REPORT ON C-MMACS

SUMMARY Many significant events took place at C-MMACS during the year. An International Conference was held on Mathematical Modelling and Scientific Computing. Modelling efforts in Earth Sciences got a major boost with Prof V K Gaur joining the Centre. Major efforts were made to reorganise C-MMACS computing facilities by relocating them in one building, by making UPS power supply available, and also by initiating action to obtain a large compute server.

Results published in a CSIR journal on application of modelling to Indian transportation sector evoked considerable interest in the national press including an editorial in the *Times of India*. Amongst other results are the encouraging comparison of predictions of a tidal simulation in the Bombay Harbour with available experimental results and new insights in the behaviour of marine ecosystems. The scientific activities at C-MMACS have progressively grown to a higher energy level, as indicated by the various academic activities: publications, reports, seminars scientific meetings, special courses and lectures.

Dr K S YAJNIK
Head

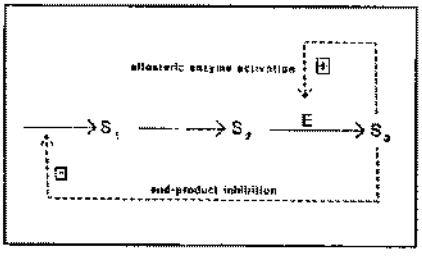
1.1 MODELLING

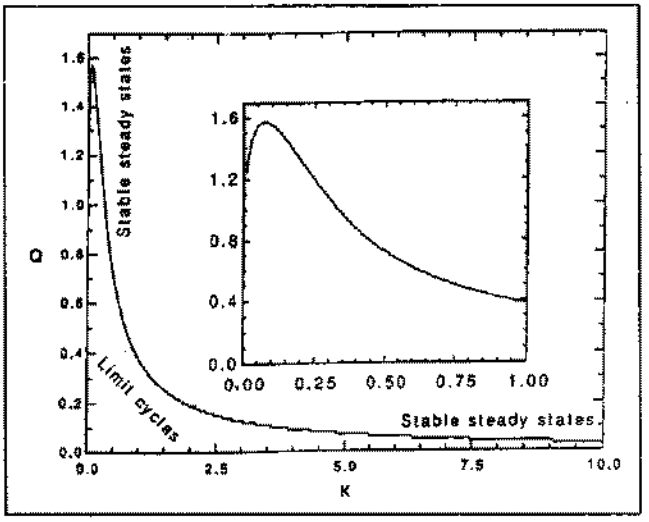
1.1A MODELLING PROBLEMS IN BIOLOGY AND CHEMISTRY

MODELLING BIOCHEMICAL REACTION PATHWAYS

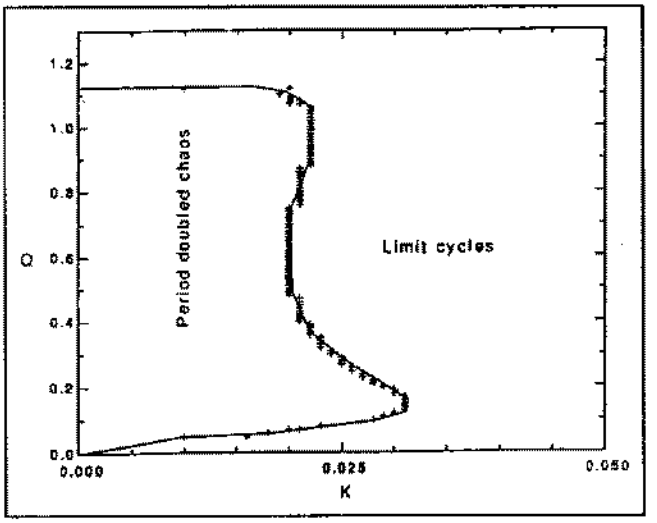
Genetic repression and induction mechanisms through small molecules and enzyme activation and inhibition are the major control elements operating on the complex circuitry of coupled biochemical reaction-cycles in cells. The various cellular functions are controlled and co-ordinated through these positive and negative feedback/feedforward loops that help in activating (sensitivity factor) and deactivating (stability factor) particular steps in the pathway at required times. Though the biochemical details of many reaction pathways are known, a general understanding of the nature of interactions among these coupled processes have not yet emerged. This can be attributed to the complex nature of these systems involving essentially nonlinear phenomena. A wide variety of dynamical behaviour is observed in living systems, namely, steady and periodic output in basal and alternate conditions, 'switching' behaviours (i.e. threshold sensitivity and multistability), excitability, transients, aperiodic or chaotic oscillations etc.; some of these may be pathological. It has become possible now a days to simulate the dynamical behaviour of these systems on high-performance computers by computing the solutions of the nonlinear model equations.

▼ *Fig. 1 Schematic of the model biochemical reaction pathway.*





▲ *Fig. 2 Hopf bifurcation surface across which the asymptotic dynamical behaviour changes from steady state to simple periodic oscillations.*



▲ *Fig. 3 Surface in k-q space across which simple periodic oscillations give way to period doubling followed by chaos.*

In a joint programme involving C-MMACS and CCMB, a model has been constructed for a possible pathway having coupled positive and negative feedback processes. Although the possible dynamical patterns in pathways that involve only positive or only negative feedback/ feedforward steps were studied earlier, not much is known about the case where a positive feedback is coupled with a negative one. Here, the feedbacks are in the form of genetic repression (end-product inhibition) and allosteric enzyme activation (see schematic in *Fig. 1*), respectively. Earlier the results of a scan of parameter space were reported for the different behavioural patterns using bifurcation diagrams, phase space and time series analysis and other methods.

