e.g. [5][6]). See Makino and Taiji (1998) [2] or Hut and Makino (1999) [7] for reviews.

For simulations of pure N-body systems, GRAPE hardwares offer huge advantage both in the absolute speed and in the price-performance. However, though many astrophysical phenomena are primarily driven by gravitational force, hydrodynamics and other physics are sometimes important. A number of research groups use GRAPE hardwares mainly for combined N-body+hydrodynamical simulations of formation and evolution of galaxies or clusters of galaxies ( [8][9][10][11]). All implementations of SPH on GRAPE use it only to calculate gravitational interaction and to construct the list of neighbors for SPH interactions. Actual evaluation of SPH interaction is performed on the host computer.

Thus, in SPH calculations on GRAPE, the speed of the host computer tends to determine the total performance of the system, since the calculation cost of the SPH interaction is, though not as large as that of the gravitational interaction, much larger than the calculation cost of the rest of the simulation program such as time integration and I/O.

The calculation cost of the SPH interaction is rather high. The average number of neighbors of a particle in modern SPH programs is around 30 to 60, and calculation cost of single SPH interaction is a few times more than that of gravitational interaction (since the expression is more complex). Thus, when one uses the tree algorithm [12], the calculation cost of SPH interaction is not much smaller than that of gravity. If we perform a pure SPH simulation without collisionless particles, the gain in speed achieved by GRAPE is a factor of few at the best. In practice, in many SPH simulations relatively large number of collisionless particles are included, and for such calculations GRAPE offers a large speedup. However, when we want to perform SPH simulations without collisionless particles, the speedup would be rather limited. Accordingly, though SPH techniques have been applied to wide variety of problems, such as the dynamics of star-forming regions and hydrodynamical interaction of stars, GRAPE hardwares have not been widely used for those kind of simulations.

In principle, one could develop a special-purpose hardware similar to GRAPE to accelerate SPH interactions [13]. Such a hardware, once completed, would offer a large speedup over general-purpose computers.

However, so far the viability of such a project has remained unproven. There are several reasons why it is difficult to develop a specialized computer for SPH. First, the calculation of the SPH interaction is quite a bit more complex compared to the calculation of the gravitational interaction. With gravity, the only thing we need to implement is the force which is proportional to the inverse square of the distance. The pipelined circuit to evaluate
this interaction comprises around 15 arithmetic units (adders and multipliers) and one unit to evaluate \( f(x) = x^{-3/2} \). In concept, the hardware for SPH is equally simple. What we need is a hardware to evaluate sum of quantities weighted by the kernel function \( W(r;h) \) or its derivative. In practice, there are numerous technical details which have to be taken care of in hardware. For example, the smoothing length \( h \) is different for different particles, and the kernel \( W \) has to be symmetrized.

The second reason is that there are rather large number of varieties in SPH algorithms. Several different ways to symmetrize \( W \) are used. In addition, there are many methods to implement artificial viscosity. For some problems, some methods work fine. For some other problems, some other methods seem to be better. Moreover, there have been several new developments in the last few years. If we design a hardware for a specific SPH algorithm, the development the hardware would be significantly more difficult and time-consuming compared to the development of a GRAPE, and yet the hardware might become obsolete even before its completion.

We can avoid the risk of becoming obsolete if we can change the hardware of the pipelined processor for SPH after its completion. Changing the hardware might sound self-contradictory, since the hardware is, unlike the software, cannot be changed once it is completed. Though the name might sound strange, such “programmable” chips have been available for several decades now. These chips, usually called FPGA (Field-programmable gate array) chips, consist of small logic elements (LE) and switching matrix to connect them. A LE is typically a small lookup table made of an SRAM, combined with additional circuits such as a flip-flop and special logic for arithmetic operations. The design procedure for an FPGA is largely similar to that for traditional gate arrays; one writes the design either in the schematics or in hardware description languages such as VHDL, and then the CAD software assigns the logic to LEs and generates the connection pattern for the switching matrix. The design is loaded to the FPGA chip either from a small ROM chip or from a dedicated write port.

