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APPLICATIONS OF NUMERICAL CODES TO SPACE PLASMA PROBLEMS

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Applications of Numerical Codes to Space Plasma Problems

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A Study of Applications of Numerical Codes to Space Plasma Problems was conducted on January 7 and 8 by the Theoretical Studies Group at Goddard jointly with the Institute for Fluid Dynamics and Applied Mathematics at the University of Maryland. The organizing committee consisted of T. G. Northrop, T. J. Birmingham, F. C. Jones (all GSFC) and C. S. Wu (University of Maryland).

The purpose of the study was to expose space plasma theorists to the capabilities of numerical codes developed at the Naval Research Laboratory, and to assess whether space plasma theory and observations have arrived at the point where a large effort of the NRL type would enormously enhance progress in space plasmas, or whether such an effort would be premature.

In order to limit the scope of the Study sufficiently to fit into two days, the committee decided to concentrate on three areas: solar wind, Earth's bowshock, and magnetospheric convection and substorms.

The aim was to have, in each of these three areas, two invited speakers; one familiar with the state of observations and another with the theory.

The NRL group was invited to speak first, describing their numerical codes and some of the problems successfully attacked with them. The invited speakers in each of the three chosen areas of concentration followed the NRL presentation. The presentations ended with a short series of spontaneously generated talks by invited attendees. The Study ended with a short discussion of the "where are we going, what should we do" variety.

A questionnaire was passed out to the attendees asking for written responses to the questions or for any other comments.

The substance of each invited presentation is summarized in the following pages.

T. Coffey (N.R.L.) "Overview"

The N.R.L. group consists of 25 theoretical physicists and 25 computational physicists. The requirements for a successful group are three: "a critical mass" of experts in computational physics and in the appropriate areas of theoretical physics, large computers, and finally a strong link to experimental programs. The rôle of computation is: 1) to serve as a tool for understanding details of physical processes not analytically tractable or experimentally accessible, 2) to extrapolate beyond the experimental state of the art and to define experiments to be performed to answer outstanding questions.

A list of 14 recent N.R.L. computational projects was given and each briefly discussed. The list included: 3 dimensional (plus time) calculations of reacting neutral fluids, 2D and 3D models of auroral arcs and of the midnight auroral oval, and 1D to 2D Fokker-Planck codes for collisional relaxation in plasmas.

Possible applications of the N.R.L. codes to NASA programs include the following areas: solar wind flow past planets, modeling of solar flares and transport in the solar atmosphere, detailed analysis of Atmospheric Explorer data, chemistry and transport of Shuttle effluents, planetary atmosphere modeling, ionosphere-magnetosphere coupling, and interplanetary plasma interactions.

J. Boris (N.R.L.) "Computational Physics"

A computer performs two functions - bookkeeping and discovering new physics. In spite of a large improvement in computer technology about 5 years ago, and better computational techniques (which gained a factor of 10), it is still impossible to compute on microscopic and macroscopic scales simultaneously. The macroscopic consequences of microscopic processes must be fed into the macro codes after being separately calculated.

Numerical experiments are desirable because: 1) actual experiments are escalating in cost; 2) increased leadtime is needed for experiments; 3) they can supply scaling laws and quick diagnostics; 4) they can supply quick evaluation of new concepts. Numerical experiments can: 1) make accessible regimes not accessible on Earth (pulsars, quasars); 2) study scaling laws over large ranges; 3) study effects of changes in parameters in the problem; 4) permit changes in the basic physics. Numerical experiments are done by: 1) choosing the governing sets of equations; 2) discretizing these equations; 3) creating algorithms to solve the discretized equations; 4) writing and running the computer code; and 5) analyzing the results. In obtaining the governing sets of equations, one must often synergize various disciplines, such as atomic physics, magnetohydrodynamics, and plasma kinetic theory from the Vlasov equation.

The capabilities of half a dozen particle codes were described. They vary in the number of dimensions in which particles are allowed to move, the types of interactions permitted among the particles, and the terms retained in Maxwell's equations. Similarly, nine fluid codes were described. N.R.L. has found that fluid codes really bring the answers to problems home to sponsors because these codes deal with macroscopic quantities which are easily measured and visualized.

