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SIMULATION PROGRAM ON THE CRAY X-MP

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EARLY MIMD EXPERIENCE WITH A PLASMA PHYSICS SIMULATION PROGRAM ON THE CRAY X-MP*

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ABSTRACT

This paper describes some early experience with converting a plasma physics simulation program to the CRAY X-MP, a current multiple instruction, multiple data (MIMD) computer consisting of two processors with architecture similar to that of the CRAY-1. The computer program used in this study is an all Fortran version of SELF, a two species, one space, two velocity, electromagnetic, Newtonian, particle in cell, plasma simulation code. The approach to converting SELF to use both processors of the CRAY X-MP is described in some detail. The resulting multiprocessor version of SELF is nearly a factor of two faster in real time than the single processor version. The multiprocessor version obtains 58.2 ± 1 seconds of central processor time in 30 ± 5 seconds of real time. For comparison, the CRAY-1 execution time is 74.5 seconds. For SELF, which is mostly scalar coding, the CRAY X-MP is about 2.5 times faster overall than the CRAY-1.

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INTRODUCTION

The purpose of this paper is to document some of our earliest experience with running a physics computer program on a commercially available multiple instruction, multiple data (MIMD) computer, the CRAY X-MP.¹ We hope thereby to encourage others to explore the new world of parallel execution of physics codes. We begin by discussing our reasons for performing this study and for making our particular choice of physics program. We then establish our terminology and describe the plasma physics simulation code SELF. Our approach to parallelizing SELF and our results are discussed. Finally, our conclusions and recommendations for future work are presented.

BACKGROUND

Accessible, usable, and useful MIMD computers are still very rare. In our view, to be useful, an MIMD computer must offer performance superior to that of the seven year old CRAY-1.² To be usable, sufficient software must be provided. To be accessible, there needs to be a fairly wide distribution of machines.

CRAY X-MPs are just now entering the field. Currently, Cray Research, Inc., has one installed at Mendota. NASA Ames Research Center has just received delivery. Her Britannic Majesty's Atomic Weapons Research Establishment and the Los Alamos National Laboratory will each install a machine during the fourth calendar quarter of 1983. Other laboratories including the Lawrence Livermore National Laboratory will follow in 1984. Table 1 contains a list of the location of the first twelve machines. Consequently, CRAY X-MP's are becoming fairly widely distributed.

The usability issue is not so easily dismissed. Because of the heretofore dearth of MIMD machines, computational physicists, numerical analysts, and computer programmers have little experience with running real physics programs on such machines. Not only is a new set of performance related issues present, but there are new issues of logical correctness, language constructs, and operating concepts. We have so little experience that we are in much the same position today with respect to the parallel world as we were in the late 1960's with respect to the vector world.

This paper also offers light on the subject of usefulness of the CRAY X-MP. The amount of work required of the computational physicist to obtain a 25% speed up is zero. To obtain a factor of 2.5 speed up requires more work. For a broad class of Monte Carlo codes, of which the particle in cell plasma simulation is a leading example, the amount of work is minimal.

TABLE 1. Current sites of CRAY X-MP machines.

<u>Location</u>	<u>Number of machines</u>
NASA - Ames	1
ECMWF	1
Chevron	1
Digital Production	1
Los Alamos National Laboratory	2
Department of Defense	2+
CEZE, France	1
AWRE, United Kingdom	1
Germany	1
Lawrence Livermore National Laboratory	1

The computer program SELF used in this study is a two species, one space, two velocity, self consistent, electromagnetic, Newtonian, particle in cell, plasma simulation code. It was chosen for a number of reasons. While small in size, SELF is a real physics research tool in that a number of papers^{3,4} have been published using it. The Fortran version of SELF used here contains the same physics as that used in published studies. It is a real code not a pale imitation or stripped down version of the real thing. SELF is extremely well documented⁵ and was also used as a benchmark in a computer acquisition.⁶

SELF is a member of a whole family of plasma simulation codes^{5,7} and a direct progenitor of a very sophisticated multi-dimensional plasma simulation code called CCUBE.⁸ In most ways, SELF is typical of a whole class of plasma simulation codes, so that what we learn from the exercise of putting SELF on the CRAY X-MP can be directly applied to other codes. Finally, the author was familiar with SELF, had a copy on his shelf, and thought that it would be straightforward to run on the CRAY X-MP. In this, he was not disappointed.