The size (in equivalent gate count) of FPGA chips has been enormously increased, from around 1K of mid-1980s to around 100K of 1997. Since the increase is driven essentially by the advance in the semiconductor device technology, we can expect that the increase will continue for the next several years. An FPGA chip with over one million gates will be available by 2001. Of course, one should not take these advertised numbers for its face value. Actual size of the circuit which can be implemented on a particular FPGA chip is limited by various factors, much in the same way as a program rarely runs at the theoretical peak speed of the computer used.

The size of the present (and future) FPGA chip is large enough to house fairly complex circuits. For example, the pipeline processor chip of GRAPE-3 is around 20K gates, and that of GRAPE-4 is around 100K. Thus, even if we assume rather low utilization ratio of 20%, a GRAPE-3 chip should fit into an FPGA chip with 100K gates.

Of course, to implement a GRAPE on FPGA would have little practical meaning, since GRAPE pipelines implemented on custom LSI chips of similar price to FPGAs are much faster. However, applications for which no custom hardware is available would find a GRAPE-like machine implemented using FPGA useful. Consider the case of SPH. We can
implement any variety of SPH algorithm, as far as it is expressed as interaction between particles and the necessary circuit fits in a target FPGA chip. The peak performance is not as large as what we can enjoy with custom LSI chips, but is still orders of magnitude faster than what is available on general-purpose computers of similar price.

We call the concept of using a programmable FPGA chip as the pipeline processor as PROGRAPE (PROgrammable GRAPE). It should be noted that PROGRAPE is not the first attempt to use FPGAs as the building blocks of special-purpose computers. There are a number of projects to develop custom computing machines using FPGAs as a main unit. The most influential are probably Splash-1 and Splash-2 project [15].

Projects like Splash did not select a specific application area as their target. Thus, machines developed in these projects can be regarded as “general-purpose”. In the sense, one could use them for any application. One of the unique features of PROGRAPE is that its architecture is specialized to a rather limited range of problems, namely the evaluation of the particle-particle interaction in many-body simulations. Thus, there is relatively little room of programmability. The only thing one can change is the functional form of interaction between particles, and all else are essentially fixed. This might sound like a limitation, but it actually means the amount of work of both the designer of the PROGRAPE hardware and the application programmer using it can be greatly reduced, compared to other FPGA-based machines like Splash. With Splash everything on board is programmable, and that means the user must program everything on board. If our main interest is in particle-based simulation, we do not need the programmability other than the possibility to change the interaction, and PROGRAPE is designed to provide just the minimal amount of programmability needed to be useful.

We have developed a GRAPE-like hardware based on FPGA chips which we call PROGRAPE-1 (PROgrammable GRAPE-1). It contains two Altera EPF10K100 FPGA chips (around 100K nominal gates). We tested its performance with a realistic application by implementing the pipeline similar to that of GRAPE-3. One pipeline was successfully fitted into one chip, and operated at 16 MHz clock. Thus, the performance of the single FPGA chips was shown to be comparable to that of a GRAPE chip used in GRAPE-3. We are currently working to implement an SPH calculation code.

In section 2, we describe the concept of the PROGRAPE system. In section 3, we describe the hardware design of PROGRAPE-1. In section 4, we describe the software and example application of PROGRAPE-1. Section 5 is for discussions.

2 PROGRAPE System

In this section, we describe the basic idea behind the PROGRAPE approach to build multi-purpose programmable computer for particle-based simulations. In section 2.1., we describe the hardware architecture, and in 2.2, how we use the hardware.
2.1 Hardware architecture

PROGRAPE is a programmable multi-purpose computer for many-body simulations. Figure 1 shows the basic structure of a PROGRAPE system. The system consists of a PROGRAPE and a host computer. The PROGRAPE calculates interactions between particles. The host computer performs all other calculations.