Recent computational advances include: 1) a solution to the Alfvén problem (i.e., how to account for Alfvén waves in low density plasmas, where these waves carry energy away, but their phases are of no direct interest in the problem); 2) asymptotic integration methods (which permit solution of "stiff" differential equation systems); 3) multi-fluid algorithms for counterstreaming fluids; 4) use of dynamic magnetic coordinates (a "natural" coordinate system); 5) development and use of triangular coordinate systems (which permit following fluid interfaces for long times); 6) flux corrected transport for solving continuity equations (which permits calculation of shock propagation without artificial damping).

Finally, the attributes of the N.R.L. Advanced Scientific Computer (to be delivered by Texas Instruments in 1976) were briefly described.

D. Papadopoulos (N.R.L.) "Multifluid Codes"

Microscopic processes in plasmas take place on a time scale of the plasma period and space scale of the Debye length. Particle codes are needed on the micro scale. Macroscopic fluid processes take place on time scales that are slower by factors of 10^4 to 10^{10} and space scales that are larger than the Debye length by 10^4 to 10^{10}. It is impossible with present computers or any on the horizon to use the micro codes on macro time and space scales. The microscopic effects must be modeled into the macro codes. For each fluid there is a continuity equation, a momentum equation, and an energy equation. And the Maxwell equations complete the set. In each of the fluid equations there are anomalous terms which really contain the plasma physics, which may take months or years to unravel, and into which go the results of microscopic calculations.

Several examples of such calculations were presented: 1) streaming of plasma across a magnetic field; 2) penetration of a magnetic field into a plasma (in a laboratory experiment); 3) non-linear damping of magnetosonic pulses; and finally 4) overtaking of slow solar wind streams by faster ones.

The computer model of this last phenomenon attempted, with some success, to reproduce observed features (ion heating without electron heating, and helium to proton temperature ratio of 4-5, as examples). However, a brief discussion (and a much more extensive one later in the Study) revealed disagreement as to the observations and raised questions re the adequacy of the computer model.

Editorial comment: Here is a problem where much more computer modeling, guided by close collaboration with the experimental work, is almost certain to yield results.

S. Ossakow (N.R.L.) "Ionospheric Irregularities"

Numerical modeling of three phenomena was reviewed: 1. Electrojet instabilities, 2. Dynamics of barium cloud releases, 3. Spread F.

1. and 3. produce ionospheric irregularities naturally, while 2. produces them artificially. Ionospheric irregularities are the result of instabilities and degrade communication and radar. To get a predictive capability is a goal of numerical simulation. The models are principally 2 dimensional, since modern computers cannot really do 3 dimensions with fine resolution. The dimension parallel to the magnetic field is usually integrated out. For the equatorial electrojet the numerical experiments succeed in generating the observed short wavelength vertically propagating instabilities from the long wavelength horizontally propagating gradient drift instabilities. The barium cloud release numerical models show that the E region conductivity should dominate what happens to the barium plasma when the release is in the F region; in fact image striations are predicted in the E region and could be looked for as a test of the model. This is an example of the predictive capability of numerical models.

Remaining ionospheric irregularity problems can probably be attacked successfully now, although much effort is required.

N. Winsor (N.R.L.) "Modeling Laser Plasmas"

Laser pulses impacting solid deuterium-tritium is being tried as a source of hot, dense, plasma for controlled thermonuclear purposes. Other applications are as an intense source of X-rays, and to produce in the laboratory highly stripped atoms of astrophysical interest.

When the laser pulse hits say an aluminum target, the metal is evaporated, ionized, and propelled outward from the surface by the pressure gradient. Densities are such that the plasma is optically thick. The numerical calculation must thus handle three types of physics, all linked - the magnetohydrodynamics, the atomic rate equations, and the radiative transport. The calculation correctly predicts the total X-ray output and spectrum. Conversion efficiency of the laser pulse to X-rays is as high as 50%. Experimentally, where the laser pulse is obliquely incident on the aluminum, rather than normally, the X-ray output is reduced. This reduction is due to decreased plasma temperature, but has not been quantitatively predicted numerically, since the numerical code is axisymmetric about the laser beam.

