UDC 519.68: 681.326

Development and Application of MASPHYC Computational Material Design System "Application Package in HPC"

●Munetaka Takeuchi ●Takahiro Ishigai ●Katashi Ishibashi

(Manuscript received April 28, 1997)

Although high performance is one of the main criteria when considering whether to introduce a supercomputer, users are paying much more attention to the quantity and quality of application packages available for a candidate machine. In response, Fujitsu has developed original packages and ported de facto standard packages for supercomputers.
This paper describes the status of application packages available for Fujitsu VX/VPP series computers. Also, this paper introduces Fujitsu's MASPHYC computational material design system and describes its performance on a VPP500.

1. Introduction

The market reputation of supercomputers used by large organizations such as universities and national institutes greatly depends on quality factors such as the hardware performance and capability of the compiler. However, as more and more for-profit enterprises, especially major manufacturers, begin using supercomputers, the quality and quantity of application packages used in the field of Computer Aided Engineering (CAE) are becoming more important.

Since 1985, when Fujitsu released its VP50 supercomputer, Fujitsu has been using two methods to promote the available application packages.

One method is to promote porting of de facto standard independent software vendor (ISV) packages used in for-profit enterprises and packages developed in universities and research institutes. The other method is to develop packages using Fujitsu-originated concepts.

This paper first looks at the status and strategies for package porting. Then this paper introduces one of the packages developed by Fujitsu, the computational material design system MASPHYC.

2. Porting and Development of Application Packages

2.1 Porting

Figure 1 shows how Fujitsu is promoting porting of application packages for supercomputers in Japan, the U.S., Australia, and Europe. Packages developed in the U.S. were popular in all these regions, but recently, packages developed in Europe are becoming popular. Therefore, in March 1996, to meet the market requirements, Fujitsu established the Fujitsu European Centre for Information Technology (FECIT), in addition to the porting centers already established in the U.S., Australia, and Europe. FECIT is engaged in porting activities and is also developing parallel application packages and making a study about the future of parallel processing. **Table 1** lists some example application packages for VX/VPP that have been ported through these activities.

The U.S. and Japan have been the dominant manufacturers of vector supercomputers, which are a main product in high-performance computing. Europe, on the other hand, has concentrated on improving parallel processing software.