Figure 2 shows the structure of a PROGRAPE. It consists of a control unit, an interface unit, a memory unit and multiple FPGA chips. This structure is the same as that of GRAPE hardwares such as GRAPE-3, GRAPE-4 and GRAPE-5.

In a rather abstract expression, a PROGRAPE evaluates the following:

\[ f_i = \sum_{j=1}^{N} g(X_i, X_j), \]  

where \( X_i \) is the vector which contains the information of particle \( i \), \( f_i \) is the resulted “force”
on particle $i$, and $g$ is a function which describes the interaction between two particles.

To give a specific example, in the case of GRAPE for gravitational force, $X_i = (x_i, m_i)$ where $x_i$ and $m_i$ are the position and mass of particle $i$, and $g$ would be given by

$$g = -m_j \frac{x_i - x_j}{(|x_i - x_j|^2 + \epsilon^2)^{3/2}},$$  

where $\epsilon$ is the softening parameter. The result, $f_i$, is the gravitational acceleration of particle $i$. Note that $X_i$ and $X_j$ in equation (1) do not necessarily contain the same amount of information, though we refer to them by the same symbol for simplicity. In the case of the gravitational interaction, mass $m_i$ is not used to calculate the acceleration $f_i$. Therefore, we can remove $m_i$ from $X_i$, though $X_j$ should contain $m_j$. If a PROGRAPE has multiple pipeline FPGA chips (or if an FPGA chip houses multiple pipelines), $f_i$ for multiple particles are evaluated in parallel.

If PROGRAPE is used to evaluate the SPH interaction, $X$ will contain density and pressure to calculate the pressure gradient, and velocity to calculate the artificial viscosity. When variable smoothing is used, the size of the smoothing length must also be included in $X$. The interaction function $g$ will be more complex than equation (2).

The calculation proceeds in the following steps. First, the host computer sends the configuration data of pipeline FPGA chips. This need to be done only once. Then, the host computer stores the data of particles into the memory unit. These particles are used as $X_j$ in equation (1), and we refer to them as “$j$-particles”. After sending the data of $j$-particles, the host computer sends $X_i$ to each pipeline. These data will be stored in registers in the pipelines, which we call $i$-registers ($i$ denotes $i$-particles, as opposed to $j$-particles). Next, the host computer sends the command to the control unit to start the calculation. Accordingly, the control units sends address (particle index) to the memory unit and control signals to the pipeline FPGA chips. Pipeline FPGA chips receive the data from the memory, evaluate the interaction function $g$ and accumulate them in their internal accumulators. Finally, when the summation is finished, the contents of the accumulators are sent back to the host computer.

Figure 3 shows the conceptual design of the circuit in a pipeline FPGA chip. As stated above, a pipeline FPGA chip consists of a memory interface, an I/O interface and a pipeline unit. A pipeline unit consists of an arbitrary number of pipelines including one. A pipeline consists of $i$-registers, an interaction unit to evaluate an interaction function, and accumulators.

Note that we can change only the content of the pipeline FPGA chips. All other parts of hardware such as an interface unit, a control unit and a memory unit are fixed. For example, once the hardware is designed and built, the amount of data transferred from the memory unit to the pipeline FPGA chips in one clock cycle is fixed. However, this is not a serious limitation, since even if $X_j$ requires the number of bits larger than what is available in hardware, we can still use the PROGRAPE hardware by designing the pipeline FPGA chip so that it uses more than one clock cycles to receive $X_j$. In the case of PROGRAPE-1 described in section 3, the memory unit can transfer 16 bytes of data per clock cycle. For most applications, this is more than necessary, and we do not have to design a complex...
Figure 3: The conceptual design of the circuit in a pipeline chip of PROGRAPE.

2.2 Software architecture

Once the content of the pipeline is designed and tested, the way we use a PROGRAPE system is very much the same as the way we use any of GRAPE systems. The application program sends the data of \( j \)-particles and \( i \)-particles, and the PROGRAPE hardware returns the result calculated for \( i \)-particles. From the point of view of the application program, only a small number of library functions are visible.

