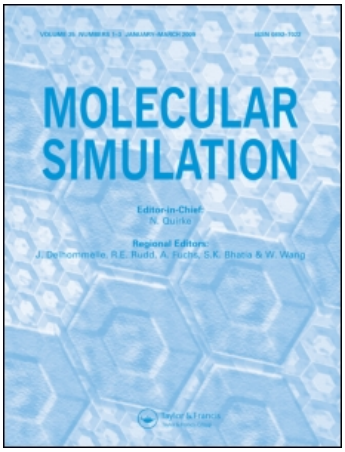

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Molecular Dynamics Machine: Special-Purpose Computer for Molecular Dynamics Simulations

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MOLECULAR DYNAMICS MACHINE: SPECIAL-PURPOSE COMPUTER FOR MOLECULAR DYNAMICS SIMULATIONS

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We are now developing Molecular Dynamics Machine (MDM), a special-purpose computer for classical molecular dynamics simulations. It accelerates the calculation of non-bonding force, Coulomb and van der Waals forces, because the calculation cost for Coulomb force dominates the total calculation time when we treat a large system of charged particles without truncating Coulomb force. When we use Ewald method, the Coulomb force can be calculated by dividing it into real-space and wavenumber-space parts. MDM is composed of MDGRAPE-2, WINE-2, and a host computer. MDGRAPE-2 calculates van der Waals force and real-space part of Coulomb force. WINE-2 calculates wavenumber-space part of Coulomb force. The host computer calculates bonding-force and updates positions and velocities of atoms. The target performance of MDM is 100 Tflops and will sustain about 30 Tflops in realistic applications. It can calculate 3.2×10^6 time-steps of MD simulation with a million atoms in a week. Total system will be completed in 1999.

Keywords: Special-purpose computer; molecular dynamics simulation; Ewald method; massive parallel processing; pipeline architecture

1. INTRODUCTION

Molecular dynamics (MD) simulations have been widely used to study the physical properties of condensed matter in an atomic level. There are strong

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motivations to perform MD simulations with a large number of atoms to study large molecular systems. In recent years, the structure of large biomolecules in the range of 10,000 to 100,000 atoms have been determined [1, 2]. Furthermore, biomolecular systems consisting of many molecules have become targets of simulations, for example, lipid bilayer [3] and protein-DNA complexes [4]. These biomolecule systems are often required to be surrounded by water molecules. In order to study the structures and dynamics of these large systems of molecules, simulations with million atoms are required. Moreover, investigating phenomena, such as the stability of biomolecules on the structure obtained by experiments, at least several hundreds of pico-seconds of MD simulations are often required.

In molecular dynamics simulations, each atom in a system is treated as a classical particle. An atom interacts with the other atoms through bonding force, Coulomb force, and van der Waals force. Calculation of Coulomb force is the most time consuming part of the MD simulation, and it is often truncated at a length of $10\,\text{Å} \sim 15\,\text{Å}$ in order to reduce the computing time to a reasonable value. However, this truncation leads a very large computational error [5]. Calculation of Coulomb force without truncation needs a huge computational power. Our way of achieving this computational requirement is to develop a highly parallelized special-purpose computer which calculates forces by a pipeline architecture. Sugimoto *et al.* [6] have developed GRAPE (GRAvity PipE) hardwares, such as GRAPE-4 [7], for the calculation of gravitational N-body simulations. They also developed special-purpose computers for molecular dynamics simulations, such as WINE-1 [8] or MD-GRAPE [9, 10]. They use the Ewald method [11] to calculate the Coulomb force. WINE-1 accelerates the calculation of wavenumber-space part of Coulomb force. MD-GRAPE accelerates the calculation of non-bonding forces, *i.e.*, Coulomb force and van der Waals force.

In the present paper, we give the hardware design of a highly parallelized GRAPE system for molecular dynamics simulations, which we named as Molecular Dynamics Machine (hereafter MDM). The target speed of MDM is about 100 Tflops. MDM will take 0.19 s per time-step for MD simulations with a million particles by Ewald method: It takes only one week ($\sim 6.0 \times 10^5$ s) to perform the simulations of a time span of 1.6 ns ($\sim 3.2 \times 10^6$ time-steps). MDM will be several ten times faster than the currently fastest supercomputers in a sustained speed for MD simulations with a million atoms. In Section 2, we presents the basic equations to calculate forces on atoms. In Sections 3 and 4 we describe the structure and the performance of MDM system, respectively.