A typical example is the Europort project,

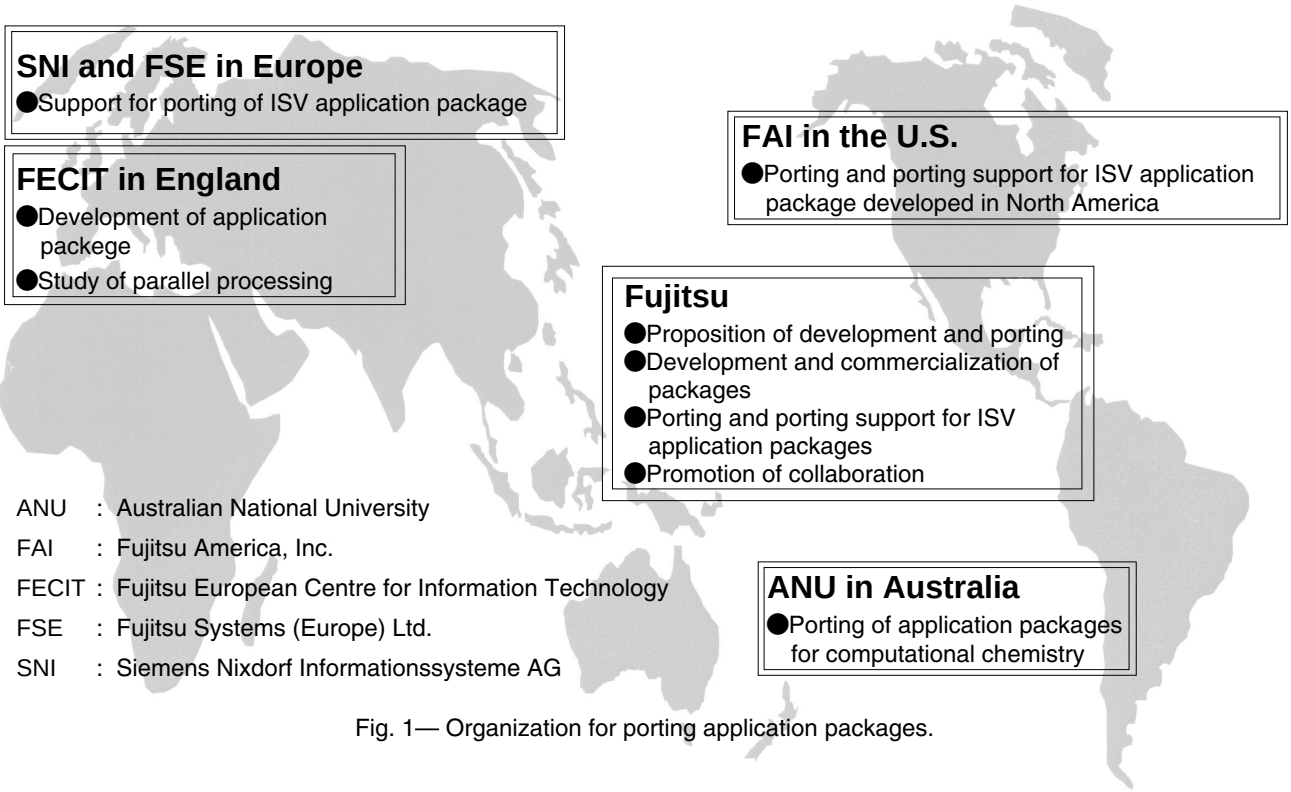

Fig. 1— Organization for porting application packages.

Table 1. Typical application packages for VX/VPP

Collision and impact analyses	Computational fluid dynamics	Computational chemistry	Electromagnetic field analysis	Mathematical library
ABAQUS/Explicit	ADINA-F	AMBER	ELF/MAGIC	IMSL (F77)
DYNA3D	FIRE	CADPAC	JMAG-DYN	IMSL C
LS-DYNA3D	FLOW3D	DISCOVER	JMAG-DYNPL	IMSL F90
PAM-CRASH	FLUENT 4.3	DMOL	JMAG-WORKS	NAG
PAM-STAMP	# FUJITSU/α-FLOW	GAMESS-US	MAGNA/FIM	# SSLII/VP
RADIOSS-CRASH	KIVA2	GAUSSIAN94	NISA/EMAG	# SSLII/VPP
Structure and vibration analyses	KIVA3	# MASPHYC		**Others**
ABAQUS/Standard	PAM-FLOW	MOLPRO94		# AVS
ADAM	PHOENICS-2	MOPAC93		BOOM
ADINA	SCRYU	# MOZYME		# CGMS
ADINA-T	STAR-CD	XPLOR (Academic)		# GRAPHMAN
FINAS	STREAM			# FSPICE/UVX
GENESIS				NCAR graphics
MARC				VisLink
MSC/ABAQUS				
MSC/NASTRAN				
NISAII				
OPTISHAPE				
# POPLAS/FEM5				
SAP4				
SURFES				

Note) This table contains scheduled products. # : Fujitsu products. The application package names are trademarks of the developers or suppliers.

which was carried out between 1994 and 1996 to promote parallel processing in practical packages. The most significant feature of this project was that not only hardware and software vendors participated, but also end users who wanted to perform complicated analyses. The Europort project resulted in success for parallel processing in packages.

Fujitsu would adopt the results of such projects effectively and promote vector parallel processing for higher performance of the VX/VPP series. Also, Fujitsu will port application pack-

Table 2. Parallel processing packages to be ported or developed

Field	VX/VPP series	AP3000 series
Mathematical library	IMSL, SSLII/VPP	BLAS, ScaLAPACK, SSLII/AP
Computational chemistry	AMBER, GAMESS-US, DISCOVER, DMo1, MASPHYC	AMBER, GAMESS-US, MOPAC93, MASPHYC
Fluid analysis	(to be determined)	(to be determined)
Collision and structure analyses	LS-DYNA3D	MARCK6.3
Electronic CAE	————	Mentor Graphics, EDA application software Cadence, EDA application software Accufield (Electromagnetic interference analysis)

Note) The application package names are trademarks of the developers or suppliers.

ages that provide higher performance on the AP3000 scalar parallel server, which was put on the market in 1996. **Table 2** lists the application packages to be ported.

2.2 Development

Porting of popular application packages is not sufficient in fields that are rapidly expanding, so for these and entirely new fields, new packages must be developed.

Therefore, for a long time Fujitsu has been developing packages based on the following three points:

1) Collaboration with leading customers and researchers
2) Participation in national development projects
3) Commercialization using Fujitsu-originated technologies.

The Research Center for Computational Science (RCCS) in the Package Business Group, and the Computer Chemistry System Department (CCS) in the Systems Engineering Group have been developing new packages for CAE and computational chemistry for advanced supercomputers.

Some typical Fujitsu packages are described below.

2.2.1 MOZYME (Computational chemistry)

MOZYME is based on MOPAC, a world-famous package for application of the semiempirical molecular orbital method. MOZYME uses a newly developed high-speed algorithm in which the computation time is proportional to N (N is the size of the system) to enable large molecules such as enzymes to be analyzed. This software was developed by Dr. Stewart, who developed MOPAC, and Fujitsu.