The big difference between PROGRAPE and GRAPE is that in the case of PROGRAPE, the user can specify every detail of the pipeline. To change its logic in a slightly different way, the user must specify literally every bit of the pipeline.

It should be noted that it is also true that the user need to specify only pipeline FPGA chips. As shown in figure 2, a PROGRAPE hardware consists of a control unit, an interface unit, a memory unit and pipeline FPGA chips. Everything other than pipeline FPGA chips are fixed. Also, a memory interface, an I/O interface, \( i \)-registers and accumulators in pipeline FPGA chips are pre-designed and provided as parametrized modules.

Figure 4 shows the conceptual design of a pipeline in a pipeline unit in the VHDL language. A pipeline receives data from an I/O interface and a memory interface and evaluates an interaction. In figure 4, the \( X_i \) and \( X_j \) are the ports of data put from an I/O interface and a memory interface respectively. The evaluated result is then fed to the accumulator module. Compared to programming other FPGA-based machines, programming
a PROGRAPE is much easier, simply because the large part of the hardware is already programmed.

Even though programming PROGRAPE is not as hard as programming other FPGA-based machines, the design and testing of a pipelined FPGA chip for particle-particle interaction is, judging from our experience of developing custom LSI chips for GRAPE hardwares, still a rather time-consuming work. As we stated earlier, the design process of the internal logic of an FPGA is essentially the same as that for a custom LSI, except that the risk of making mistakes is small.

In practice, this smaller risk is a significant factor. With a custom LSI, a serious mistake in the design would cost several tens of million yens and cause the delay of several months in schedule. Even if one makes no mistake, several tens of million yens is still necessary to get first samples of the chip. On the other hand, even most advanced FPGA chips would cost around hundred thousand yens. In addition, if the mistake is found in the design of an FPGA, it can be fixed in a few hours or even minutes. This difference means the iteration in the design is much quicker with FPGA, and therefore the design process as a whole is also a lot quicker. Even so, the design of the pipeline still looks like a serious project, which would require considerable investment even for an expert in programming general-purpose computers.

There are several reasons for the difficulty of the programming. The first obstacle is that there are too much freedom. An FPGA chip can be used to implement any logic circuit, as far as it fits into the chip. Thus, the programming of FPGA is done essentially in the lowest level of logic, in which one specifies basic logic gates (AND/OR gates) and flip-flops. To make an analogy, an FPGA is something like a universal Turing machine without any high-level language, library functions or even operating systems. Thus, when one designs a machine using FPGA, all these infrastructure must also be developed by someone.

This complete freedom is available for all operations to be implemented in FPGA. Thus, even for a simple addition, there are infinitely many possibilities, which would cause very large variation in the size and speed of the implemented circuit. For many applications, it would be necessary to determine what number format and accuracy are appropriate for each operation, otherwise, the pipeline would not fit into available FPGA chips. Even if they fit, the performance would be rather low. Thus, unlike a program on a general-purpose computer, a design of the pipeline for a PROGRAPE requires in-depth understanding of both the arithmetic operations in digital circuit and the effect of the round-off error in the target application. In many application areas, little is known about the effect of the round-off error. Thus, in many case the user need to conduct systematic experiments to understand the error propagation mechanism.

In principle, if FPGA chips are large and fast enough, we can just implement standard 32- or 64-bit floating-point arithmetic operations. Unfortunately, we need to wait several years before such large FPGA chips become available. Currently, even the largest FPGA chips would not be able to house a single 64-bit multiplier. Moreover, even when large chips are available, we can achieve very large speedup by adjusting the size of arithmetic units according to the required accuracy. Thus, to achieve a good performance, it will always be necessary to select right arithmetic units for each operation.
entity pipeline is
    generic (  
      JDATA_WIDTH : integer;  
      IDATA_WIDTH : integer;  
      FDATA_WIDTH : integer;  
      ADR_WIDTH : integer;  
      NVP : integer  
    );
    port(  
      Xj : in std_logic_vector(JDATA_WIDTH-1 downto 0);  
      Xi : inout std_logic_vector(IDATA_WIDTH-1 downto 0);  
      adr : in std_logic_vector(ADR_WIDTH-1 downto 0);  
      we, run, iclk, pclk : in std_logic;  
      RESULT : out std_logic_vector(FDATA_WIDTH - 1 downto 0)  
    );
end pipeline;