2. BASIC EQUATIONS

The force, $\vec{F}_i$, on particle i is the sum of Coulomb force, $\vec{F}_i(\mathrm{Clb})$, van der Waals force, $\vec{F}_i(\mathrm{vdW})$, and bonding force, $\vec{F}_i(\mathrm{bd})$, by covalent and hydrogen bonds:

$$\vec{F}_i = \vec{F}_i(\mathrm{Clb}) + \vec{F}_i(\mathrm{vdW}) + \vec{F}_i(\mathrm{bd}). \tag{1}$$

Coulomb force is calculated by Ewald method, when the periodic boundary condition is imposed. In Ewald method, $\vec{F}_i(\mathrm{Clb})$ is divided into two parts, *i.e.*, real-space part, $\vec{F}_i(\mathrm{re})$, and wavenumber-space part, $\vec{F}_i(\mathrm{wn})$:

$$\vec{F}_i(\mathrm{Clb}) = \vec{F}_i(\mathrm{re}) + \vec{F}(\mathrm{wn}). \tag{2}$$

Here, $\vec{F}_i(\mathrm{re})$ and $\vec{F}_i(\mathrm{wn})$ are expressed as follows when the computational box is a cube:

$$\vec{F}_i(\mathrm{re}) = \frac{q_i}{4\pi\varepsilon_0} \sum_j^{r_{ij}<r_{\mathrm{cut}}} q_j \left[\frac{\mathrm{erfc}(\alpha r_{ij}/L)}{r_{ij}} + \frac{2\alpha}{\pi^{1/2}L} \exp(-\alpha^2 r_{ij}^2/L^2) \right] \frac{\vec{r}_{ij}}{r_{ij}^2}, \tag{3}$$

$$\begin{aligned} \vec{F}_i(\mathrm{wn}) = \frac{q_i}{2\pi\varepsilon_0 L^3} \sum_{\vec{k}}^{k<k_{\mathrm{cut}}} \frac{\vec{k}}{k^2} \exp(-\pi^2 L^2 k^2/\alpha^2) \\ \times \left[\sin(2\pi\vec{k}\cdot\vec{r}_i) \sum_j q_j \cos(2\pi\vec{k}\cdot\vec{r}_j) \right. \\ \left. - \cos(2\pi\vec{k}\cdot\vec{r}_i) \sum_j q_j \sin(2\pi\vec{k}\cdot\vec{r}_j) \right]. \end{aligned} \tag{4}$$

where $\vec{r}_i$ is the position of particle i, $\vec{r}_{ij}$ is the relative vector from particle j to particle i, r_{ij} is the distance between particle i and particle j, q_i is the electrostatic charge of particle i, $\vec{k}$ is the wavenumber vector, k is the length of $\vec{k}$, L is the length of a side of the computational box, r_{cut} and k_{cut} are the cut-off length of relative vector and wavenumber vector, respectively, ε_0 is the dielectric constant of vacuum, α is a parameter to adjust the computational cost for real and wavenumber part of the Coulomb force calculation, and $\mathrm{erfc}(x)$ is the complementary error function:

$$\mathrm{erfc}(x) = 1 - \frac{2}{\pi^{1/2}} \int_0^x \exp(-t^2)dt. \tag{5}$$

We assume the computational box to be a cube for simplicity in the present paper, though MDM can treat a non-orthogonal as well as orthogonal parallelepiped for a computational box.