2.2.2 MASPHYC (Material Design)

MASPHYC is a general-purpose molecular dynamics package developed independently by Fujitsu. MASPHYC can calculate macroscopic characteristics of materials from microscopic features. Details of this software are given later.

2.2.3 FUJITSU/α-FLOW (Fluid analysis)

α-FLOW is a 3-D general-purpose fluid dynamics analysis system created by Fujitsu as a commercial product. It is based on the results of the α project, which was conducted to promote development of fluid analysis software between manufacturers, public offices, and institutes. α-FLOW enables high-speed processing on a supercomputer and it has an easy-to-use interface.

2.2.4 POPLAS/FEM5 (Structure analysis)

POPLAS/FEM5 is a structure analysis system for analyzing linear static/dynamic stress and heat conduction of three-dimensional structures with arbitrary shapes using the finite element method. This software can operate on a supercomputer, engineering workstation, or personal computer and interacts well with other well-known CAD and LA systems.

2.2.5 FSPICE (Circuit analysis)

FSPICE is Fujitsu's commercial enhancement of the SPICE circuit analysis software developed at the University of California. It is an exclusive vectorized circuit simulator that is very useful for analyzing large-scale circuits. FSPICE has reinforced I/O systems.

3. Computational material design system MASPHYC

3.1 Material design using computational simulation

It was said that the application of computational chemical simulation to actual material designs was premature because memory capacities and CPU performance were too low. However, current computer hardware with its high processing speed, large memory capacity, and rapidly progressed visualization technology have made the application practical.

The performance of the molecular orbital method[Note1)] and molecule dynamics method[Note2)] is immediately improved by vector and parallel processing. These fields now show promise.

Particularly, in materials fields such as advanced ceramics and functional materials such as liquid crystals for display devices, highly technical experiments are being done to control the structures at the molecular and atomic levels and to use high-resolution analytical devices. However, recent requests for quicker development cycles for new products are casting doubts on the carpet bombing experimental method, which is expensive and takes a long time.

Therefore, to promote the material sciences, not only more experiments but also more computational simulations should be done.

Fujitsu predicted the above situation 10 years ago, and responded by independently developing a supercomputer package based on molecular dynamics. In 1992, Fujitsu released a computational material design system called MASPHYC that came from this development effort. MASPHYC has been repeatedly upgraded to simplify its operation, enhance its functions, improve performance, and obtain higher quality.

3.2 About MASPHYC

MASPHYC (MAterial design System by means of computational PHYsics and Chemistry) is an application package for computational material design systems using the molecular dynamics method. The molecular dynamics method is a typical procedure in computational chemistry. It enables the macroscopic characteristics of materials such as thermal expansion and elastic modulus to be calculated using masses and velocities of atoms or molecules and interactions (called potentials hereafter) between atoms or molecules. It also makes it possible to trace the dynamical properties to be simulated.

MASPHYC has various features that are not provided in other molecular dynamics software, namely:

1) Easy handling of the mouse and an advanced visualization system make it easy to set up the

Note 1) An approximation describing the electronic states in molecules. This method uses the viewpoint that all electrons in a molecule belong to a molecular orbital diffused over the entire molecule. There are many types of approximation procedures for obtaining a molecular orbital: for example, all electrons are handled, only specific electrons are handled, the precise value of the required energy is obtained from integral calculation (ab-initio), or some integral values are regarded as empirical parameters (semiempirical molecular orbital method). Progress in computers has greatly advanced the molecular orbital methods for studying electronic structure, optical/electromagnetic characteristics, and reactions of molecules.

Note 2) A method of studying the macroscopic characteristics of a system by regarding the atoms as mass points in motion according to Newtonian mechanics, obtaining time-sequenced microscopic data about positions and velocities of atoms through numeric integration of the motion equation, analyzing the data using statistical mechanics, and calculating the physical properties. Molecular dynamics is used not only to study the thermodynamical properties of a system, but also to examine its dynamical properties.

initial configuration of even complex models (e.g., the bilayer structure of lipids which form the fundamental framework of cell membranes, and adsorption of gases in porous crystals like silica gel).
2) Simulations can be made for any temperature/pressure combination.
3) Includes Potential Library, which is a Fujitsu-originated product (described later).
Unlike conventional software, MASPHYC can handle not only organic material systems such as amino acids and crystals, but also inorganic material systems such as metals and ceramics.
4) The highly tuned vector and parallel processing enables extremely high-performance calculation on the VPP series.

3.3 MASPHYC system configuration

Figure 2 shows the system configuration of MASPHYC. MASPHYC consists of MASPHYC/WB and MASPHYC/MD. MASPHYC/WB is the workbench that controls the pre-processing and post-processing. MASPHYC/MD handles the calculations for molecular dynamics.