architecture std of pipeline is

signal idata : std_logic_vector(IDATA_WIDTH-1 downto 0);
signal fdata : std_logic_vector(FDATA_WIDTH - 1 downto 0);
signal runr : std_logic;

begin
  u1: i_register GENERIC MAP(IDATA_WIDTH => IDATA_WIDTH, NVP => NVP)  
     PORT MAP(datai => Xi, we =>we, adr =>adr, run => run,  
               idata => idata, iclk => iclk, pclk => pclk);

  u2: interaction GENERIC MAP(JDATA_WIDTH => JDATA_WIDTH,  
                               IDATA_WIDTH => IDATA_WIDTH)  
      PORT MAP(jdata => Xj, idata => idata, run => run,  
               runr => runr, fdata => fdata, clk => pclk);

  u3: accumulators GENERIC MAP(FDATA_WIDTH => FDATA_WIDTH, NVP => NVP)  
      PORT MAP(fdata => fdata, run => runr, adr => adr,  
               datao => RESULT, iclk => iclk, pclk => pclk);

end pipeline;

Figure 4: The conceptual design of a pipeline of PRPGRAPE in the VHDL language.
The second obstacle is the simple fact that what is designed is a hardware, not a software. Though the design of a hardware is not necessarily more difficult than that of the software, they are different and require different kinds of expertise. To some extent, the situation is similar to that of programming parallel computers. The programming of a parallel computer is not necessarily more difficult than that for a sequential computer. However, the lack of experience and the lack of good software environment make the development of parallel program a difficult task. This is true of the case of the hardware design.

At present, those who wish to use PROGRAPE must write the design of the pipeline in VHDL, unless the application has been developed by somebody else. We are developing some kind of design environment which will be discussed elsewhere.

3 PROGRAPE-1

PROGRAPE-1 is the first machine of the PROGRAPE architecture. Figure 5 shows the block diagram of PROGRAPE-1. It is connected to the host computer through a PCI interface board [16]. The interface protocol used between PHIB and PROGRAPE-1 is the Hlink protocol described in Makino et al. [17].

The PROGRAPE-1 board consists of two pipeline FPGAs, a memory unit, an interface unit and a control unit. Thus, PROGRAPE-1 is a minimal realization of the concept of PROGRAPE (figure 2) with two pipeline FPGA chips. In the following subsections, we will describe each of these units.

3.1 Pipeline FPGA

We adopted Altera EPF10K100 chips as the pipeline FPGA. This FPGA has 4992 logic cells, each of which has a look-up table with 4-bit input and a flip-flop, and 12 SRAM...
blocks, with the size of 2 Kbits each. The manufacturer claims that the chip has the capacity equivalent to about 100,000 gates.

This FPGA chip from Altera was not the only possibility. Similar chips were available from Xilinx and Lucent Technologies. The main reason we chose Altera was that we had some experience with its design software.

The configuration data of the pipeline FPGAs are written from a special port connected to the interface unit. Thus, the pipeline can be programmed by software on the host computer.

Figure 6 shows the I/O specification of the pipeline FPGA. It has one data input port (JDATA[127:0]), one bidirectional data port (IDATA[31:0]), one address port (ADR[9:0]), four control input pins (CS, RE, WE, RUN) and one clock pin (CLK). The data input port (JDATA) is used to supply the data of j-particles from the memory unit. The bidirectional data port (IDATA) and address port (ADR) are used to read or write the on-chip registers, whose organization is specified by the configuration data fed from the host computer. The control pins (CS, RE, WE) are used to control the read and write operations to the on-chip register. The CLK pin supplies the clock signal. The RUN pin is used to start operations of a interaction unit and accumulators in a pipeline unit of a pipeline FPGA chip.