The wavenumber-space part of Coulomb force, $\vec{F}_i(\mathrm{wn})$, is actually calculated with MDM by the following equations. Equation (4) can be rewritten as:

$$\vec{F}_i(\mathrm{wn}) = \frac{q_i}{\pi\epsilon_0 L^3} \sum_n^{N_{\mathrm{wv}}} a_n \sin(2\pi\vec{k}_n \cdot \vec{r}_i + \theta_n) \cdot \vec{k}_n, \tag{6}$$

where, a_n and θ_n are calculated by:

$$a_n = \frac{\exp(-\pi^2 L^2 k_n^2/\alpha^2)}{k_n^2} (S_n^2 + C_n^2)^{1/2}, \tag{7}$$

$$\theta_n = \begin{cases} -\sin^{-1}[S_n/(S_n^2 + C_n^2)^{1/2}] & \text{for } C_n \geq 0, \\ \pi + \sin^{-1}[S_n/(S_n^2 + C_n^2)^{1/2}] & \text{for } C_n < 0, \end{cases} \tag{8}$$

where, S_n and C_n are:

$$S_n = \sum_{j=1}^{N} q_j \sin(2\pi\vec{k}_n \cdot \vec{r}_j), \tag{9}$$

$$C_n = \sum_{j=1}^{N} q_j \cos(2\pi\vec{k}_m \cdot \vec{r}_j). \tag{10}$$

Here, N is the number of atoms, and N_{wv} is the number of wavenumber vectors to be taken into account; It is the half of the number of wavenumber vectors whose lengths are shorter than k_{cut}:

$$N_{\mathrm{wv}} \simeq \frac{2}{3}\pi L^3 k_{\mathrm{cut}}^3, \tag{11}$$

where we used the fact that the term in the summation of $\vec{k}$ in Eq. (4) takes exactly the same value for the case of $\vec{k}$ and $-\vec{k}$.

The van der Waals force, $\vec{F}_i(\mathrm{vdW})$, is calculated by

$$\vec{F}_i(\mathrm{vdW}) = \sum_{j}^{r_{ij}<r_{\mathrm{cut}}} \varepsilon(at_i, at_j)\left\{2\left[\frac{\sigma(at_i, at_j)}{r_{ij}}\right]^{14} - \left[\frac{\sigma(at_i, at_j)}{r_{ij}}\right]^{8}\right\}\vec{r}_{ij}, \qquad (12)$$

where $\varepsilon(at_i, at_j)$ and $\sigma(at_i, at_j)$ are the coefficients which depend on both of atom types at_i and at_j, where at_i is the atom type of particle i. We adopt Lennard-Jones potential for a van der Waals force in the present paper, though MDM can treat any potential type in the form of a central force.

3. HARDWARE DESIGN

MDM is composed of a host computer and two special-purpose computers: MDGRAPE-2 and WINE-2. Figure 1 shows the conceptual structure and calculation flow of MDM. A host computer is a general-purpose computer, such as a workstation, which works as a front-end processor. Two special-purpose computers, which we are newly developing, work as back-end processors.

The host computer calculates bonding forces $[\vec{F}_i(\mathrm{bd})]$ for covalent and hydrogen bonds and updates the positions and velocities of particles. The non-bonding forces, which dominates the total calculation cost, are calculated by MDGRAPE-2 and WINE-2. MDGRAPE- 2 calculates real-space part of Coulomb force $[\vec{F}_i(\mathrm{re})]$ and van der Waals force $[\vec{F}_i(\mathrm{vdW})]$, while WINE-2 calculates wavenumber-space part of Coulomb force $[\vec{F}_i(\mathrm{wn})]$. Since the load on MDGRAPE-2 and WINE-2 is much heavier than those for host computer and communication interfaces among them, the total performance of the system is determined by the super-highspeed

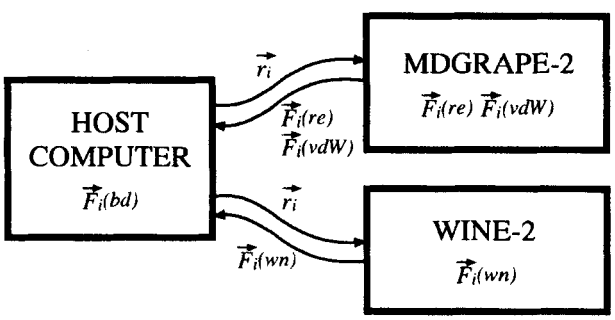

FIGURE 1 Conceptual structure and calculation flow of Molecular Dynamics Machine.

special-purpose computers rather than the host computer or communications, for a large number of particles. MD simulations under the constant-temperature [12] and constant-pressure [13] conditions can be applied on MDM with a little increase in calculation time.