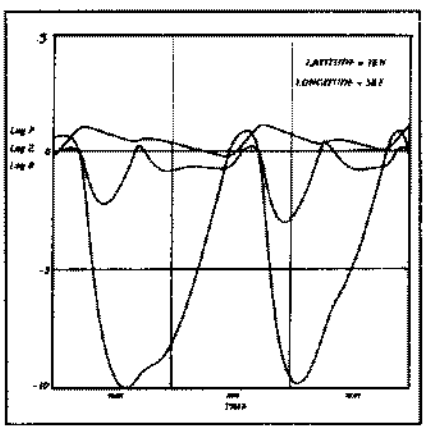
During the last year, domains in the parameter space were mapped for particular types of dynamical behaviour. Two parameters were varied namely, the degradation rates of S_1 (= k) and S_3 (= q). Other parameters were held fixed at the likely basal values. *Fig.2* shows the boundary separating the domain of the stable steady states and the domain of the autooscillation (limit cycles). The limit cycles grow in amplitude as one moves away from the curve and ultimately, for low values of k, period doubling bifurcations to chaos are observed; *Fig. 3* delineates the k-q boundary across which transition to period doubling occurs.

MODELLING IN MARINE BIOLOGICAL SYSTEMS

Marine biota play an extremely important role in the global carbon cycle. The biological pump transfers a considerable amount of carbon from the euphotic zone to the deep ocean as organic matter, the basic mechanism being fixation of inorganic carbon into organic molecules during photosynthesis. Also, the dependence of development of fish larvae on the available phytoplankton is an example of interest from the viewpoint of marine productivity.

Ocean carbon-cycle models coupled with ocean-atmosphere general circulation models, can describe the long-term responses of ocean system to global change scenarios. As a first step towards the development of such coupled, basin scale models of ocean circulation and biogeochemical cycles, a study was initiated at C-MMACS with a class of dynamical models of marine ecosystems. Initially, a 3-component model of the marine ecosystem was

▼ *Fig. 4 The logarithmic variations of phytoplankton (LP), zooplankton (LZ) and bacteria (LB) during March to May.*



studied using phase plane analysis / CM 23/. At present, a 7-component model proposed by Fasham et al (1990) is being studied at four stations in Arabian Sea which are the proposed sites for intensive time-series studies under JGOFS. /CM35/ It was observed that the marine ecosystem shows periodicities in the range of 15-45 days at these stations. The variability associated with these periodicities is quite large. Bacteria show smaller periodicities than other components. In the study of sensitivity of the response to parameters, it was found that the asymp-

totic grazing rate has a significant effect on variability of phytoplankton.

Fig.4 shows typical variations at one station. Variability in phytoplankton far exceeds variability in zooplankton or bacteria. Primary peaks of zooplankton and bacteria occur soon after peaks in phytoplankton. Also, a very weak peak in zooplankton is seen soon after a secondary peak in bacteria which follows rapid decline in zooplankton population. This simulation carried out for climatological variations of solar radiation and mixed layer depth shows that further studies and refinements in the model are required to ensure realism.

COMPUTER AIDED CHEMISTRY: CONFORMATIONAL STUDY OF PEPTIDES

Conformation of a molecule defines its characteristics and most of the molecular properties are functions of its geometry. Since most of the molecules are conformationally very flexible, the choice of their preferred conformations is a daunting problem. For example, a grid type search performed to arrive at the structure of peptides, would take with the present state-of-the-art computers, the computation times of the order of the age of the universe! Other conventional minimization methods would suffer from the local minimum problem.

The conformational study of peptides also attempts to answer another of the mysteries of nature, namely, protein folding. From the knowledge of the rules that govern protein folding, it would become possible to synthesize "Designer Proteins", which would have the desired shape and as a consequence of which would have a predefined functionality.

Secondary structural prediction has been primarily been carried out using statistical methods. But recently approaches based on the usage of Simulated Annealing (SA) has been attempted to provide a solution to the global minimum problem. A study has been initiated at IICT on the modelling of some polypeptides using a combined approach of experimental techniques (NMR) and molecular modelling. The recourse to SA proved to be attractive for the input to such a program would be just the aminoacid sequence and the structure is being calculated in an ab initio manner. The molecular mechanics program chosen was AMBER 4.0. SA studies were carried out for four peptides in order to determine their secondary structure. The peptides studied were 12-26, 15-23, 15-33 [Trp > Ser] fragments of tendamistat and an LHRH antagonist. The results obtained were consistent with the available experimental data. Studies are now being carried out at C-MMACS under a collaboration project with IICT to generate a cost-effective protocol for SA studies.

The study of cyclic peptides has another constraint of ring closure which is critical to obtain the most preferred conformation of cyclic peptides. IICT has a collaborative program with one of the Schools in Japan to develop a computer code using the AMBER suite of programs. It is hoped that this code will prove an invaluable tool for studying cyclic peptides. The program AMBER-CONFLEX is now undergoing extensive testing.