Editorial comments: 1. The geometry of a laboratory problem can be adjusted in contrast to many space problems. This simplifies numerical work. 2. The laser fusion effort has profited greatly by having a sizable group of theorists of diverse expertise and computational experts working closely with the experiments.

L. Burlaga (Goddard) "Solar Wind"

Burlaga reviewed the particle fluxes in the solar wind. He then described the geometry of colliding streams. There is a thin layer between the temperature and density peaks at the interface between the streams.

This cannot be reproduced numerically without introducing shocks and more plasma effects than (Burlaga) used so far. Papadopoulos has started with different initial conditions, but no one knows what the correct conditions to be imposed are, particularly at the photosphere.

J. Hollweg (High Altitude Observatory) "Solar Wind"

The basic problem in solar wind models is to find a mechanism that will heat the protons to the extent observed. Furthermore, the electron heat flux is only about 1/40th of that predicted by classical (i.e., Chapman-Enskog) electron thermal conductivity.

Possible mechanisms for increasing the calculated ion temperatures are the following: 1) Fast MHD waves and Alfvén waves radiate from the Sun and deposit their energy. Numerical calculation may be useful in studying non-linear damping and energy deposition by these waves. 2) Two stream instabilities due to currents in the presence of large magnetic field shears at colliding stream interfaces. However, this preferentially heats the electrons, so has the wrong effect. 3) Helmholtz instability at the interface does in fact preferentially heat protons, but only there.

The heat flux discrepancy is also difficult to resolve. The electron velocity distribution is observed to have a central "core", peaked at the solar wind velocity, plus wings on either side (the "halo" electrons) which carry the heat flux. Another possibility (due to Perkins) is that electrons are trapped between the Sun and an electrostatic potential hill some distance from the Sun.

The most fruitful area for computer simulation is in understanding the role of instabilities in controlling the electron heat flux and in increasing electron-proton coupling so as to increase ion temperature.

In the discussion Forslund said the electromagnetic ion cyclotron instability is the most likely candidate. One needs to use the quasilinear theory of this instability. Perkins said that a multidimensional Fokker-Planck equation should be solved numerically.

Editorial comment: Resolving the difficulties encountered in explaining the solar wind will require use of the correct "non-classical" transport coefficients. By contrast, the laser plasma problem is much easier to handle. There may be microscopic instabilities there also, but the densities are so high that classical collisions control the transport. The controlling physics is all-known. By contrast, this is not so in the solar wind, and moreover the geometry has less symmetry.

D. Forslund (Los Alamos) "Solar Wind and Bowshock"

Observed proton angular distributions in the solar wind show flow along the magnetic field. The velocity distribution is double-humped near colliding streams. The Los Alamos group is using the complete linear dispersion relation for a plasma in a magnetic field to test the stability of observed distribution functions. The philosophy is that the wave mode controlling the transport of heat and the exchange of energy among species will be the one closest to marginal stability. The dispersion relation must be solved numerically. One finds that the complete dispersion relation must be used; nothing can be neglected. This makes it difficult to predict whether electrostatic or electromagnetic instability will dominate.

The coarsest categorization of bowshocks is into two classes: laminar and turbulent, depending on how regular the magnetic field transition is. The two classes correspond to whether electron whistlers have sufficient velocity to phase stand in the upstream region. If they can, a turbulent shock results. Otherwise, laminar. The whistler decays parametrically into other waves, the type of decay depending on the plasma parameters. Numerical simulation (with particles) has demonstrated strong ion heating, as is observed by spacecraft instrumentation. The numerical calculation to date has been one dimensional as far as the whistler decay is concerned. One could probably do a 2-dimensional simulation, using a hydrodynamic code for the electrons and treating the protons as particles. A 2-dimensional simulation is desirable because whistlers are unstable to decay into waves over a wide cone. The result would be more turbulence than predicted by the 1-dimensional simulation.

Editorial Note: This is an area where more numerical simulation should be supported, particularly in view of the future I.S.E.E. missions designed to make bowshock solarwind and magnetospheric observations. Better theoretical guidance would be most desirable.