MDM is divided into 8 nodes connected with each other by a communication switch (Fig. 2) in the actual hardware. A node is composed of a node computer, MDGRAPE-2, and WINE-2 (Fig. 3). MDGRAPE-2 and WINE-2 have MDGRAPE-2 and WINE-2 chips, respectively, which we newly develop. Total number of MDGRAPE-2 and WINE-2 chips is 2,560 and 3,072, respectively. The peak speed of MDM is about 100 Tflops,

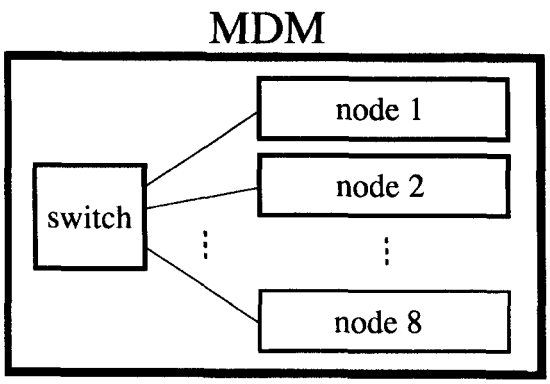

FIGURE 2 Block diagram of Molecular Dynamics Machine.

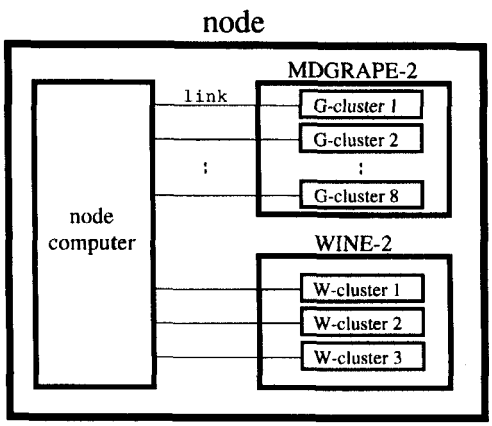

FIGURE 3 Block diagram of a node.

and the total system will be completed in 1999. Total budget for MDM is about 5 million dollars.

In the following subsections, we briefly describe the hardware of a host computer, MDGRAPE-2, WINE-2. Detailed descriptions are presented in the separate paper [14].

3.1. Host Computer

A host computer is composed of 8 node computers which are connected with each other by a switch. We need 8-point-8 switch whose transfer speed between any pair of nodes is faster than 180 Mbyte/sec. The total calculation speed of a host computer is 12 Gflops in sustained.

3.2. MDGRAPE-2

MDGRAPE-2 is composed of 8 G-clusters (Fig. 3). Each G-cluster is connected to a node computer through a link. We plan to use PCI (Peripheral Component Interconnect) bus (64-bit wide and 33 MHz clock frequency) as a link. Each G-cluster (Fig. 4) has 4 MDGRAPE-2 boards (hereafter, G-boards; Fig. 5) and each G-board has 10 MDGRAPE-2 chips (hereafter, G-chips; Fig. 6). A G-chip has four G-pipelines (Fig. 7).

A G-board calculates pairwise central forces such as real-space part of Coulomb and van der Waals forces with the cell-index method [15] as:

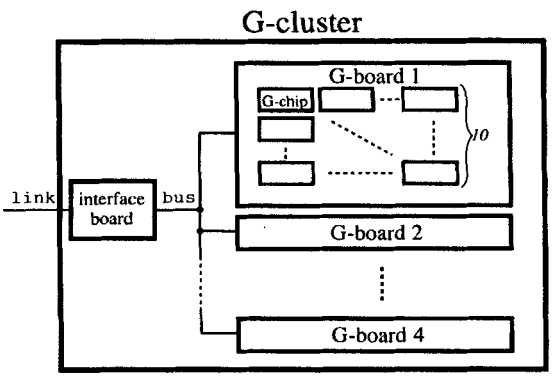

FIGURE 4 Structure of a G-cluster.