1.1B MODELLING PROBLEMS IN EARTH SCIENCES

MODELLING STRESSES IN THE INDIAN LITHOSPHERE

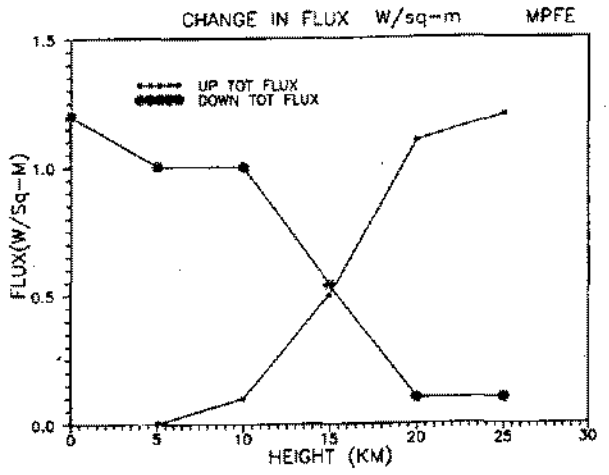
The Indian lithosphere: a basic canvas for the exploration and delineation of fracture-controlled lineaments: resources and hazards.

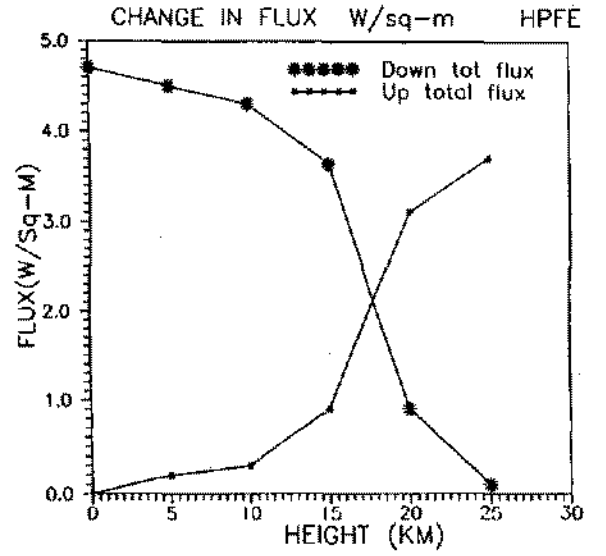
Prevailing stresses in the lithosphere are the immediate cause of its fragmentation at various scales thereby carving the basic tectonic framework which, in turn, controls the evolution of its structure and geomorphic features that are of great interest to us. These range from broad scale landforms that determine our habitat and activities in many ways, to shallow textural features that influence the course of mineralization and groundwater regimes.

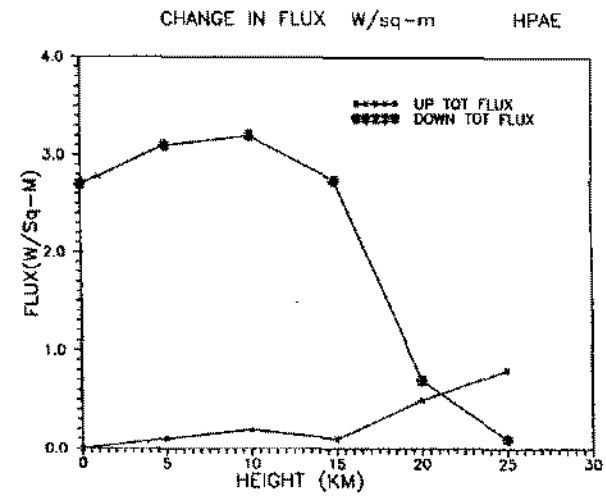
The stress regime of the lithosphere also determines the response of this outer brittle shell on which we live, to intensifying exploitation of the earth resources: land use, mining and containment of long life hazardous waste. Knowledge of the stress field thus provides an understanding of the natural grain of the earth which can prove valuable in engineering design of land use and other large scale industrial systems. As our burgeoning human family stretches its reach to colonize every available ecological niche for habitat and resource development exposing large investment activities to ever greater risks, the need for a knowledge based approach becomes all the more imperative.

Furthermore stress distribution in the lithosphere, being the net result of boundary forces and its 3-D lithospheric geometry & composition, can shed significant light on these features which would in turn, help constrain models of earth structure and evolution. This, indeed is our ultimate objective, towards creating a rational basis for addressing diverse problems of development and earth use with deeper insight and understanding of its intrinsic texture. These considerations put stress modelling of the lithosphere high on the research agenda of earth physics with important implications to development activities

In the case of Indian lithosphere, considerable new knowledge has been gained about some significant intra-plate features notably flexure of the lithosphere in response to topographic loads, and the intense deformation zone in the equatorial Indian ocean lithosphere as well as







its rheological properties. These developments in turn call for a more realistic modelling of stresses in the Indian lithosphere simulating all important features known to date that influence the state of stress.