E. Greenstadt (TRW) "Bowshock"

The categorization of bowshock crossings into types has been refined, and the number of categories increased over the original two (laminar and turbulent). Magnetic field and plasma property tracings for the different types were shown. The categorization is based on a few dozen cases.

Editorial comment: Greenstadt is well aware that his categorization is subjective, to some unknown degree. Of course, if the number of categories approaches the number of cases studied, the categorization is not very meaningful. There is a question whether the types of bowshocks form a discrete spectrum or a continuum. More numerical simulation like Forslund's would help sort this out.

P. Kellogg (Univ. of Minesota) "Bow Shock"

Electric field measurements have been made with antennas on IMP-6. Electron whistlers are not the only wave seen upstream of the bowshock. There is a sharp peak in the power spectrum at 20 kilohertz, which is the electron plasma frequency. This mode is excited by electrons reflected upstream from the shock and is not seen on field lines that miss the shock. Only the more energetic electrons make it upstream (low energies are swept back into shock), so that the upstream electron energy distribution is peaked.

Downstream of the shock one sees "runout" noise. This noise has a much broader power spectrum than the upstream noise. The spectrum (and angular distribution) of the electric field is the same in the shock as downstream. Hence the instabilities operative in the shock should be ascertainable from the runout waves. The runout noise spectrum is different at different points on the bowshock: This means that several instabilities are at work over the entire shock. The dawnside has more runout noise than elsewhere.

The only case in which the direction of the electric field in the shock was steady enough to be measured was that of a magnetosonic shock (magnetic field up and downstream parallel to the shock surface). In this case the electric field was also in the plane of the shock and perpendicular to the magnetic field. This would be consistent with a current driven instability in the shock.

Editorial comment: In the discussion following this talk, Forslund pointed out that in the laboratory shock experiments at Garching, the operative instabilities had been fully diagnosed.

R. McPherron (UCLA) "Substorms"

The UCLA group consists of 32 people, 30 of whom are supported by outside contracts. They have handled the data for about 2000 substorms, and this group is best known for this area of research. The Earth's magnetic field is never steady, but goes repetitively through a sequence of geometric changes on about a 3 hour time scale on the average. One cannot yet predict when a substorm will occur, but the morphology is well studied.

NASA does not devote enough resources to theory or to data analysis. Experimenters tend to avoid seeking out intensive interaction with theorists because such an interaction may become at least a year's undertaking. But by the end of a year the project is being closed down (hopefully to be replaced by another project to support the group). There is only sufficient life and dollars in the project to go through the data file once and to get the data in the literature. And the project is being closed down by the time the theorists learn of and get interested in the data.

Another problem is that hardware overruns rob data analysis funds. The situation is exacerbated by the tendency to underestimate the cost of data reduction and analysis, and to underestimate the time required to do it by a factor of 3 or more.

Recommendations: 1) Increase data analysis dollars at the cost of experiments. 2) Separate hardware and data analysis dollars. 3) After each project, support 4 years of data analysis at the level of: 2 graduate students + 1 postdoctoral + 1/3 senior scientist + 1 full time programmer. The postdoctoral should be half theoretical and half experimental. The third and fourth years should be contingent upon cooperation with theorists. For the price of just one flight experiment, 20 theorists can be supported for a year.

Editorial comment: This talk stimulated a considerable amount of valuable discussion. McPherron was not aware, until this Study, of the amount of work that has gone into the N.R.L. codes. He does not believe that we are far enough advanced with magnetospheric survey to use these codes to great advantage for substorms. Krall, (Science Applications, Inc.) commented that full documentation of a code is not sufficient to permit a stranger to use it. Responsiveness and help of the computational physicist who designed it is essential.

R. Wolf (Institute for Advanced Study) "Magnetospheric Convection"

No system of equations simpler than that presented in his talk can really represent magnetospheric convection. From the N.R.L. presentation, he believes the system is slightly beyond current capabilities. Whether or not these equations would produce substorms in the presence of a perfectly steady solar wind is unknown - i.e., whether solar wind fluctuations are necessary to trigger substorms is not known.