3.3.1 MASPHYC/WB

All instructions for MASPHYC/WB are executed by clicking the mouse basically, and all required MASPHYC/WB submodules are automatically launched. MASPHYC/WB can be used with no technical knowledge of computers. MASPHYC/WB consists of the five submodules explained below.

1) Database control system

The database control system consists of the crystal database, molecule database, and potential library. The potential library is based on a concept unique to MASPHYC. The potential li-

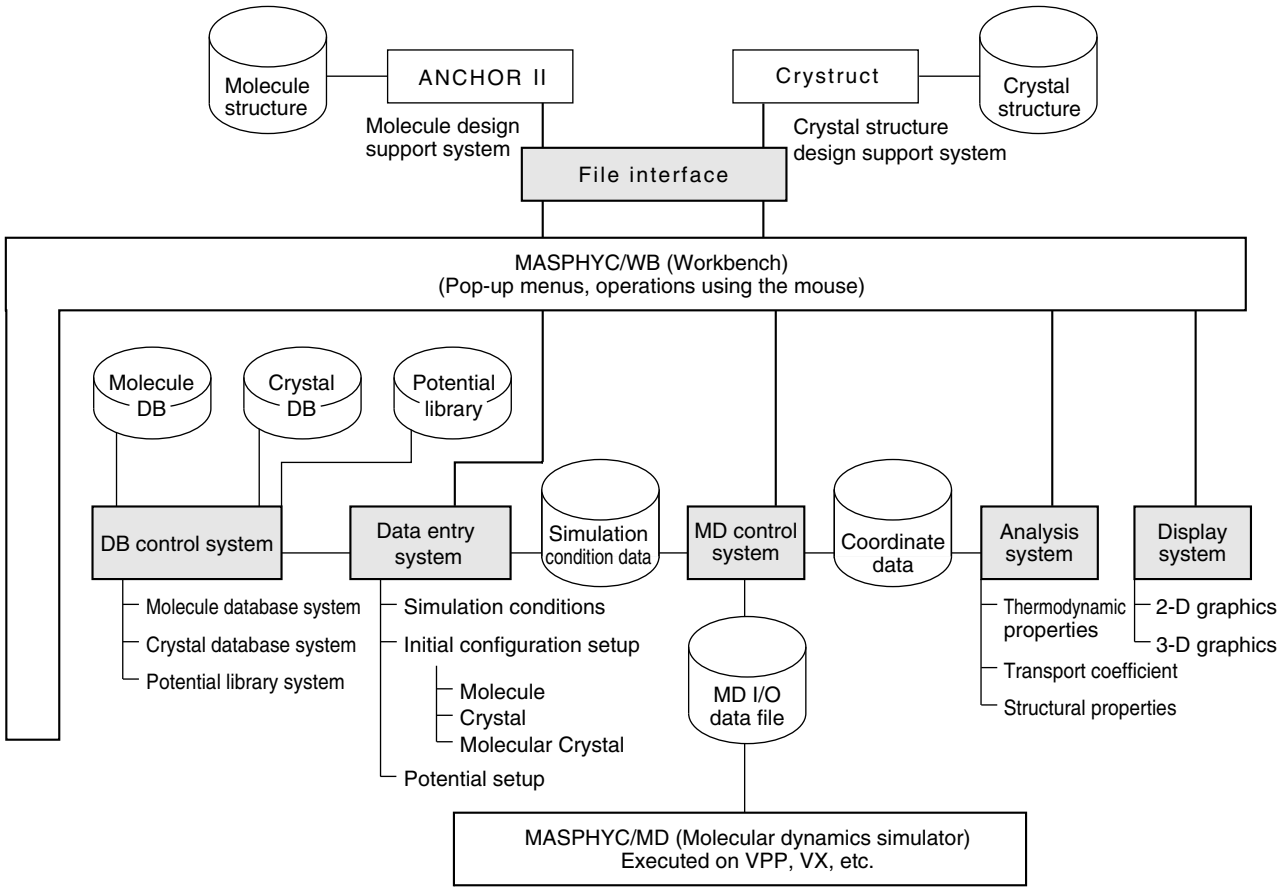

Fig. 2— Outline of MASPHYC.

brary records and controls the potential functions and parameters between atoms, which are fundamental to calculations related to molecular dynamics. By adding new potential functions to the potential library, users can enhance the scope of their computational objectives. This system can easily handle ceramics, semiconductor materials, and metals, which have been hard to handle with previous packages.

Table 3 lists the potential function names and applicable materials currently registered. The major feature of the potential library is its expandability; more potential functions will be added to it in the near future.