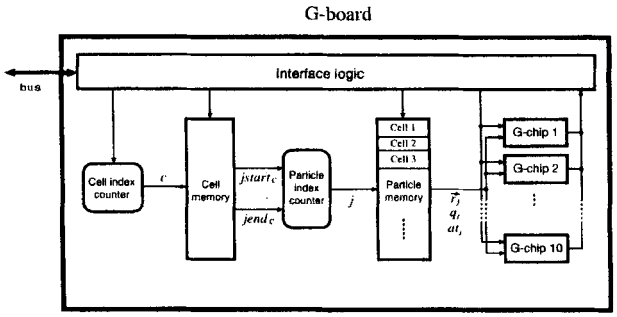

FIGURE 5 Block diagram of a G-board.

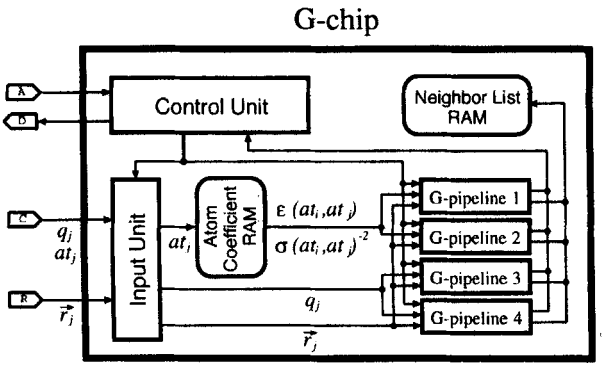

FIGURE 6 Block diagram of a G-chip.

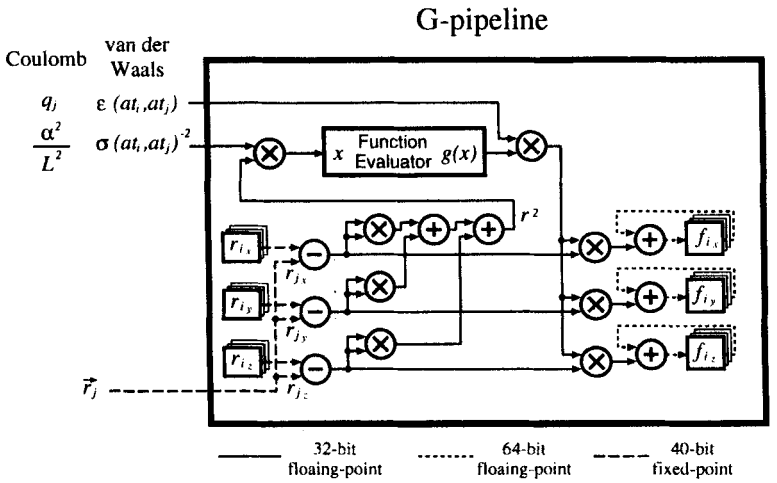

FIGURE 7 Block diagram of a G-pipeline.

$$\vec{f}_i(\mathrm{re}) = \sum_{c=1}^{27} \sum_{j=j\mathrm{start}_c}^{j\mathrm{end}_c} \vec{f}_{i,j}(\mathrm{re}),$$

$$\vec{f}_i(\mathrm{vdW}) = \sum_{c=1}^{27} \sum_{j=j\mathrm{start}_c}^{j\mathrm{end}_c} \vec{f}_{i,j}(\mathrm{vdW}), \tag{13}$$

where c is the index of the neighboring cells and $j\mathrm{start}_c$ is the index of the first particle in a cell c, $j\mathrm{end}_c$ is the index of the last particle in a cell c, and $\vec{f}_{i,j}(\mathrm{re})$ and $\vec{f}_{i,j}(\mathrm{vdW})$ are the pairwise real-space part of Coulomb and van der Waals forces between particles i and j, respectively. Here, indices of particles in a cell are assumed to be contiguous.

Real-space part of Coulomb force, $\vec{F}_i(\mathrm{re})$, on a particle i is calculated from $\vec{f}_i(\mathrm{re})$ as:

$$\vec{F}_i(\mathrm{re}) = \frac{q_i}{4\pi\varepsilon_0}\vec{f}_i(\mathrm{re}). \tag{14}$$

Van der Waals force, $\vec{F}_i(\mathrm{vdW})$, on a particle i is the same as $\vec{f}_i(\mathrm{vdW})$.

