Another project is to reveal the region of validity of perturbation methods in Hamiltonian mechanics. A canonical Lie series method was implemented to calculate perturbations of systems close to those encountered in celestial mechanics. The classical perturbation methods do not result in good approximations in the whole phase space, that is, both far from and close to the resonances. A perturbation theory with extended validity is now being sought. In the course of this study some problems encountered in algebraic manipulations in MACSYMA were corrected. This allowed a fast and efficient algorithm for canonical perturbation theory to be implemented.
Dear Ms. Kurtti

This is a copy of an interim report that I sent to J. Chandra and A. Wouk at ARO in March of 1986.

This is an interim report on the grant AFOSR-85-0092, which is a DoD-URIP grant for the year 1985-86. The grant was titled "Symbol Manipulation and Applied Mathematics"; Prof. Stanly Steinberg is the PI. It was cost-shared with the University of New Mexico, and had two parts. The first consisted of installing a LAN (local area network) in the mathematics and statistics department and connecting this to the university wide CDCN (campus data communication network). The second part involved the installation of a network of workstations for four professors in the department.

The LAN is now nearing completion; some parts have been usable for approximately a month. The departments has about 25 terminals connected to the network. Most of the terminals are located in the offices of the faculty and graduate students, with a few in a joint-use equipment room. The initial response is that this has greatly improved the computing environment. In addition, 7 faculty members have been given microcomputers by the university, and these have been connected to the LAN. This configuration seems to provide an excellent computing environment. Some of the faculty have found that current microcomputers are too small and have too little software, so the university will soon replace some of these with more powerful micros, which will also be connected to the LAN.

The network of workstations consists of four Sun-2/160 minicomputers; each has a tape and disk drive. They are connected via an ethernet, and this is connected to the university CDCN. (There is currently an incompatibility between the Sun network and the CDCN; the university is buying equipment to correct this.) The Sun workstations will soon be upgraded to Sun-3 class workstations.

What follows are short reports by each of the faculty members who are using workstations. The faculty members are Professors Steinberg, Gibson, and Kyner.

Professor Steinberg has been using his workstation for both general
computation and research work. The general computing includes text processing such as the preparation of research papers and course materials. The research projects include symbolic symmetry calculations and symbolic and numeric grid-generation calculations. One of the workstations was for Prof. Buys who is on a two year leave at the University of Arizona. During this time, two of Professor Steinberg’s students are using her workstation.

One of the main uses for the workstations is to do symbolic calculations. In the fall of 1985 the symbol manipulators MACSYMA and SMP were installed on the system. The manipulators Maple and Reduce are still on order. The workstations have now been used to do many symbolic calculations; the system provides an excellent environment for doing symbolic calculations. The additional speed that will be provided by the Sun-3 upgrades will make the system even more useful.

Professor Steinberg has developed a set of MACSYMA programs for calculating symmetries of ordinary and partial differential equations. He and Professor Buys have been using these programs to calculate the symmetries and integrals of rigid bodies including the Euler, Lagrange, and Kovalewski tops. During the fall 1985 break between classes, several of these computations were run on a university VAX computer. The jobs take between 20 and 40 cpu hours, with a total cost of about $8,000.00. It would be impossible to run such jobs during the semester. About 5 times as many of these calculations have now been run on the workstation. This type of research would be impossible, from both time and money considerations, without the workstation.

Professor Steinberg has also been working on a project that uses variational methods to generate adaptive numerical grids. An important step in the methods uses the symbol manipulator MACSYMA to write some FORTRAN subroutines. In the early stages of this project, the subroutines were very expensive to write; some required about 10 cpu hours on the workstation. As our techniques improve, the subroutines are shortened and consequently less computing power is need to write them. However, the initial (poorly written) subroutines are critical because they dictate what improvements are needed. Again, such research would be difficult or impossible to carry out on the university computers, so the workstations have been critical in this project. In addition, all of the hand-written FORTRAN code necessary for the grid generation project is being developed on the workstation. Soon, a high-resolution color graphics capability will be incorporated into the grid generation codes.

Two of Professor Steinberg’s Ph.D. students are using the workstations in their thesis work. Mr. Michael Wester is working on a project to implement a powerful symbolic matrix eigen package for MACSYMA. He is programming much of this work in LISP, which will give the programs enhanced speed and versatility. Mr. Jose Castillo is working on generating adaptive grids by directly minimizing variational integrals. He uses one of the workstations for writing and running his FORTRAN programs.