The stress in the Indian lithosphere is modeled using a realistic set of boundary conditions in a finite element procedure. Plate boundary forces simulated, include 1) Slab pull at subduction zones, 2) Ridge push, 3) Resistive forces acting on the down going slab at trenches, 4) basal drag at the base of the plate, 5)Suction forces along the Tonga-Kermadec trench and 6)Bending moments along the Himalayan collision zone. In addition to these, the plate will also be loaded vertically by known seamounts and thick sedimentary deposits notably the Afanasy - Nikitin seamount load on the highly deformed central Indian basin and sediment loading of the northern Indian plate.

Modelling of stresses in the Indian plate using the above boundary conditions is being carried out using finite element software packages on PC 486 machine. Fortran routines for calculation of forces such as slab pull, ridge push and resistance forces at the trenches have been developed. Lithospheric ages required to calculate ridge push and slab pull have been taken from the maps compiled by Sclater et al. (1980). To begin with the Indian plate has been approximated by a flat model. The finite element mesh generated consists of triangular elements in a plane stress approximation.

NEGATIVE RECENCY IN EARTHQUAKE MIGRATION

This work relates to proposed activity of developing nonlinear prediction schemes. It is a preparation for

▲ ***Fig. 5*** *Perturbations in the radiation budget for (a) fresh moderate volcanic (MPFE), (b) fresh high volcanic (HPAE) aerosols, (c) aged high volcanic (HPFE). The reductions in fluxes when compared to the background aerosol case are shown. A reduction in the downward flux indicates cooling of the layers below while a reduction in the upward flux indicates trapping (hence heating) of outgoing radiation.*

that objective and establishes a new form of predictability in earthquakes sequences. By earthquake migration conventionally one means either a systematic migration of earthquake foci in one particular direction on a long linear fault system or such a migration preceding and following a major earthquake on a fault segment. The present work deals with earthquake migration on long linear fault systems and studies it in its entirety rather than looking for systematic migration in a particular direction. The pattern found is called negative recency. That is, if the recentmost movement of earthquake foci is in a particular direction, the next earthquake is more likely to reverse that trend than to follow it. Historical earthquakes along the Alpide belt, Southern California fault system, Himalayan arc and Japan trench have been analyzed. The negative recency is generally seen to get stronger as the magnitude threshold for the earthquakes included in the analysis is raised. The next step would be to use spatial migration of earthquakes for prediction using nonlinear prediction strategies /CM 12,30/.

GLOBAL CLIMATE CHANGE: EFFECT OF VOLCANIC AEROSOLS ON TROPICAL RADIATION BUDGET AND SATELLITE MEASUREMENTS

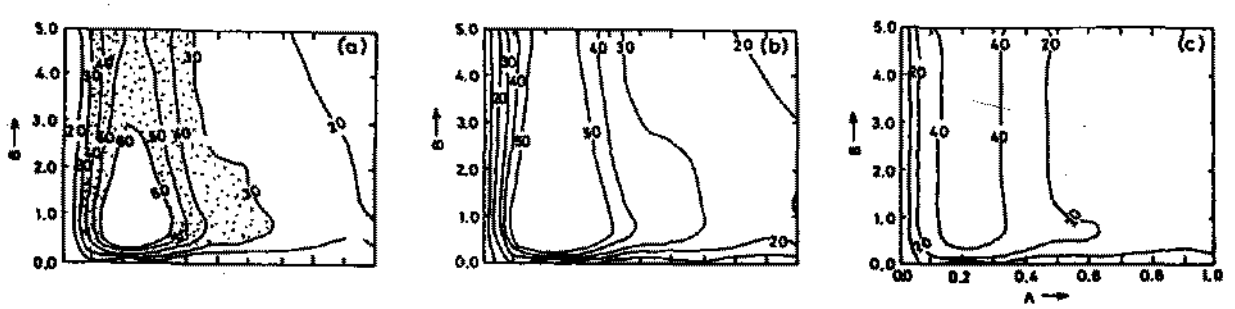
The recent multiple eruptions of Mt. Pinatubo have spewed an enormous amount of volcanic aerosols in to the stratosphere. A significant part of this is still trapped in the tropical stratospheric belt and is expected to have a lifetime of 1-3 years (Watson et al, 1990). The effect of these aerosols on atmospheric radiative transfer are manifold; they interfere with satellite observations of the earth and also perturb the radiation budget leading to climate change..

It is generally believed that an increase in stratospheric aerosols will cool the earth on account of attenuation of direct sunlight (Harshavardhan 1979). But there are other aspects of this problem which also require attention, i.e., the increase in diffuse radiation due to multiple scattering and trapping of ground and atmosphere emitted long wave radiation. It is recognised that the influence of aerosols on climate are far more difficult to assess than trace gases because of temporal and spatial variations in concentration,size distribution, chemical and optical properties (Watson 1990).