A G-chip has four G-pipelines, and each of them calculates pairwise force, $\vec{f}_{i,j}$, between particles i and j as:

$$\vec{f}_{i,j} = b_{ij}g(a_{ij}r_{ij}^2)\vec{r}_{ij}, \tag{15}$$

where $g(x)$ is an arbitrary central force, and a_{ij} and b_{ij} are coefficients determined by atom types of particles i and j.

Pairwise real-space part of Coulomb force, $\vec{f}_{i,j(\mathrm{re})}$, is calculated when:

$$g(x) = \frac{2\exp(-x)}{\pi^{1/2}x} + \frac{\mathrm{erfc}(x^{1/2})}{x^{3/2}}, \tag{16}$$

$$a_{ij} = \alpha^2 L^{-2}, \tag{17}$$

$$b_{ij} = q_j. \tag{18}$$

On the other hand, pairwise van der Waals force, $\vec{f}_{i,j}(\mathrm{vdW})$, is calculated when:

$$g(x) = 2x^{-7} - x^{-4}, \tag{19}$$

$$a_{ij} = \sigma(at_i, at_j)^{-2}, \tag{20}$$

$$b_{ij} = \varepsilon(at_i, at_j). \tag{21}$$

Figure 7 shows the block diagram of a G-pipeline. An arbitrary function, $g(x)$, is approximated by segmented 4-th polynomial interpolation in Function Evaluator in a G-pipeline. Coefficients of the polynomials are stored in the RAM in Function Evaluator.

A G-chip can also calculate potential of particles from particles in its potential mode as:

$$\Phi_i = \sum_j b_{ij} G(a_{ij} r_{ij}^2). \tag{22}$$

The calculation speed of a G-chip corresponds to about 16.4 Gflops at a clock frequency of 100 MHz.

Design of a G-chip is now in the final stage and engineering sample chips will be shipped in the third quarter of 1998. We use SA-12 technology by IBM Corp., whose design rule is 0.25 μm and operation voltage is 2.5 volt. The number of transistors in a G-chip is 5 million.

3.3. WINE-2

WINE-2 is composed of 3 W-clusters (Fig. 3). Each W-cluster is connected to a node computer through a link. Each W-cluster (Fig. 8) has 8 WINE-2 boards (hereafter, W-boards; Fig. 9) and each G-board has 16 WINE-2

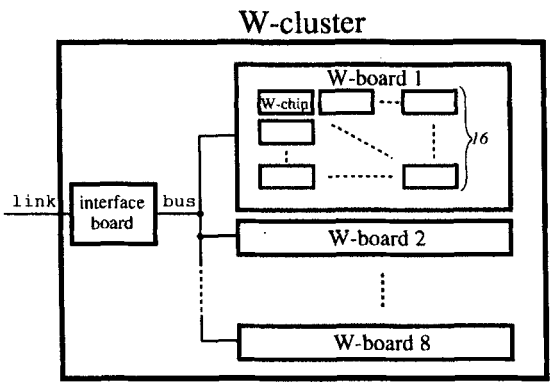

FIGURE 8 Structure of a W-cluster.

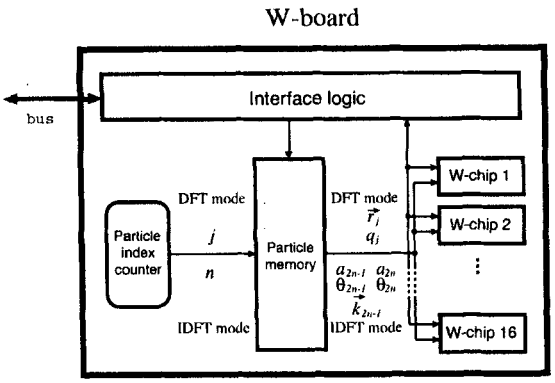

FIGURE 9 Block diagram of a W-board.

chips (hereafter, W-chips; Fig. 10). A W-chip has eight W-pipelines (Figs. 11 and 12).

W-chips on a W-board perform DFT (Discrete Fourier Transform) based on Eqs. (9) and (10) in DFT mode, and IDFT (Inverse DFT) based on Equation (6) in IDFT mode.

Figures 11 and 12 show W-pipelines in DFT and IDFT modes, respectively. A W-pipeline calculates $\sin(x)$ and $\cos(x)$ by segmented second polynomial interpolation. Coefficients of the polynomials are stored in a ROM in a W-pipeline.