2) MD data entry system

This system is used to input data. All operations can be handled using the mouse, so there is no need to enter cumbersome line commands. The created data is stored in a file, then the MD control system reads the input data, inputs it to MASPHYC/MD, and starts the simulation.

3) MD control system

MD input data created on the MD control system is transferred to a computer (referred to as the host hereafter) in which MASPHYC/MD is installed. Then, MASPHYC/MD starts execution using the MD input data. The MD control system can display simulation status details about MASPHYC/MD such as the CPU elapsed time, processing status, and memory-usage amount. **Figure 3** shows how the status is displayed.

After checking that the simulation was normal ended , the output data of MASPHYC/MD can be transferred to MASPHYC/WB by simple mouse operations.

4) Analysis system

The analysis system reprocesses the output data of MASPHYC/MD to calculate the self-diffusion constants or radial distribution functions of the atoms, etc. The results of the calculation are displayed on the display system described in the next paragraph. All calculation conditions can be set on the windows. MASPHYC/WB executes all analyses.

Table 3. Potential functions currently registered

Potential function name	Applicable system
LJ potential	Rare gas, organic material, biochemical materials
BMH potential	Ionic crystal, inorganic oxide, silicate glass
Johnson potential [1)]	Iron, nickel
Stllinger-Weber potential [2)]	Silicon, germanium
RGL potential [3)]	Metal
Finnis-Sinclair potential [4)]	Metal
Tersoff-Ohhira potential [5), 6)]	Semiconductor, carbon, hydrogen
Bond-stretch potential (2 types)	Organic materials, biochemical materials
Bond-bending potential (3 types)	Organic materials, biochemical materials
Dihedral angle potential (3 types)	Organic materials, biochemical materials
Out-of-plane potential (3 types)	Organic materials, biochemical materials

5) Display system

The display system directly displays the results from MASPHYC/MD and the outcome of the analysis system using 2-D or 3-D graphics. The following information is displayed: diffusion constants, radial distribution functions, voronoi polyhedron analysis, thermodynamic properties such as temperatures and pressures, and changes in the microscopic structures and the coordinates of atoms and molecules.

3.3.2 MASPHYC/MD

MASPHYC/MD is a simulator for molecular dynamics that can operate on various platforms, for example, the VX or VPP series.

The algorithm used in MASPHYC/MD is outlined below.

1) Equation of motion (for particle system)

The simultaneous equation below is Newton's equation.V is the potential energy of the system. r_i indicates the coordinates of the i-th particle, and $\{r_i\}$ indicates the set $\{r_1, r_2, r_3 \ldots r_N\}$, where N is the number of particles in the fundamental cell.

$$\frac{d}{dt}\left(m_i \frac{\boldsymbol{r}_i}{dt}\right) = -\frac{dV(\boldsymbol{r})}{d\boldsymbol{r}_i}$$

To keep a constant temperature and pressure, it is necessary to artificially incorporate the external force or heat flow into the equation of motion. An approximation of this incorporation is obtained