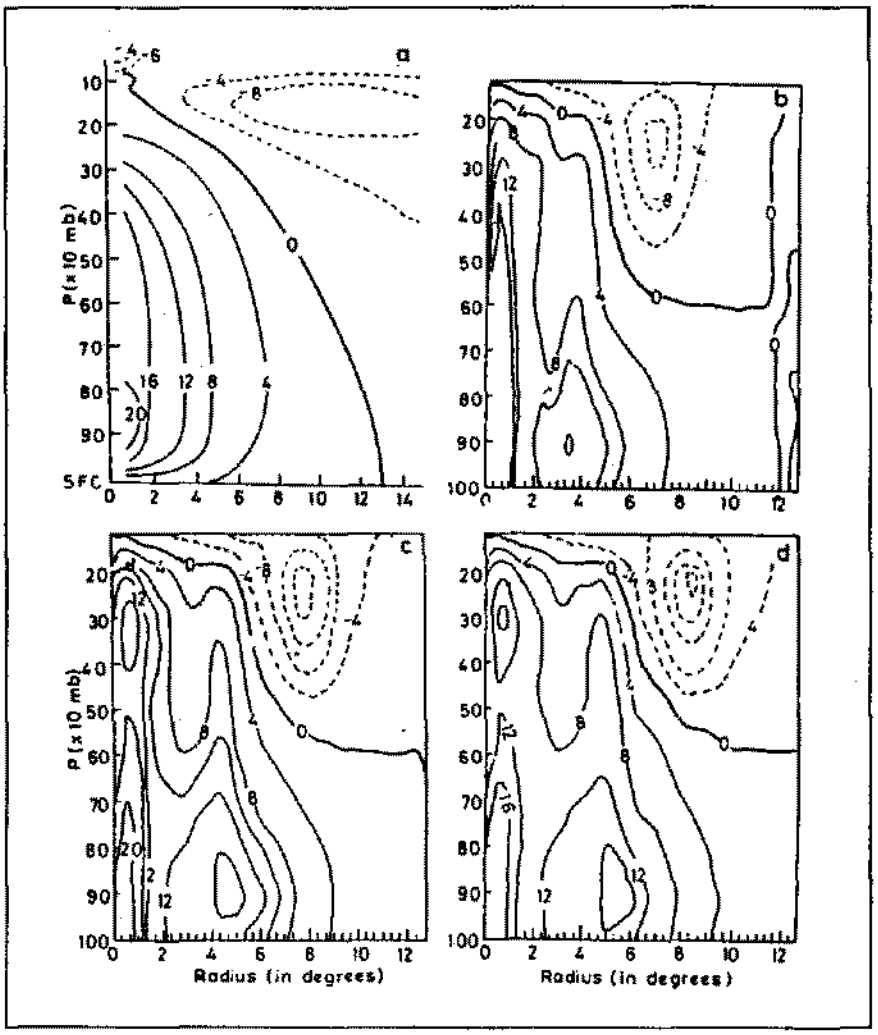
C-MMACS has initiated a programme to study the effects of aerosols on climate and satellite remote sensing. The objectives of the study are a) modelling radiative transfer through the atmosphere as accurately as possible with a view to making reliable inferences about aerosol effects and (b) generating models which are specific to tropical conditions. At C-MMACS, radiative transfer through the atmosphere has been accurately modelled using LOWTRAN 7, a state-of-the-art software package (Kneizys et al 1988). Spectral calculations (300 lines covering the solar and long wave spectrum) have been integrated to yield total upward and downward fluxes.

Four types of stratospheric aerosols, (a) background, (b) fresh moderate volcanic, (c) aged high volcanic and (d) fresh high volcanic have been considered in our simulations. Of these case (a) prevails in the absence of any volcanic activity and the fresh and aged indicate the conditions which exist a few months and a few years after the eruption, respectively. These four cases cover a wide variety of possible scenarios.

The reduction of downward (which includes direct, diffuse and downward emitted atmospheric radiation) fluxes when compared to the background case for cases (b), (c) and (d) are 1.2, 2.7 and 4.8 W/sq-m, respectively. The trapping of long wave radiation in the stratosphere is also significant with values of 1.2, 0.8 and 3.8 W/sq-m for the three cases. When both upward and downward fluxes are considered together there is a net cooling upto a height of 15, 22



▲ *Fig. 6 Variation of the properties of the maximally growing equatorial Kelvin wave in presence of evaporation wind feedback and convective time lag: (a) behaviour of the periodicity in A-B plane (b) behaviour of the associated wavelength in A-B plane (c) behaviour of the e-folding time in A-B plane, where A is a nondimensional evaporation wind feedback parameter and B is the convective time lag in nondimensional units. Length scale L_e = 1047 km, time scale T_e = 0.66 day.*



▶ *Fig. 7 Radial vertical profiles of tangential velocity in m/s. (a) observed profiles for a mean hurricane. Model simulated profiles at (b) 12 hr, (c) 18 hr and (d) 24 hr.*

and 17 km and net heating thereafter for the three cases. The magnitude of these changes in fluxes can lead to significant changes in the thermal circulation pattern in the short term. Besides, the heating observed at larger altitudes is expected to deplete the ozone layer by assisting the vertical transport of ozone to higher altitudes (see *Fig.5*).

The effect of volcanic aerosols on satellite remote sensing is currently under study at C-MMACS under a project sponsored by DOD. Preliminary results indicate a depression of 1-2K in the brightness temperatures sensed by the infrared channels of the AVHRR radiometer. A complete analysis of the aerosol effect is expected to yield correlations which may be applicable in SST determination in the presence of aerosols.

The determination of radiative properties of aerosols from measured profiles and size distributions by the application of Mie theory is also currently under progress. These will be incorporated into future versions of the radiative transfer model.