3.2 Memory Unit

The memory unit supplies the data of j-particles to pipeline FPGA chips according to the address supplied by the control unit. Two pipeline FPGA chips receive the same data. The memory unit consists of four 512 Kbit (16 Kwords × 32bits) SRAM modules. The
width of the data port from the memory unit to pipelines is 128-bit width. The width of the data port from the interface unit to memory unit is 32-bit width. We adopted 7MC4032 made by Integrated Device Technology, Inc, which is 512K bits SRAM module with separate I/O.

3.3 Interface Unit

The interface unit handles the communication between the host computer and PROGRAPE-1. There are 5 communication modes: (1) The host computer sends a command to the control unit. (2) The host computer sends the data to memory unit. (3) The host computer sends the data to the pipeline FPGA chips. (4) The pipeline FPGA chips send the calculated result to the host computer. (5) The host computer sends the configuration data to pipeline FPGA chips. The interface unit consists of an Altera EPF10K20 chip and several transceiver and buffer chips.

3.4 Control Unit

The control unit generate all control signals for all other units, according to the command sent from the host computer. The control unit is implemented in the same FPGA chip as used for the interface unit.

3.5 Miscellaneous Aspect

We have packaged PROGRAPE-1 in a board of a size 37cm by 40cm. Figure 7 is a photograph of the PROGRAPE-1 board. The total number of chips is 84. All of the chips are wire-wrapped on the boards. It operates at the clock frequency of 16MHz.

4 Application of PROGRAPE-1

In section 2.2., we discussed the general aspect of programming a pipeline FPGA chip in PROGRAPE. Here, we discuss practical aspects of programming, using a pipeline to calculate gravitational interaction as an example.

4.1 The programming model

Figure 8 shows the internal structure of the pipeline FPGA chip. It consists of the memory interface (MI), the I/O interface (IO), the pipeline unit (PU). The PU consists of \(i\)-particle register unit (IREG), the accumulator unit (ACC), and the interaction function pipeline unit (IFP). The application programmer need to design the IFP. All else are designed as configurable library modules. Both the design of IFP and the rest of the chip are written in VHDL. Figure 9 shows the skeleton of the top level source of the pipeline chip.

The design flow for an application programmer would be the following
Figure 7: The PROGRAPE-1 board.

Figure 8: The internal structure of the pipeline chip of PRPGRAPE-1.
entity pipeline_top is
  generic(
    JDATA_WIDTH : integer;
    IDATA_WIDTH : integer;
    FDATA_WIDTH : integer
  );
  port(
    i_jdata : in std_logic_vector(JDATA_WIDTH-1 downto 0);
    i_data : inout std_logic_vector(IDATA_WIDTH-1 downto 0);
    i_adr : in std_logic_vector(9 downto 0);
    i_cs, i_we, i_re, i_run : in std_logic;
    i_clk : in std_logic
  );
end pipeline_top;

architecture std of pipeline_top is
  signal jdata : std_logic_vector(JDATA_WIDTH-1 downto 0);
  signal datai : std_logic_vector(IDATA_WIDTH-1 downto 0);
  signal adr : std_logic_vector(9 downto 0);
  signal run, we : std_logic;
  signal datao : std_logic_vector(FDATA_WIDTH downto 0);
begin
  u1: io GENERIC MAP(FDATA_WIDTH => FDATA_WIDTH)
    PORT MAP(i_data => i_data, i_adr => i_adr,
      i_cs => i_cs, i_we => i_we, i_re => i_re,
      i_run => i_run, clk => i_clk,
      datai => datai, adr => adr, run => run,
      we => we, datao => datao);

  u2: mi GENERIC MAP(JDATA_WIDTH => JDATA_WIDTH)
    PORT MAP(i_jdata => i_jdata, clk => i_clk, jdata => jdata);

  u3: pu GENERIC MAP(JDATA_WIDTH => JDATA_WIDTH,
    IDATA_WIDTH => IDATA_WIDTH, FDATA_WIDTH => FDATA_WIDTH)
    PORT MAP(datai => datai, jdata => jdata, we => we,
      adr => adr, run=>run, clk => i_clk,
      datao => datao);
end pipeline_top;

Figure 9: The skeleton of the top level source of the pipeline chip of PROGRAPE-1.
1. Determine the detailed specification of the pipeline, including the number format used in each operation.