MULTITASKING

Since the terminology used to discuss parallel processing has not yet been standardized, this section establishes some of the common concepts and terms. In general, we have attempted to follow that suggested in the Cray Research, Inc., Multi-tasking User's Guide.⁹

Multitasking is a mode of operation that provides for parallel processing of a single program by two or more processors. Parallelism may be achieved by dividing a program into two or more parts that can be executed at the same time. A program that can efficiently be multitasked will see its wall clock time as measured from start to finish on a dedicated system, reduced when compared with an identical single task program.

It is commonly believed that the best theoretical gain that can be achieved from multitasking is a factor of n where n is the number of processors. On real processors, this hypothesis is known to be untrue. The best theoretical gain may actually be greater than n because of reduced memory conflicts, and improved instruction buffer management.

In general, less than a factor of n improvement will be seen in real programs. A program may not be separable into parts which execute in the same amount of time. Even where identical code without explicit logical data dependencies executes with different input data, execution times will not be identical because of memory conflicts. Those parts that can be multitasked may have dependencies on one another that result in one or more tasks having to wait until another completes some operation. Finally, depending on the primitives concepts provided by the compiler, library and operating system and on their efficiency of implementation, some amount of multitasking overhead will occur.

As indicated previously, the parallel world is potentially a much more perilous world. Many of us have had programs go astray when only one compute task was being multitasked with one or more input/output operations. Asynchronous errors are especially difficult to track down, because sometimes you see them, sometimes you don't - all depending on system activity and task timing. When two or more parts of a program may be executed at the same time, the potential for even more timing problems arise. Again these problems are often not reproducible. In addition, there are few tools available to help track them down. Worse, it is not entirely clear what tools would prove useful and usable.

Multitasking is today at the same state as vectorizing was in the late 1960's. There is little automatic help in code analysis. There are many who believe such analysis is impossible. And there are very few working at solving the problem. As with vectorization, so too with multitasking. Once adequate experience is gained, we will be able to find the right concepts and figure out what primitive operations are useful and what tools are needed and what language constructs are viable. At that point, at least some of the impossible will become possible. This paper is one of the first steps along the road to a better understanding of the multitasking world.

At the present time, only COS,¹⁰ the CRAY Operating System from Cray Research, Inc., supports multitasking on the CRAY X-MP. CTSS, the LTSS/NLTSS dual system and

NLTSS do not yet support multitasking. COS, CFT,¹¹ the CRAY Fortran Compiler, and their support libraries define a number of useful concepts, chief among them are TASKS, LOCKS, and EVENTS.

For simplicity, we use only the task concept. The task primitive operations which we use, are TSKSTART and TSKWAIT. TSKSTART initiates a task and TSKWAIT waits for the task to complete. Table II provides additional information.

TABLE II. Description of TSKSTART and TSKWAIT.

TSKSTART initiates a task

CALL TSKSTART (task-array, name, list)

task-array	A two or three word task control array to be used for this task. Word 1 must be set to the length of the array, either 2 or 3. Word 3, if used, must also be set. On return, word 2 will be set to a unique task identifier that must not be changed by the program.
name	External entry point at which task execution is to begin. This name must be declared EXTERNAL in the program or subroutine making the call to TSKSTART.
list	The list of arguments to be passed to the new task when it is entered. This list may be of any length.

TSKWAIT waits for the task to complete execution

CALL TSKWAIT (task-array)

task-array	Task control array as defined above.
------------	--------------------------------------

SELF

This section describes the SELF computer program for the one-dimensional numerical simulation of collisionless plasmas. SELF solves the Vlasov equation in very limited regions of phase space by means of a simple Monte Carlo technique, that of following trajectories of simulation particles as they move under the influence of self-consistent electromagnetic fields.

A time-centered difference approximation of the Lorentz force law, formulated in Newtonian form, is used to advance the particle positions and velocities. Only the X position of each particle is carried in the calculation, while both X and Y velocity components are used. In the limited region of phase space described by the code,

velocities and positions can vary continuously up to the computer round-off error. The particles move through a periodic grid of uniform spacing, a particle disappearing out one end of the grid reappearing at the other end. Charge and current densities are calculated at cell centers by inverse linear interpolation of particle positions and velocities. From these, electromagnetic fields are determined at the cell edges using Maxwell's equations. The particles are then moved using the linearly interpolated fields. This loop is continued for as long as necessary to obtain a solution to the problem of interest.