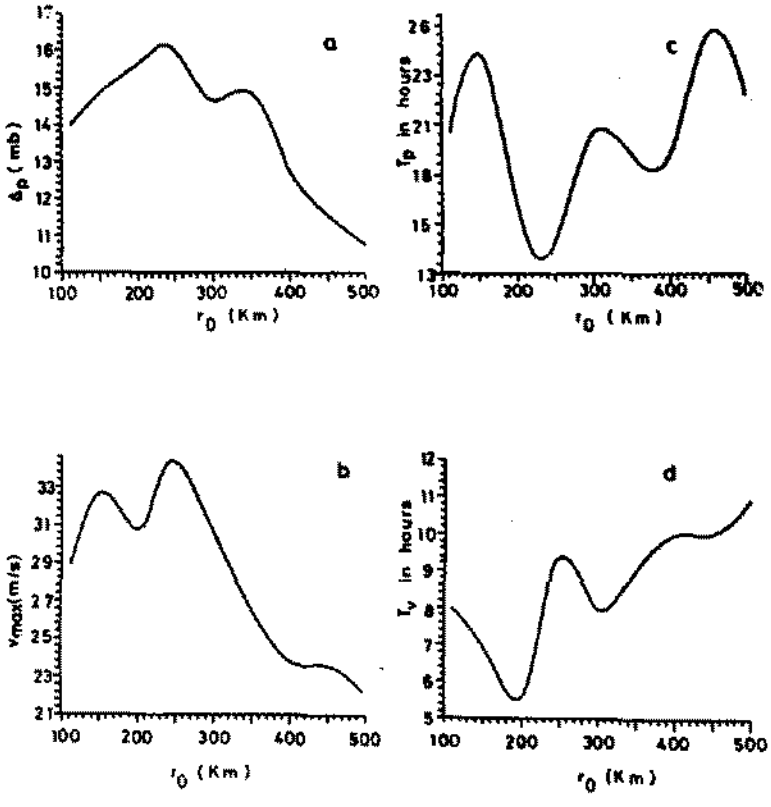
MODELLING MOISTURE FEEDBACK FOR LARGE SCALE TROPICAL CIRCULATION

The 30-50 day tropical oscillation is an important component of monsoon variability and monsoon prediction. An analytical model for the tropical 30-50 day intraseasonal oscillation was modelled as the Kelvin mode of a shallow water model on an equatorial plane driven unstable by moist processes. Unlike in similar models, here precipitation is modelled as a relaxation process based on the hypothesis that the large scale flow is not in quasi equilibrium with convective heating. The introduction of such a convective time lag naturally gives rise to a scale selection of the Kelvin wave in the low frequency regime. The structure and properties of the maximally growing wave closely resemble those of the observed 30-50 day tropical oscillation. The variation of the periodicity, wavelength and e-folding length of the maximally growing wave as functions of two feedback parameters. A (Evaporation wind feedback) and B (Convective time lag) are shown in *Fig.6*. Thus using this model we could give for the first time, a consistent description of the 30-50 day oscillation as in intrinsic mode of the linearized tropical atmosphere. Extension of the model to account for the other low frequency tropical oscillation is in progress.