The magnetosphere can be divided into three regions. Region I is the magnetosheath, where isotropic pressures and magnetohydrodynamic (MHD) equations are valid. No systematic anisotropies are observed. Region II is the far tail and high latitude tail. The magnetic field is weak in portions of this Region, and MHD equations do not apply. It is a completely 3-dimensional problem. Region III is the inner magnetosphere, where adiabatic theory applies, and bounce averaging permits reduction to a 2-dimensional problem.

The present status of solving such sets of equations is that a steady state with one species with a given magnetic moment has been tried at Rice University. The computer time even for so simple a model is about one hour per hour of magnetospheric time. Because the magnetosphere has been separated into three regions, there are critical problems with choosing boundary conditions.

Five Minute Talks

Contributed papers of 5 minutes each were given by Burch (Simulation of Shuttle Experiments), Kaiser (Numerical Simulation of Cosmic Ray Diffusion), Goldstein (Ditto), Stern (Particle Motions in Neutral Sheets), Perkins (Necessity for Obtaining a Predictive Capability).

Discussion

After the 5 minute talks, approximately one hour was devoted to general discussion. For the most part what followed was an elaboration and development of questions and ideas that had first arisen during the previous day and a half.

A considerable portion of the time was devoted to the question of what constitutes a "critical mass" of workers and what sort of skill mix is required. The N.R.L. group consists of about 50 people involved in many different programs. A "critical mass" can be as small as 2 people for a simple calculation, but many more for large scale modeling. The skill mix, according to Boris, should be about half and half, theoretical physicists and computational physicists, but almost entirely physicists because a thorough understanding of the <u>physical</u> problem must permeate all phases of the development of the numerical codes. One can burn a lot of money with a computer unless the physics is well understood.

There was no unanimity on the applicability of the N.R.L. codes to problems in space physics. The opinion was expressed by Krall that almost all of the codes would be useful to space physicists practically without modification. On the other hand it was asserted by Hollweg with equal vigor that space physicists should develop their own codes rather than rely on existing ones. Most opinions fell between these two limits.

A question was raised concerning the size of the computer required to run the codes that had been discussed. The answer was given that commercially available computers of large but non-gigantic capacity are quite adequate for many problems (i.e., an IBM 7094 or larger). However, Boris in his presentation had stated that in spite of the large improvement in computer technology which occurred about 5 years ago, plus improvements in computational techniques, it was still impossible to compute on a microscopic scale for macroscopic times and distances. The list of fifteen particle and fluid codes presented by Boris contained only two three-dimensional codes. Three-dimensional codes are expensive to run and can only be run at coarse resolution that hides some of the physics. It will be several years before 3D codes get where 2D is now. Most of the 15 N.R.L. codes have been developed in the last 5 years.

All in all there appeared to be a widespread opinion that computer simulations should play an increasingly important role in space research and that it was high time if indeed not past due that space theorists turn their attention to this approach. Furthermore the opinion was overwhelmingly expressed that space science in general and NASA in particular should devote far more effort to theory than has been the case up to now. It was further asserted that this theoretical effort should take place both before and after (and indeed in some cases instead of) the launching of a space experiment.

Response to Questionnaire

At mid-morning of the second day the following short questionnaire was distributed to all participants.

> We would like your written comments on what the future role of numerical computations in space plasma physics should be. As a guide you might consider answering the following questions. Although we have rather arbitrarily limited this study to three areas (solar wind, bow shock, and substorms), your discussion need not be limited to these.
>
> 1. What do you think of the present balance among theoretical, computational and experimental activities in NASA?
>
> 2. In <u>your area</u> of space research, what do you perceive the role of numerical computation to be in the future? Is the most urgent need presently for additional data, for mathematical modeling and analysis, or for numerical computation?
>
> 3. Of the NRL codes or any others that you are now aware of, would any be useful to you? Which ones and what would be the application?

Thirty participants (about 75%) completed and returned them. Identification of the responder was optional: twenty signed, ten preferred anonymity.

