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Creation of Fully Vectorized FORTRAN Code for Integrating the Movement of Dust Grains in Interplanetary Environments

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July 1989

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NASA Johnson Space Center
Space and Life Sciences Directorate
Solar System Exploration Division

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University of Houston · Clear Lake

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The RICIS Concept

The University of Houston-Clear Lake established the Research Institute for Computing and Information systems in 1986 to encourage NASA Johnson Space Center and local industry to actively support research in the computing and information sciences. As part of this endeavor, UH-Clear Lake proposed a partnership with JSC to jointly define and manage an integrated program of research in advanced data processing technology needed for JSC's main missions, including administrative, engineering and science responsibilities. JSC agreed and entered into a three-year cooperative agreement with UH-Clear Lake beginning in May, 1986, to jointly plan and execute such research through RICIS. Additionally, under Cooperative Agreement NCC 9-16, computing and educational facilities are shared by the two institutions to conduct the research.

The mission of RICIS is to conduct, coordinate and disseminate research on computing and information systems among researchers, sponsors and users from UH-Clear Lake, NASA/JSC, and other research organizations. Within UH-Clear Lake, the mission is being implemented through interdisciplinary involvement of faculty and students from each of the four schools: Business, Education, Human Sciences and Humanities, and Natural and Applied Sciences.

Other research organizations are involved via the "gateway" concept. UH-Clear Lake establishes relationships with other universities and research organizations, having common research interests, to provide additional sources of expertise to conduct needed research.

A major role of RICIS is to find the best match of sponsors, researchers and research objectives to advance knowledge in the computing and information sciences. Working jointly with NASA/JSC, RICIS advises on research needs, recommends principals for conducting the research, provides technical and administrative support to coordinate the research, and integrates technical results into the cooperative goals of UH-Clear Lake and NASA/JSC.

Creation of Fully Vectorized FORTRAN Code for Integrating the Movement of Dust Grains in Interplanetary Environments

Preface

This research was conducted under the auspices of the Research Institute for Computing and Information Systems by Walter Colquitt, of the Houston Area Research Center. A. Glen Houston, Director of RICIS, served as technical representative for this activity.

Funding has been provided by the Solar System Exploration Division, Space and Life Sciences Directorate, NASA/JSC through Cooperative Agreement NCC 9-16 between NASA Johnson Space Center and the University of Houston-Clear Lake. The NASA technical monitor for this activity was Herbert Zook, of the Space Science Branch, Solar System Exploration Division, NASA/JSC.

FINAL REPORT

"Creation of Fully Vectorized FORTRAN Code For Integrating the Movement of Dust Grains in Interplanetary Environments"

Submitted to

UNIVERSITY OF HOUSTON CLEAR LAKE
RICIS Research Activity
Houston, Texas 77058-1096

RICIS RESEARCH ACTIVITY NO. MS.2
NASA COOPERATIVE AGREEMENT NCC9-16

by

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July, 1989

Final Report

As both the calendar time and the computer allotment are coming to a close it is time for the final report of all that has happened. The purpose of this contract was to improve the performance of a specific FORTRAN computer code from the Planetary Sciences Division of NASA/JSC when used on a modern vectorizing supercomputer. The code is used to calculate orbits of dust grains that separate from comets and asteroids. This code accounts for influences of the sun and 8 planets (neglecting Pluto), solar wind, and solar light pressure including Poynting-Robertson drag. Calculations allow one to study the motion of these particles as they are influenced by the Earth or one of the other planets. Some of these particles become trapped just beyond the Earth for long periods of time. These integer period resonances vary from 3 orbits of the Earth and 2 orbits of the particle to as high as 14 to 13.

The code is about 700 lines of fairly generic Fortran and it has run on a variety of computers - VAX, PC, SX-2, and Cray. Initial runs showed the code not well structured for vector computers; this is hardly surprising as this code was never run on a vector machine before. Initially there were three problems that hampered vectorization:

- o vectors too short with length of 8 (planets) or 3 (x-y-z components of motion)
- o computed GOTOs in the most inner loop of the integrator
- o subroutine calls embedded in inner loops

The first of these degrades performance because of the overhead of vector loop start up while the latter two cancel any vectorization attempts by the compiler.

Several runs using the Analyzer were made to isolate the "hot spots" so we could concentrate our tuning efforts where they would do the most good. A series of modifications were made to improve the performance. At first the computed GOTO's were removed by placing the selected code "behind" an IF test (see below). This vectorized on the NEC but not on the Cray. We also made an attempt to increase vector length by using the three orthogonal elements of the motion vectors for each of the 8 planets. This increased vector length to 24 and improved run time by more than 50%. Unfortunately the data structures became too complicated for easy maintenance and modification. This data layout was not in conformance with the practice of the art so it was very difficult to implement outside suggestions. Finally this attempt was laid by the side.