2. Verify the design using a software simulator linked to the application program.

3. Develop the VHDL source program for the pipeline.

4. Verify the design by comparing with the simulator.

5. Integrate the VHDL source of the pipeline with other modules.

6. Generate the configuration data from the design using CAD softwares.

7. Develop the driver software on the host computer.

8. Configure pipeline FPGA chips.

9. Verify the pipeline FPGA by comparing with the application program linked to the software simulator.

10. Run the application program.

We can see that a rather large amount of work is involved in developing a pipeline FPGA chip. In principle, most of the softwares, such as the simulator and the driver software on the host computer, could be automatically generated from the design specification or the VHDL source of the pipeline. We have not yet developed such software simply because of the limitation in the available human resources.

In the rest of this section we describe the implementation of the gravitational interaction pipeline.

4.2 Pipeline for Gravitational Force

We have implemented a pipeline for the gravitational force on the pipeline FPGA chip. It calculates the right-hand side of equation (2). Figure 10 shows a block diagram of the pipeline for the gravitational force, which is almost same as the GRAPE chip. We omitted the circuit to handle mass of particles and the circuit to accumulate the potential energy for simplicity. The number formats are the same as those used in the GRAPE chip.

The pipeline for the gravitational force consumes about 50% of the logic cells of the pipeline FPGA chip. The nominal gate count of the pipeline FPGA chip is 100K, while the transistor count of the GRAPE chip was 110K. Since our implementation of the gravitational pipeline lacks several functions implemented in the GRAPE chip, the transistor count of the circuit equivalent to our pipeline implementation would be around 90K. Thus, for the case of the GRAPE chip, one nominal gate of FPGA corresponds to about 1.8 transistors. The FPGA chip successfully operated at 16 MHz clock. Thus, assuming that the number of floating-point operations per one interaction is 30, the peak speed of a chip is 480 Mflops and that of PROGRAPE-1 is 0.96 Gflops.
Figure 10: Pipeline for the gravitational force.

Whether these numbers are good or not depends on the point of view. The FPGA chip we used contain more than one million transistors in 0.5µm process, while a GRAPE chip really contains 110K transistors in 1µm process. A custom LSI fabricated using the same technology as the pipeline FPGA chip of PROGRAPE-1 would contain around 2 pipelines operating at 100 MHz. Thus, performance penalty of the programmability of an FPGA is as large as a factor of 100 or more. One can reduce this factor by carefully optimizing the design of the FPGA chip and by increasing the clock period, but even after such tuning the performance could not be three times as high as that of pre-optimizing design.

When compared with a general purpose computer, however, the speed achieved with PROGRAPE-1 is pretty high. For example, a workstation with an Alpha chip (EV56, 533MHz) has the theoretical peak speed of 1066 Mflops. However, actual speed for the calculation of the gravitational interaction is less than 100 Mflops \[^2\] even after a heroic effort of tuning. On the other hand, PROGRAPE-1 does deliver the performance close to the peak for real applications. In addition, it’s pretty easy to achieve massive parallelism with PROGRAPE.

5 Discussion

5.1 Comparison with other FPGA machines

There are a number of research project to use FPGA in the form of attached processors. As a well known and successful example, here we discuss Splash-2 \[^4\]. Figure 11 shows the architecture of a Splash-2 board. It is connected to SBus of a Sun workstation. Up to 16 processor boards can be housed in a chassis. The architecture of Splash-2 is an array of basic processing units (PU). A PU consists of an FPGA chip and its local memory. Processing
units are connected through one shared data bus, one linear network and one crossbar switch. Thus, we can see that Splash was designed with wide range of applications in mind. For some applications, linear network allowed the programmer to implement a deep pipeline which spans over multiple FPGA chips. For other applications, the programmer can use the 16 PUs in an SIMD fashion. It is also possible to program the crossbar to implement a complex dataflow.