To facilitate comparison of calculated results with those of others and to increase program running speed, the relativistic "external" scaling shown in Table III is used (Relativistic Scaling Scheme). The unit of time is $1/\omega_p$, where ω_p is the plasma frequency. The unit of velocity is c , the speed of light; and hence, the unit of distance is c/ω_p . The electric and magnetic fields have units

$$\sqrt{4\pi n_e m_e c^2}$$

where n_e is the number density of electrons and m_e is the electron mass. This choice for the fields allows easy display of field energies in keV/particle for direct comparison with electron and ion temperatures. This scheme is "external" in the sense that results are printed out in these units. In addition to this external scaling, SELF has "internal" scalings which are used further to increase computational speed. These are discussed below.

The organization of SELF is along the following lines. There is a main program in which all constants are defined and scale factors computed and from which the subroutines doing the actual calculations are called. The structure of the calling sequence is divided into four parts. First, the particle positions and velocities are loaded, with the particle positions distributed uniformly and the velocities distributed in a shifted Gaussian. In addition, arrays are zeroed and any other necessary initial conditions are set. Second, fields are calculated. Third, the electrons are moved, then the ions are moved. After a number of iterations of field solving followed by pushing of electrons and ions, the program prints out appropriate energy diagnostics.

Printed output begins with a summary of all the initial parameters. All of these are first given in cgs units and a few are then given in machine units. Next, the time step number, the X electric field energy, the Y electric field energy, the total electric field energy, the magnetic field energy, the average particle thermal energies in both directions for the electrons and ions are given for each time step.

TABLE III. External scaling in SELF.

Variable in usual units		Dimensionless variable multiplied by scale factor
TIME	t(sec)	$\tilde{t} * (1/\omega_p)$
PARTICLE VELOCITY	V(cm/sec)	$\tilde{V} * c$
PARTICLE POSITION	X(cm)	$\tilde{X} * (c/\omega_p)$
ELECTRIC FIELD	E(statvolts)	$\tilde{E} * \sqrt{4\pi n_e m_e c^2}$
MAGNETIC FIELD	B(gauss)	$\tilde{B} * \sqrt{4\pi n_e m_e c^2}$

n_e = electron number density

m_e = electron mass

c = speed of light in vacuum

ω_p = $\sqrt{4\pi n_e e^2/m_e}$ = plasma frequency

e = charge on the electron

DIFFERENCING SCHEME

The differencing scheme used to move the particles assumes that particle positions, the electric fields, and the magnetic field are known at integral time steps and that particle velocities are known at odd half-integral time steps. So that current may be calculated after the particles have moved half their distance, the particles are pushed twice in a single time step.

Thus we use

$$X^{n+1/2} = X^n + V_x^{n+1/2} \frac{\Delta t}{2} \quad (1)$$

$$X^{n+1} = X^{n+1/2} + V_x^{n+1/2} \frac{\Delta t}{2} \quad (2)$$

$$V_x^{n+1/2} = V_x^{n-1/2}$$

$$V_x^{n+1/2} = V_x^{n-1/2} + \frac{\Delta t}{1 + \left(\frac{\Delta t}{2}\right)^2 (B_z^n)^2} \left[E_x^n + V_y^{n-1/2} B_z^n + \frac{\Delta t}{2} (B_z^n E_z^n - V_x^{n-1/2} B_z^{n2}) \right] \quad (3)$$

$$V_y^{n+1/2} = V_y^{n-1/2} + E_y^n \Delta t + \frac{B_x^n}{2} (V_x^{n+1/2} + V_x^{n-1/2}) \quad (4)$$

Equation (3) is first used to calculate $V_x^{n+1/2}$; then $V_y^{n+1/2}$ is calculated from Eq. (4). The particles are then pushed using Eq. (1) and the current in each cell calculated directly thereafter. The final push using Eq. (2) is then made; it is followed immediately by a calculation of the particle (charge) density in each cell. The area weighting scheme is used in computing charge density and current.