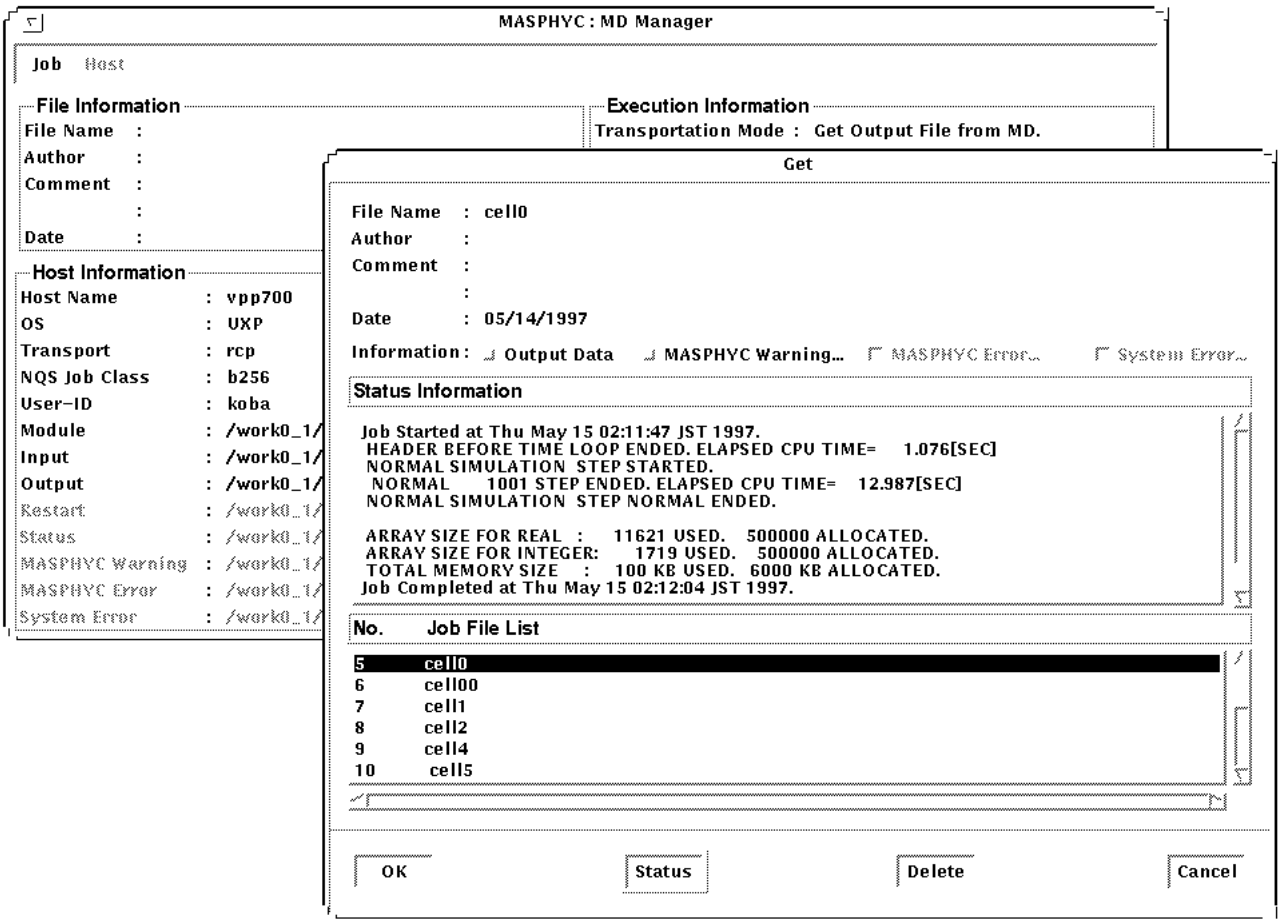

Fig. 3— Example of host status window.

by using the concept of an expanded system.

The canonical equations shown below indicate the equations of motion for particles and an MD cell and heat bath when NTP ensemble simultaneously controls the temperature and pressure.

$$\frac{d}{dt}\left(m_\alpha \frac{d\boldsymbol{s}_\alpha}{dt}\right) = -\boldsymbol{h}^{-1}\frac{d\varphi(\boldsymbol{q})}{d\boldsymbol{q}_\alpha} - m_\alpha \boldsymbol{G}^{-1}\frac{d\boldsymbol{G}}{dt}\frac{d\boldsymbol{s}_\alpha}{dt} - \frac{m_\alpha}{f}\frac{df}{dt}\frac{d\boldsymbol{s}_\alpha}{dt}$$

$$\frac{d}{dt}\left(W\frac{d\boldsymbol{h}}{dt}\right) = \sum_\alpha m_\alpha \boldsymbol{h}\frac{d\boldsymbol{s}_\alpha}{dt}\left(\frac{d\boldsymbol{s}_\alpha}{dt}\right)^t - \sum_\alpha \frac{\partial\varphi(\boldsymbol{q})}{\partial\boldsymbol{q}_\alpha}\boldsymbol{s}_\alpha^t - \boldsymbol{P}\boldsymbol{\Lambda} - \boldsymbol{h}\boldsymbol{\Gamma} - \frac{W}{f}\frac{df}{dt}\frac{d\boldsymbol{h}}{dt}$$

$$\frac{d}{dt}\left(Q\frac{df}{dt}\right) = f\left(\sum_\alpha \frac{\boldsymbol{\pi}_\alpha^t \boldsymbol{G}^{-1}\boldsymbol{\pi}_\alpha}{m_\alpha} + \frac{1}{W}Tr\left(\boldsymbol{\Pi}^t\boldsymbol{\Pi}\right)\right) + \frac{Q}{f}\left(\frac{df}{dt}\right)^2 - fgk_BT$$

$$\left.\begin{aligned}\boldsymbol{s}_\alpha &= \boldsymbol{h}^{-1}\boldsymbol{q}_\alpha \\ \boldsymbol{\pi}_\alpha &= \boldsymbol{h}^t\boldsymbol{p}_\alpha\end{aligned}\right\}$$

$\boldsymbol{s}$ and $\boldsymbol{\pi}$ are canonical-transformed coordinate $\boldsymbol{q}$ and momentum $\boldsymbol{p}$, respectively. $\boldsymbol{h}$ is the matrix indicating the shape of the cell (the cell is a parallelepiped). $\boldsymbol{\Pi}$ is the momentum of the cell conjugate to $\boldsymbol{h}$. f is the scaling variable (Nose variable[7), 8)]) used to incorporate into the equations of motion the particle velocity changes due to transition of heat supplied from the heat bath to maintain a constant system-temperature. In the equations above, α indicates atom. Although MASPHYC can handle constrained-dynamics systems, it is not suitable for describing the equations of motion because the equations are too complex.