With PROGRAPE, the dataflow outside the FPGA chips is fixed, and there is only one memory unit. This design greatly simplifies the development of the hardware. In addition, this limitation in the programmability actually made it easier to program, provided the architecture of PROGRAPE is suited to the target problem. Thus, as far as the target application is the evaluation of the particle-particle interaction, the architecture of PROGRAPE is probably better than other more flexible architectures. Of course, more flexible architectures can be applied to wider range of problems. So we cannot simply say which architecture is better.

At least one group [18] has tried to implement the pipeline similar to that of GRAPE-2 [20] onto a programmable FPGA board. What they used is an Altera RIPP-10 FPGA board, which is composed of eight Altera EPF81188 FPGA chips and and 2MB of SRAM chips. They implemented all operations in 32-bit floating-point arithmetic. A fully-parallel multiplier was too large to be implemented, so they designed arithmetic units which require four clock cycles to generate one result. They implemented one pipeline which operated at 10 MHz clock, resulting in 2.5 million interactions per second or 75 Mflops. The nominal gate count of the Altera RIPP-10 board was about the same as what is available
on PROGRAPE-1. The difference in the speed comes mainly from the difference in the number format.

5.2 Other Applications

As we described in the introduction, our main target of PROGRAPE is SPH calculation. Compared with the calculation of gravity, the calculation of SPH interaction is much less expensive. Nonetheless evaluation of the SPH interaction becomes the dominant part of the calculation once the calculation of gravity is accelerated by GRAPE.

We are currently working on an implementation of SPH, and the result will be described elsewhere. Here, we discuss what else would be suitable for PROGRAPE.

Short-range particle-particle interactions are good candidates for the implementation on PROGRAPE. Those include, beside SPH, van-der-Waals force in molecular dynamics calculation and Coulomb force with cutoff used in Ewald method or PPM method. As we have seen, the actual performance of an FPGA depends very strongly on the required accuracy. Since relatively little is known about what level of the accuracy is required for these calculations, we cannot predict whether PROGRAPE is useful for these applications or not.

Though the overall architecture of PROGRAPE is determined so that it is optimized for the evaluation of particle-particle interaction, it can be used for other operations which can be expressed in the form of equation (1). One example is the discrete Fourier transform used in the direct Ewald method. Both the discrete Fourier transform and the inverse transform can be expressed in the form of equation (1) [19], and therefore can be efficiently implemented on PROGRAPE. In the case of the Ewald method, the required accuracy is relatively low (since it handles higher-order correction of the force due to “image” particles). Thus PROGRAPE would be a good alternative to an implementation on a general-purpose computer.

It is also possible to use PROGRAPE hardware for applications which cannot be expressed in the form of equation (1). As one example, consider the matrix multiplication

\[ C = A \cdot B \]  

(3)

We can use the memory unit to store matrix \( A \), and internal memory available in FPGA chips to store one row of matrix \( B \). Thus, we can perform the multiplication in the so-called inner-product form. We can also use the same configuration to implement the Gaussian elimination. Here again, the consideration of the accuracy would determine the effectiveness of PROGRAPE.

5.3 Future Prospect

We plan to develop a massively parallel PROGRAPE, the PROGRAPE-2. It will consist of around 1000 FPGA chips, and 2-4 FPGA chips will share the memory unit. The overall architecture will be the same as that of GRAPE-6 [22]. The only difference between GRAPE-6 and PROGRAPE-2 will be that the FPGA chips are used in the place of the GRAPE-6 chip. The performance of PROGRAPE-2 system will vary depending on
applications, but it will be in the range of 1-10 Tflops. We plan to complete PROGRAPE-2 by 2001.
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