From the new particle charge densities, a new E_x^{n+1} is determined by direct integration. The wave equation for A_y in terms of J_y is solved by

$$A_y^{n+1/2} = 2A_y^{n+1/6} - A_y^{n-1/6} + (\nabla^2 A_y^{n+1/6} + J_y^{n+1/6}) \left(\frac{\Delta t}{3}\right)^2 \quad (5)$$

$$A_y^{n+5/6} = 2A_y^{n+1/2} - A_y^{n+1/6} + (\nabla^2 A_y^{n+1/2} + J_y^{n+1/2}) \left(\frac{\Delta t}{3}\right)^2 \quad (6)$$

$$A_y^{n+7/6} = 2A_y^{n+5/6} - A_y^{n+1/2} + (\nabla^2 A_y^{n+5/6} + J_y^{n+5/6}) \left(\frac{\Delta t}{3}\right)^2 \quad (7)$$

where we take

$$J_y^{n+1/6} = J_y^{n+1/2} \quad (8)$$

$$J_y^{n+5/6} = J_y^{n+1/2} \quad (9)$$

After A_y is advanced using the above three equations, the magnetic field and the Y component of the electric field are given by

$$B_z^{n+1}(X) = \{ [A_y^{n+7/6}(X+1) + A_y^{n+5/6}(X+1)] - [A_y^{n+7/6}(X) + A_y^{n+5/6}(X)] \} / 2\Delta X \quad (10)$$

$$E_y^{n+1}(X) = \{ [A_y^{n+5/6}(X+1) + A_y^{n+5/6}(X)] - [A_y^{n+7/6}(X+1) + A_y^{n+7/6}(X)] \} / 2(\Delta t/3) \quad (11)$$

OPTIMIZATION

To decrease running time, SELF has been optimized. In addition to the previously mentioned "external" scaling, the equations of motion have been rescaled.

The rescaling is accomplished as follows:

Redefine the following variables: $\tilde{X}$, $\tilde{V}_x$, $\tilde{V}_y$, $\tilde{E}_x$, $\tilde{E}_y$, and $\tilde{B}_z$ as shown below.

$$\tilde{X} = X/\Delta X \quad (12)$$

$$\tilde{V}_{(x,y)} = V_{(x,y)} \frac{\Delta X}{2\Delta X} \quad (13)$$

$$\tilde{B}_z = -B_z \Delta t \quad (14)$$

$$\tilde{B}_z (\text{ion}) = B_z \Delta t \frac{m_e}{m_i} \quad (15)$$

where m_e = mass of electron and m_i = mass of ion.

$$\tilde{E}_x = -E_x \frac{(\Delta t)^2}{2\Delta X} \quad (16)$$

$$\tilde{E}_y = -E_y \frac{(\Delta t)^2}{2\Delta X} \quad (17)$$

$$\tilde{E}_x (\text{ions}) = -E_x \frac{(\Delta t)^2}{2\Delta X} \frac{m_e}{m_i} \quad (18)$$

$$\tilde{E}_y (\text{ions}) = E_y \frac{(\Delta t)^2}{2\Delta X} \frac{m_e}{m_i} \quad (19)$$

Then the particle equations of motion become

$$\tilde{X}^{n+1/2} = \tilde{X}^n + \tilde{V}_x^{n+1/2} \quad (20)$$

$$\tilde{X}^{n+1} = \tilde{X}^{n+1/2} + \tilde{V}_x^{n+1/2} \quad (21)$$

$$\tilde{V}_x^{n+1/2} = \tilde{V}_x^{n-1/2} + \frac{1}{1 + (\tilde{B}_x/2)^2} \left[\tilde{E}_x^n + \tilde{V}_y^{n-1/2} \tilde{B}_z^n + \frac{\tilde{B}_z^n}{2} \tilde{E}_y^n - \tilde{V}_x^{n-1/2} \frac{\tilde{B}_z^n}{2} \tilde{B}_z^n \right] \quad (22)$$

$$\tilde{V}_y^{n+1/2} = \tilde{V}_y^{n-1/2} + \tilde{E}_y^n - \frac{\tilde{B}_z^n}{2} (\tilde{V}_x^{n+1/2} + \tilde{V}_x^{n-1/2}) \quad (23)$$

Also, to save time in linear interpolation, the changes ΔE_x , ΔE_y , ΔB_z at each cell edge in the various fields across the cell in the direction of increasing X from the edge are defined.

A brief description of subroutine functions is given in Table IV. Table V contains a simplified Warnier-Orr diagram of SELF.

TABLE IV. SELF Subroutine functions.