As might be expected, a wide spectrum of opinion was obtained. Categorization of the responses is hence difficult: some answered the questions, others contributed interesting and relevant observations on other aspects of the topic. We here report what we judge to be the most significant comments gleaned from these questionnaires.

1. There was almost unanimous agreement that the balance in NASA's scientific program is too heavily weighted toward the experimental side. Data analysis is short changed, plasma theory is poorly appreciated and inadequately supported; and computational physics is non-existent. Two people cited the Atmospheric Explorer effort as one in which pre-

and post-launch collaboration between theorist and experimentalist has greatly enriched the value of the project. AE is, however, a singular (highly commendable) example.

2. Several people commented that NASA allows too short a period for data analysis: project money is cut-off before a thorough run-through of the data can be accomplished. A more extended funding period would permit the closer data examination needed to come up with substantial conclusions. The examination should preferably be by both theorists and experimenters. As a result of the present NASA policy, large amounts of significant data from past projects lies unused.

3. As a corollary to 2, it was suggested that mini-computers be used for data handling. Such usage would be cost-effective and free larger computers for modeling efforts of the type discussed by the NRL people.

4. There was a general feeling that many areas of space exploration are ready, at least in part, for computer simulation; among these are the three discussed at this Study. A major reservation on the part of participants, however, was the unavailability of experimentally determined boundary conditions for input to the simulations. The NRL people answered this concern by arguing that boundary conditions can be left as explorable free parameters in simulation work. Boundary conditions to which the calculation is sensitive are the important ones to measure.

5. It was emphasized that computer simulation is a task for Ph.D. level computational physicists. Experience has shown that only they have the motivation and understanding needed to come up with sensible results in reasonable time intervals. Further the computational physicist is most effective when working closely not only with the space plasma theorist, who has an overview detached from the numerics, but also with

experimenters, who provide him input and with whom he compares output.

Modeling is a team effort.

6. It was pointed out that an essential ingredient of global codes, such as a solar wind code, is an understanding of the fundamental plasma physics involved. This includes both basic theoretical analysis and the numerical study of micro-physics, and is by no means a closed book. Fundamental plasma physics should be accorded a support by NASA commensurate with any large modeling support.

7. Model studies of plasma magnetospheric, and auroral experiments for the Space Shuttle were suggested.

8. It was suggested that a catalog of the codes available at NRL and elsewhere be made available to space plasma physicists. Further, it was suggested that a vehicle be found for transmitting new developments in the modeling area to potential users.

9. Significant concern was expressed about the utilization of NRL codes without the direct involvement of the code developer. For example, boundary conditions are often such a fundamental ingredient of a code that changing them to space conditions might be as much work as re-writing the code itself.

STUDY OF APPLICATIONS OF NUMERICAL CODES TO SPACE PLASMA PROBLEMS

Tuesday, January 7, 1975

8:30 - 9:00 Introductory Formalities

9:00 - 12:00 NRL Presentation

Tim Coffey: "Overview"	15 min.
Jay Boris: "Computational Physics"	25 min.
Dennis Papadopoulos: "Multifluid Codes"	25 min.
Sid Ossakow: "Ionospheric Irregularities"	20 min.
Neils Winsor: "Modeling Laser Plasmas"	25 min.

12:15 - 1:30 Lunch in Building 1 Executive Dining Room
($2.00 tickets available at Information Desk)

1:30 - 5:00 Other Invited Speakers

Len Burlaga	30 min.	Solar Wind
Joe Hollweg	30 min.	
Dave Forslund	20 min.	
Gene Greenstadt	20 min.	Bow Shock
Paul Kellogg	30 min.	
Bob McPherron	30 min.	Substorms/Convection
Dick Wolf	30 min.	

5:30 - 6:30 Reception, Room 200, Building 26, tickets $3.00 at Information Desk

Wednesday, January 8, 1975

Wednesday morning we are leaving informal. If the Tuesday afternoon session runs late, we will postpone one or two talks until Wednesday. We also would like a contributed talk from anyone. If you wish to talk, please tell one of us (Northrop, Birmingham, Jones, or Wu) sometime Tuesday.

Attendees

Study of Applications of Numerical Codes to Space Plasma Problems

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