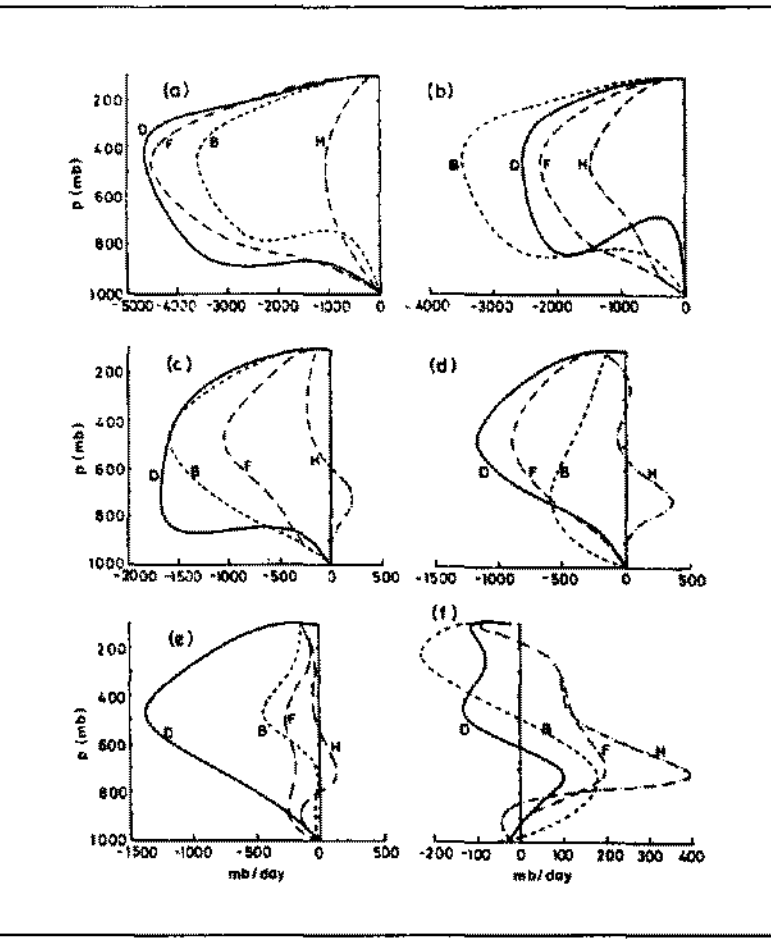
SIMULATION OF A TROPICAL CYCLONE BY AN AXISYMMETRIC MODEL

An axisymmetric model of the tropical cyclone that uses Arakawa Schubert parametrization scheme was used to simulate the evolution and structure of a tropical cyclone, using 20 year mean climatological data for Calcutta Station. The simulated results were then compared with the observed profiles for a *mean* mature hurricane. This set of experiments was carried out both for testing the suitability of the model for studying the Bay of Bengal cyclones and to estimate the deviation of the latter from the mean hurricane in other ocean basins. The results show good agreement between observed and simulated structures with allowance for deviation of individual systems from the mean structure. Vertical profiles of the model simulated tangential velocity at various time steps are compared with observed mean profiles in *Fig.7*. The adopted (Wada) model therefore provides an excellent research tool for studying evolution and structure of tropical cyclones.

▶ *Fig. 8 Dependence of intensification of tropical disturbances on the size of the incipient vortex. (a) maximum fall of the central pressure (in mb): y-axis shows the maximum difference between the environmental pressure and the low-level central pressure, (b) maximum tangential wind attained in m/s vs. r_o (c) time (t_p) in hours for attaining maximum P vs. r_o, (d) time (t_v) for attaining v_{max} vs. r_o.*



▶▼ *Fig. 9 Vertical profiles of vertical velocity (mb/day) averaged over 3° latitude for incipient vortices B (110 km), D (240 km), F (350 km) and H (450 km) at (a) 3 hr (b) 6 hr (c) 9 hr (d) 12 hr (e) 18 hr (f) 24 hr.*



Most of the cyclones in the Bay of Bengal region evolve from intensification of tropical disturbances that develop *in situ* or drift into these areas. An important and long standing problem in tropical cyclone warning and prediction is an early warning of these 'coastal' cyclones. Based on the above simulation studies a set of experiment was conducted to investigate the role of the incipient vortex size in the subsequent evolution of a tropical disturbance, and the possible use of the incipient vortex size as an early warning parameter. The most significant findings of this set of experiments are (1) the intensification of tropical disturbances is not uniform or linear with the incipient vortex size r_o (for 100 km<r_o < 500 km); there is a peak in the intensification curve at about 250 km. *Figure 8* shows the distribution of (a) maximum sustained tangential v *v* (b) minimum low level central pressure difference (Δ) attained with the size of incipient vortex size r_o. There is a clear maximum at about r_o equal to 250 km. (2) The vertical profiles of w (vertically velocity for the maximally growing vortex (r_o ~ 250 km) shows a distinctive oscillation in time, absent in the other vortices. In *Fig.9* are shown the vertical profiles to 30° radial mean vertical velocity for different vortices at different time steps. Notice the oscillation of the vertical

position of the maximum vertical velocity for the vortex D (r_o ~ 250 km).

The first of these results hints at the possibility of use of the incipient vortex size as an early warning parameter for tropical cyclones; the second result points to an intricate dynamical mechanism, hitherto unreported, that gives rise to the maximal growth at a particular scale.

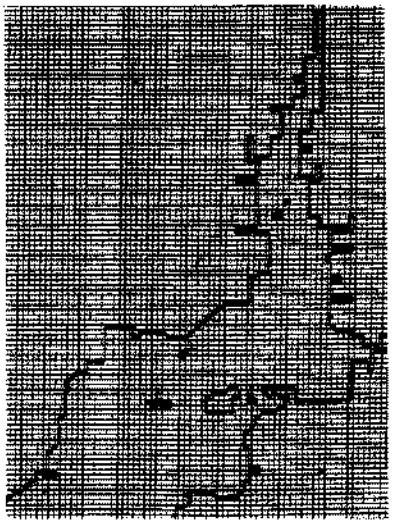
Development of a dynamical mechanism for the effects observed as well as investigation of the sensitivity of the results to various mean conditions are in progress.

BASIN SCALE OCEAN MODELLING

One of the striking features of the circulation in the Indian Ocean is the seasonal variation in surface currents in response to reversal in the wind direction due to monsoons. Efforts are underway at C-MMACS to generate a realistic model of the Indian Ocean by incorporating monthly climatology data and realistic topography.