Subroutine	Function
SELF	Main program Initial conditions Calls other routines
INPT	Prints out initial conditions
INPTA	Prints out calculated parameters
VEL9	Sets initial particle distribution
FIELD	Calculates E_x , E_y , B_z from charge density and current
PUSH13	Particle pusher for electrons Calculates charge density and current
PUSH14	Particle pusher for ions Calculates charge density and current
EPRINT	Prints out energies

TABLE V. Simplified Warnier-Orr Diagram of the original SELF

SELF	collect beginning processor and wall clock times	
	specify parameters	
	set constants	
	compute parameters	
	initialize arrays	
	print initial data	
	print computed data	
	set up initial particle velocities and positions	
	primary loop iteration	increment cycle number
	print results	increment time
	collect ending processor and wall clock times	calculate fields
	print timing information	push electrons
	quit	push ions

TABLE VI. Simplified Warnier-Orr diagram of the two task SELF. Only the differences with respect to Table V. are shown.

SELF		increment cycle number
		increment time
		calculate fields
		start task - push electrons
	primary loop iteration	push ions
		wait for task to complete
		compute total charge from electron and ion charges
		compute total current from electron and ion currents

TABLE VII. FORTRAN of primary loop of original SELF.

```

130 ncy=ncy+1
    time = dt * ncy
    call field (rho, jy, exen, eyen, een, bzen)
    call push13 (rho, jy, x1, vx1, vy1, ven1x, ven1y)
    call push14 (rho, jy, x2, vx2, vy2, ven2x, ven2y)
    if (ncy .lt. nt) go to 130
140 continue

```

TABLE VIII. Flow trace summary of original SELF for 50 timesteps.

	Routine	Time	%	Called	Average T
<hr/>					
1	SELF	0.004464	0.11	1	0.004464
2	WALCLK	0.000208	0.01	2	0.000254 Called by SELF
3	CPCLK	0.000052	0.00	2	0.000026 Called by SELF
4	INPT	0.007400	0.19	1	0.007400 Called by SELF
5	INPTA	0.000887	0.02	1	0.000887 Called by SELF
6	VEL7	0.235414	5.94	1	0.235414 Called by SELF
7	FIELD	0.014776	0.37	50	0.000296 Called by SELF
8	PUSH13	1.815548	45.79	50	0.036311 Called by SELF
9	PUSH14	1.859253	46.89	50	0.371852 Called by SELF
10	EPRINT	0.023150	0.58	1	0.023150 Called by SELF
11	PRNTIM	0.003390	0.09	1	0.003902 Called by SELF
***	<u>TOTAL</u>	3.964843			
***	Overhead	0.004781			

NOTE: These results were obtained on the CRAY 1-S

TABLE IX. FORTRAN of primary loop of two task SELF.

```

130 ncy=ncy+1
    time = dt * ncy
    call field (rho, jy, exen, eyen, een, bzen)
    tasklary(1)=3
    tasklary(3)= task 1 ' 1
    call tskstart (tasklary, push13, rhoe, jye, x1, vx1, ven1x, ven1y)
    call push14 (rho1, jy1, x2, vx2, vy2, ven2x, ven2y)
    call tskwait (tasklary)
    do 135 i=1, npt
        rho(i) = rhoe(i)+rho1(i)
        jy1(i) = jye(i)+jy1 (i)
135 continue
    if (ncy .lt. nt) go to 130
140 continue

```

TABLE X. Timings for three runs of two task SELF.

<u>Wall Clock (sec.)</u>				<u>CP Clock (sec.)</u>		
			<u>Run 1</u>			
Begin	End	Total		Begin	End	Total
16359.00	16389.000	30.000		0.492	58.656	58.165
			<u>Run 2</u>			
Begin	End	Total		Begin	End	Total
65572.000	65601.000	29.000		4.574	62.719	58.144
			<u>Run 3</u>			
Begin	End	Total		Begin	End	Total
42303.000	42060.000	30.000		63.511	121.627	58.116

TABLE XI. Timings of single task SELF on CRAY I-S and CRAY X-MP.

<u>Wall Clock (sec.)</u>			<u>CP Clock (sec.)</u>		
CRAY I-S					
Begin	End	Total	Begin	End	Total
64635.000	66685.000	2050.000	0.651	75.167	74.517
CRAY X-MP					
Begin	End	Total	Begin	End	Total
65550.000	65608.000	58.000	0.459	58.457	57.998

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