The calculation speed of a W-chip corresponds to about 19.2 Gflops in DFT mode and 23.7 Gflops in IDFT mode at a clock frequency of 80 MHz.

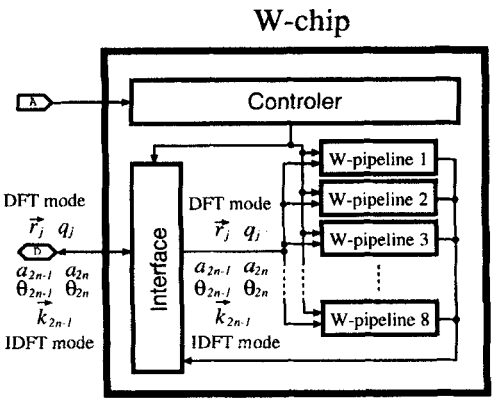

FIGURE 10 Block diagram of a W-chip.

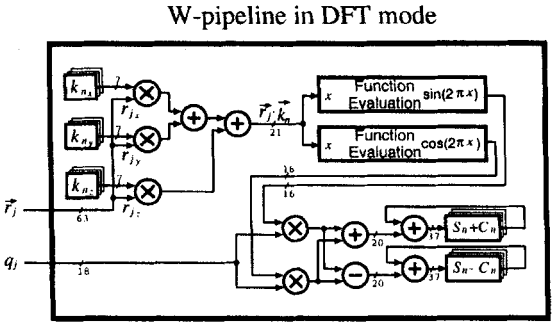

FIGURE 11 Block diagram of W-pipeline in DFT mode.

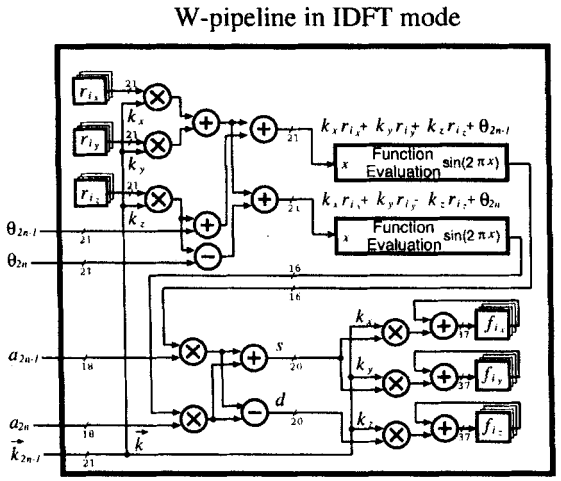

FIGURE 12 Block diagram of a W-pipeline in IDFT mode.

Engineering samples of a W-chip has been developed with LCB500K technology by LSI Logic Corp., whose design rule is 0.5 μm and operation voltage is 3.3 volt. The number of transistors of a W-chip is about 1.2 million.

4. PREDICTED PERFORMANCE

The calculation time, T_{step}, of MDM for one time-step is calculated by:

$$T_{\text{step}} = T_{\text{host}} + T_{\text{pipe}} + T_{\text{com}}, \tag{23}$$

where T_{host} is the calculation time in the host computer, T_{pipe} is the calculation time in MDGRAPE-2 and WINE-2, and T_{com} is the time for communications. They are expressed as:

$$T_{\text{host}} = N_{fp} N t_h, \tag{24}$$

$$T_{\text{pipe}} = \frac{\beta\gamma}{\pi}(54 t_g t_w)^{1/2}(-\ln\xi)^{3/2} N^{3/2}, \tag{25}$$

$$\begin{aligned} T_{\text{com}} = \{&25N + \gamma[620(t_w/t_g)^{1/2} + 110(t_g/t_w)^{1/2}] \\ &\times (-\ln\xi)^{3/2} N^{1/2}\} t_c, \end{aligned} \tag{26}$$