Ms. Megan Florence is writing a master’s practicum project under the direction of Professor Steinberg. She is creating a library of MACSYMA programs that can be used to solve and analyze an arbitrary higher-
order system of ordinary differential equations. She has completed some programs that can take a system of higher-order odes, reduce them to a first order system, and then write the FORTRAN subroutines that are required to solve the system numerically. An undergraduate student, David Scott-Collett, is just starting a project to analyze whether or not various symbol manipulators can do all of high school mathematics.

Professor Archie Gibson has installed one of the SUN workstations in his office, and it is being used by him and his collaborator, Professor Colston Chandler of the UNM Physics Department. It is also being used by three of their Ph.D. students, Barbara Bertram, Bill Pletsch, and Henry Taljeron, and by Pal Doleschall, a National Science Foundation exchange visitor from Budapest, Hungary. The work involves their research in N-body quantum-mechanical scattering theory, and the workstation has been used for the writing and running of symbolic manipulation codes using MACSYMA, and also for considerable number crunching of FORTRAN-code calculations.

Dr. Pal Doleschall, of the Central Research Institute for Physics in Budapest, visited UNM in September, 1985, and he will return again in April, 1986. In September, he brought with him his complete 3-body Faddeev code and installed it on Professor Gibson's workstation. This code is probably the world's most sophisticated code based on Faddeev's equations. It was a laborious task getting this huge code to run on the SUN, but all of the necessary modifications were made, and several calculations have already been run. Some of these calculations have taken as many as 50 cpu hours, but these times will be greatly reduced once the MC68020 upgrades have been installed.

Professors Chandler and Gibson and their Ph.D. students have ported almost all of their FORTRAN and MACSYMA software to the SUN workstation, and all of it runs satisfactorily. This has almost eliminated their need to use the UNM mainframe computers and, consequently, has already saved thousands of dollars in computer expenses. The N-particle scattering code being developed by this group of researchers is based on the Chandler-Gibson equations. They have completed the code development for the elastic channel scattering of an alpha particle by a deuteron (a six body problem), and they are now working on the incorporation of breakup channels into the code. This work is presently supported by two grants (PHY-8303738 and INT-8400053) from the National Science Foundation. The four SUN workstations and the campus LAN purchased by the UNM Mathematics Department DoD\URIP grant has greatly facilitated the research of this group of investigators, and they will continue to benefit from the availability of this computer equipment for many years.

Professor Kyner is using his workstation to study autoradiographic methods and inverse problems in neurobiology. Autoradiographic methods are used to study the formation and movement of brain interstitial fluid. If a thin slice of brain tissue containing a radioactive tracer is left on a sheet of x-ray film, the gray levels of the developed film correspond to concentrations of the tracer. Image processing equipment can be used to quantify, display, and store the information contained in the x-ray picture of the brain tissue. With the aid of false color, patterns of transport of radioactive tracers can be investigated, and
used in the construction of mathematical models.

W.T. Kyner, of the Department of Mathematics and Statistics, and G.A. Rosenberg, of the Department of Neurology, have been collaborating on a study of brain interstitial fluid and its regulating factors for several years. The equipment of the Image Processing Laboratory, UNM College of Engineering is being used for both the image processing and analysis aspects of the problem. The staff of the UNM Computing Center has helped set up a system for storing the images on tape and transferring them to a Sun Work station in Professor Kyner's office. Programs are now being written that will enable us to investigate the transport of an extracellular tracer from the injection site in the brain of a laboratory animal. Agents that alter interstitial fluid transport will be injected along with the marker to determine their influence. The color graphics of the Sun Work station, as well as its accessibility, will be of great assistance in this research.

Professor Ferenc Varadi, who is visiting Professor Kyner from Eotvos University in Hungary, is working on perturbation problems in applied mathematics. He is using MACSYMA to solve a perturbation problem connected to a nuclear spin-resonance method in oil-field research. The mathematical problem is to solve a non-autonomous linear system of differential equations with an exponentially decreasing non-autonomous part. This system can be solved using numerical methods or iterations, but these do not yield information on the solution for arbitrary values of the parameters. A special Lie series method can be used to find an approximate analytical solution. The method is a non-canonical version of the so-called Deprit method, modified to exploit some special properties of the problem. The MACSYMA program works for the first-order approximation, but the second-order calculation requires unreasonable computer resources. This is a typical phenomenon of algebraic manipulation on computers. Research on further optimization of this program is continuing. The final result of this project would be a fast algorithm for determining the ratio of the solid and liquid part of the soil. As a generalization of the method, it may be possible to find algorithms to carry out the so-called Lyapunov transformation using Lie series methods.

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Sincerely Yours,

Professor Stanly Steinberg
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