The numerical integrator used is the implicit Runga-Kutta formulation by Edgar Everhart. This integrator has achieved great popularity in the study of planetary motions because of its predictor-corrector capability which yields high performance while still maintaining excellent accuracy and stability. A second time step integrator was also investigated. The popular Everhart integrator was replaced with a Bulirsch-Stoer integrator(see ref #1). This integrator produced very good answers but its performance deteriorated and became unacceptable on highly eccentric orbits.

By this time many spots of inefficiency in the code had been found and were corrected. These were such things as common subexpression identification by enclosing items in parentheses, precalculation prior to a DO-loop, strength reduction such as low power exponentiation replaced by repetitive multiplication and the like. Several cases of stride problems were corrected by reversing the order of subscripts in local work arrays. Also the compiler was given more information by changing the dimension statement for dummy subroutine arguments from DIMENSION X(1) to X(*) indicating the length needs to be calculated at run time - it is NOT of length 1! The cumulative effect of these improvements gradually became quite noticeable.

Finally a clean version of the Everhart integrator with the planets moved in first order eccentric Keplerian orbits was created. This code finally showed the kind of performance we were looking for - about 100,000 to 150,000 simulation years per hour of chargeable CPU. This version was run for a short simulation period of 200 years of planetary motion on the SX-2, a Cray XMP-24, and on the SuperTek. Run times were respectively 5.5 sec, 11.2 sec, and 107 sec.

A series of final runs were made in a real production mode and one of these found resonance trapping by the Earth.

The following is the major change that was made to Everhart's integrator to create the version RA15SX.FOR.

```
      DO 40 I=1,3
      GOTO (10,20,30),I
10    CONTINUE
      do something when I=1
      GOTO 40
20    CONTINUE
      do something when I=2
      GOTO 40
30    CONTINUE
      do something when I=3
      GOTO 40

40    CONTINUE
```

was changed to

```
      DO 40 I = 1, 3
      IF ( I .EQ. 1 ) THEN
      do something when I=1
      ENDIF
      IF ( I .EQ. 2 ) THEN
      do something when I=2
      ENDIF
      IF ( I .EQ. 3 ) THEN
      do something when I=3
      ENDIF
40    CONTINUE
```

On the SX-2 the latter vectorizes and the former does not - this is because of the vector mask test registers in the machine. In the Cray neither fully vectorizes but the latter creates a "vector scalor" loop; whatever that is. Even so however relative performance was very good considering hardware speeds.

Enclosed with this report are two 5 1/4" floppy disks. One contains the results of the test runs made on the Cray. There are two groups of four files - submitted JCL, compilation listings, day file listings, and final output answers.

The second disk is the final delivery product. It's contents are as follows:

NOFF.FOR a utility program to remove tabs, blank lines, and nonprintable characters from a file. This is a very handy preprocessor for files to be shipped over DECNET.
RA15.FOR original Everhart integrator with the code cleaned up for easier reading. Carefully verified to provide same results as the original.
RA15SX.FOR Everhart integrator modified for vectorization. Produces the same answers as the original.
DELIVERY.JCL SX-2/OS JCL to run the job.
E9E_MAIN.FOR final version run of Encke run that produced trapping.
FOURL.FOR and E9E.MAIN two versions (four planets only and full planet stepwise integrated motion. The former had problems with accuracy and the latter with performance)
HALLEY.JCL Final version a Halley dust grain run; no trapping found
X171361.SXO A full blown run including JCL, FORTRAN expanded listing, and results of this run. Processed by NOFF.FOR.
FINL_ENC.JCL This is input JCL, including the final fully cleaned up source code with vector version of RA15SX. THIS IS THE FINAL PRODUCT OF THIS CONTRACT.

The Future

There are at least two possibilities for further investigation. One would be more code improvements. This might be to take the integrator inner loop and pull it inside of the IF tests replicating the total loop each time. I'm not fully convinced this could be made to work, or even that the improvement would be worth it. Performance improvement would probably be slight because the overhead of the IF test is very low on the NEC and fairly low on the Cray but the inner loops behind the IF would be very short so vector startup would be expensive and this would especially penalize the Cray.

Current:

```
DO J = 1, N
      DO K = 1, L
      IF ( J.EQ.1 ) THEN
      do k code for when J=1
      etc
```

would be changed to

```
DO J = 1, N
IF ( J.EQ.1 ) THEN
      DO K = 1, L
      each time replicate the entire do k loop as appropriate for J.
```

The second possibility would be to use the current code and begin to investigate the parameter space of initial dust particle orbital elements in order to limit the areas of interest. This would be especially useful for the 100-200 micron particles which seem more susceptible to trapping but these larger particles are harder to calculate as they decay slower.

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