where N_{fp} is the number of floating-point operations required for the calculation of bonding force, time integration of a particle, and coordinate transformation, t_h is the time required to perform one floating-point operation in a host computer, t_g is the time required to calculate one pair-wise interaction for real-space part of Coulomb or van der Waals force in MDGRAPE-2 in a peak speed, t_w is the time required to calculate one pair-wise interaction for wavenumber-space part of Coulomb force in WINE-2 in a peak speed, t_c is the time required for transferring a word (64-bit) through a link, ξ is the truncation error of Ewald sum [16], β is the loss parallel efficiency of pipelines because of the mismatch of the number of parallelism with the multiplication of total number of pipelines, and γ is the loss of efficiency of pipelines caused by the mismatch of α from optimal value due to the discreteness of the number of cells for cell-index method. Values for these parameters are shown in Table I. When N becomes larger, T_{pipe} becomes dominant because it is proportional to $N^{3/2}$, while other parts are proportional to N or $N^{1/2}$. The trend of the coefficients, β and γ, is decrease, and they approaches to 1 as the number, N, of particles increases. When $N = 5 \times 10^5$, $\beta = 1.1$. When $N > 2 \times 10^5$, γ is less than 2. Details for the performance including the analysis of β and γ will be presented elsewhere.

TABLE I Constant values

Parameter	*Value*	*Description*
N_{fp}	4.0×10^2	
t_h	8.3×10^{-11}	12 Gflops
t_g	9.8×10^{-13}	
t_w	5.1×10^{-13}	
t_c	8.0×10^{-10}	10 Gbyte/sec
ξ	1.0×10^{-5}	

Figure 13 shows the time span of MD simulation against the number, N, of atoms. Thick solid and dashed curves show the effective and the peak performances of MDM, respectively. We assumed 7 days (6×10^5 seconds) of CPU time and 0.5 fs of a time-step. Thin short-dashed curves above and beneath are plotted for $\beta = \gamma = 1$ and $\beta = 1$, $\gamma = 2$, respectively [see Eq. (23)]. Since the effective speed (thick solid curve) is almost between these two curves, the estimation by Eq. (23) is satisfactory.

The loss of efficiency (γ) of pipelines due to the discreteness of the number of cells for cell-index method causes the shallow dips around $N = 10^5$ and $N = 10^6$. Small cliffs in the curve are caused by the loss of parallel efficiency (β) due to the mismatch of the number of parallelism with the multiplication of total number of pipelines. The difference between peak and effective performances is relatively small (less than a factor of 3) for N larger than 10^6. The peak performance is calculated by neglecting the calculation time for a host computer, loss of efficiency of the pipelines, and communication time, *i.e.*, $T_{\text{host}} = T_{\text{com}} = 0$ and $\beta = \gamma = 1$. When $N = 10^6$, MDM will achieve about 1/3 of a peak performance (33 Tflops). It can calculate 3.2×10^6 time-steps (1.6 ns) of an MD simulation with a million atoms in a week.

On the other hand, the number of atoms is limited to several tens of thousands, when we perform 1 ns of MD simulation by a moderate speed of

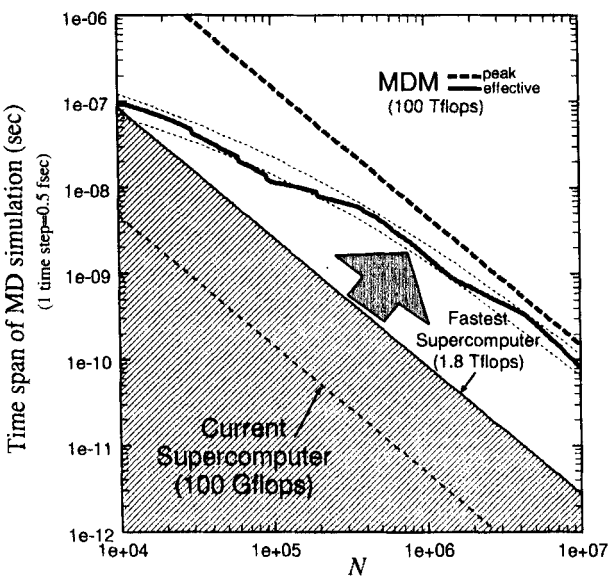

FIGURE 13 Time span of MD simulation.

supercomputer with a peek speed of 100 Gflops (thin long-dashed line). Even with the currently fastest supercomputer (1.8 Tflops; thin solid line), you can only perform up to 85 ps of MD simulation with a million atoms at its peak speed: MDM is about 20 times faster than the fastest supercomputer.

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