2) Numeral integration

The time evolution of an equation of motion

can be obtained using numeral integration. Although several procedures are known for direct solutions of second-order differential equations, MASPHYC uses a highly precise method, Gear[9]. The Gear method is a kind of predictor-corrector method.

3.4 MASPHYC application examples

As described above, MASPHYC has been applied to simulations of various materials such as biochemical materials (e.g., proteins and nucleic acids), polymers (e.g., plastics), and functional materials (e.g., liquid crystals), advanced ceramics, and metals and some remarkable results have been obtained. This section describes a practical application to dimyristoylphosphatidylcholine (DMPC) in liquid crystal phase that was done jointly by the Institute of Physical and Chemical Research and Fujitsu.

DMPC's lipid bilayer structure is the fundamental framework of cell membranes and has characteristics that reveal various important functions of organic membranes. To investigate the origin of its characteristics, it is necessary to analyze the structure and motion of lipid molecules and the water molecules around them at the atomic level; an efficient way to do this is to use molecular dynamics.

Table 4 lists the simulation conditions. **Figure 4** shows the status 600 picoseconds (1 picosecond = 1×10^{-12} seconds) after the start of the calculation.

In the initial configuration, the surfaces of the lipid bilayer are flat and parallel to each other. Then, when the simulation is started, the thicknesses of the two layers vary at local points in a random fashion. Also, it is clearly observed that the lipid bilayer prevents the passage of water molecules. This simulation is being continued to allow us to observe motions occurring over a longer time scale.

The atomic-level, picosecond-order motions that can be simulated using MASPHYC are absolutely impossible to observe in real experiments, even using the most advanced methods. MASPHYC therefore provides us with a means of discovering previously hidden mechanisms of biochemical organization, which, for example, can lead to breakthroughs such as new medicines.

Table 4. Simulating conditions for dimyristoylphosphatidylcholine

Ensemble	NTP (constant temperature and constant pressure)
Temperature	300 K
Pressure	1 atm
Time interval	0.2 fs (femtosecond)
Basic cell	$50 \times 50 \times 82$ Å (1 Å= 0.1 nanometer.)
Periodic boundary condition	Three-dimensional
Simulation system	Lipid molecule (DMPC) : 54molecules = 188×54 = 6 372atoms Water molecules : 1 080molecules = $3 \times 1\,080$ = 3 240atoms Total = 9 612atoms

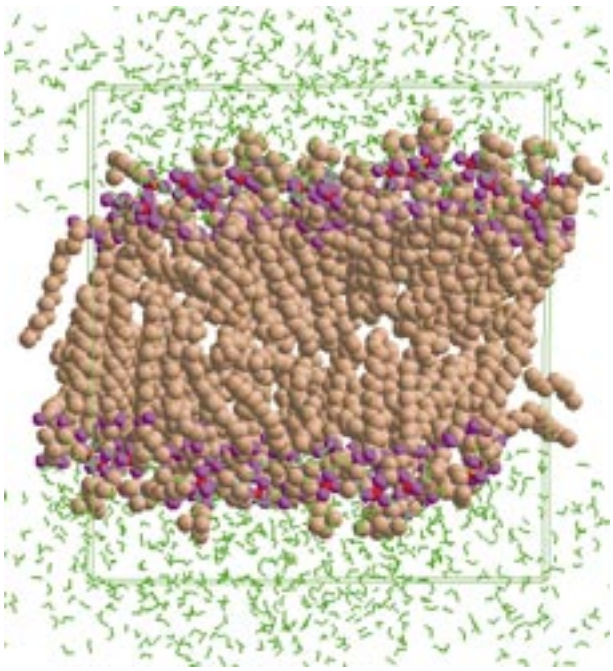

Fig. 4— Snap-shot of lipid bilayer structure.

3.5 Achieving high performance

The model used in the simulation contains 54 DMPC molecules and 1,080 water molecules, making a total of 9,612 atoms (DMPC is a large molecule; it contains 118 atoms). The CPU time re-

quired for a simulation depends on the length of simulation steps and the time interval between each simulation step. The time interval chosen for the lipid bilayer simulation was 0.2 femtosecond (1 femtosecond = 1×10^{-15} seconds), and to reach thermal equilibrium, the simulation must be run for several nanoseconds (1 nanosecond = 1×10^{-9} seconds).

As mentioned above, because of the large number of atoms and large simulation steps in the lipid bilayer simulation, and the fact that the most of CPU time consumed by two-body potential force calculations increases at a rate that is roughly proportional to the square of the number of particles, the simulation will take far too long to complete using general computer resources.

Figure 5 shows the structure of MASPHYC/MD. After vector tuning, CPU analysis indicated that two routines — two-body interaction calculation and coulomb interaction calculation — occupied more than 90% of the total CPU time. Therefore, parallel processing control lines were added to these two routines. **Table 5** lists the CPU times on a VPP500 for the lipid bilayer data described above. When two PEs were used the parallelization efficiency was 97%, and when 16 PEs were used the efficiency was 67%, showing that the parallelization is very effective.

A simulation covering 2 nanoseconds of real time and having 0.2-femtosecond steps would have a total of 10 million steps. Since the fastest workstation needs about 80 seconds to process each step, 10 million steps will take 8 billion seconds (about 25 years), making the calculation unfeasible if only a single PE is used. If we use only one PE of the VPP500, it would take as many as 17,388 hours (about two years). However, when 16 PEs are used, as shown in Table 5, processing a single step takes 0.58 seconds, so the 10 million steps can be completed in only 1,600 hours (about 67 days), which is feasible. This is a typical example of the benefit obtained by running the vector parallel processing application MASPHYC on a high-speed vector parallel processing computer.

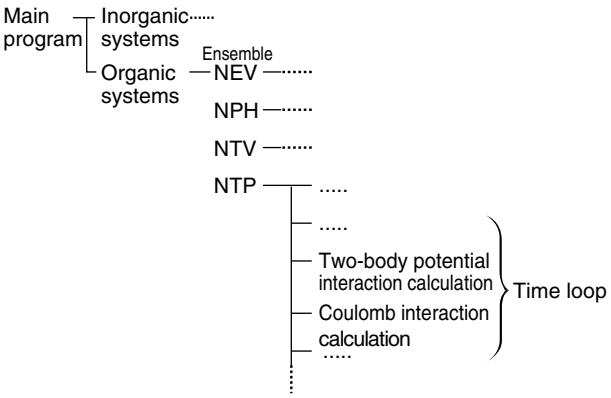

Fig. 5— Structure of MASPHYC/MD.

Table 5. Measured CPU time

Number of processors	1PE	2PE	4PE	8PE	16PE
CPU time (s/step)	6.26	3.25	1.68	0.96	0.58
Velocity rate (relative value)	1.0	1.9	3.7	6.5	10.8
Parallelization effect (%)	–	97	93	82	67

3.6 Current use of MASPHYC and future developments

The number of MASPHYC packages shipped is increasing year by year. Some notable users of the system are the Institute of Physical and Chemical Research, Nagoya University Computational Center, and Kanazawa University, all of which have VPP and VX systems for parallel processing. In addition, the Supercomputer Center of Kyushu University and two private enterprises have installed MASPHYC systems for parallel processing. MASPHYC is now being applied to simulations of liquid crystals, cell membranes, ceramics, semiconductors, metals, and other materials.

MASPHYC-SP (Surface Phenomena), which incorporates new concepts and original techniques, has been scheduled for release in the spring of 1997. This package supports simulations of deposition processes in materials that are essential to advanced technologies such as molecular beam epitaxy (MBE) and sputtering. The new package can also handle various surface phenomena such as adsorption, damage, and interface

structures.

Because of the ever growing demand for new materials and the increasing number of parallel processing computers in use, we are confident that MASPHYC will become very popular.

4. Conclusion

This paper explained how Fujitsu is developing and porting application packages for supercomputers, and gave an example of how one such package has been put to practical use.

Currently, various major application packages for the VX/VPP series are available. Application packages suited to parallel processing are being ported for the AP3000 series of parallel computation servers.

As well as MASPHYC, Fujitsu has developed and released various other packages which have become highly valued by users. Only a few supercomputer manufactures are developing and providing new application packages. Fujitsu is one of these manufacturers and will continue to meet its customers' needs in its own unique way.

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Munetaka Takeuchi received the M.E. in Chemistry from Hokkaido University in 1985.
He jointed Fujitsu Laboratories Ltd., Kawasaki in 1985, where he was engaged in research and development of advanced ceramics. He moved to Fujitsu Limited, Kawasaki in 1991, where he is currently developing and supporting computational chemistry software.

Katashi Ishibashi received the M.E. in Control Engineering from Kyushu Institute of Technology in 1968.
He jointed Fujitsu Limited, Kawasaki in 1968, where he was supporting laboratory and engineering automation systems. He is now working in the High Performance Computing Group.

Takahiro Ishigai received the M.E. in Nuclear Engineering from Nagoya University in 1976.
He joined Fujitsu Limited, Kawasaki in 1976. He is currently supporting scientific and engineering application software at Fujitsu's High Performance Computing Group.