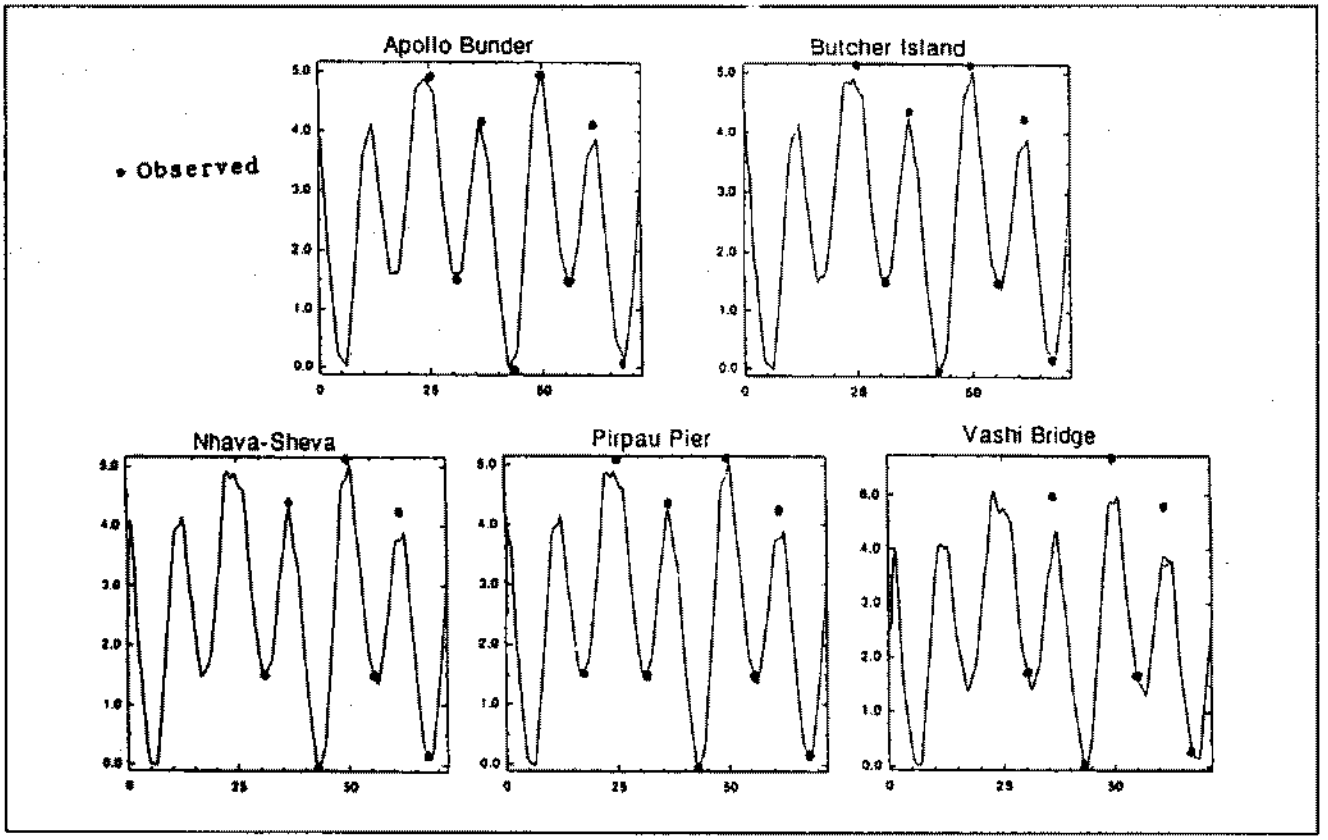
The Modular Ocean Model (MOM), recently acquired from GFDL, Princeton, was successfully installed and tested for coarse resolution runs on the SUNSPARC1 workstation. This is a 3-D primitive equation model of the ocean incorporating both wind driven and thermohaline circulation over a wide range of space and time scales and is due to Bryan and Cox (K.Bryan 1969, M.D.Cox 1970, 1984). C-MMACS has obtained a comprehensive climatological data base containing 1°*1° Scripps topography, Hellerman windstresses (monthly means and annual average), Levitus temperature and salinity profiles (monthly means and annual averages) and Oort's air temperatures. This data base can be used to generate realistic models of ocean basins using variable grids and a choice of mixing and filtering schemes to facilitate the calculation of velocities, mass transport stream functions and tracers to the desired accuracy.

MOM is intended to be run on large multiprocessor machines like the



▲ *Fig. 10 Locations of the observation stations (Thane Creek) at (1) Apollo Bunder (2) Butcher Island (3) Nhava Sheva (4) Pirpau Pier and (5) Vashi Bridge*

▼ *Fig. 11 Comparison of predicted and observed tidal variations in Thane creek*



CRAY Y-MP. At present, with the computing resources available at C-MMACS, smaller scale problems or coarse resolution studies are being attempted. The full potential of MOM will be exploited when C-MMACS acquires a large compute server.

SEA LEVEL VARIATIONS

Sea level changes can have marked effects on habitat in coastal regions. These changes when caused by global warming can be quite widespread. It is therefore important to study sea level data to ascertain trends and to make estimates of changes in future. Stochastic time series methods are available to construct empirical models. It is also possible to use fractal approach for this study, which has the advantage that the information around regions of data scatter is not lost. A study was undertaken in C-MMACS for Bombay, Cochin, Madras, Vishakhapatnam and Sagar (Calcutta). The fractal dimension was calculated using iterative function systems technique given by Barnseley (*Fractals Everywhere* (1988), Academic Press, N.Y.). It was found that the dimension lies between 1.2 and 1.3. Also stochastic time series methods are being applied to the available data for the Indian coastal region to arrive at empirical models.

COASTAL CIRCULATION AND MARINE POLLUTION MODELS

Results of the version 3 of the coastal pollution model for Thane Creek were presented to the local organisations in Bombay. Detailed discussions and feedback have led to the version 4. In this version, the tides are represented more realistically by including 34 spectral components by using the tide data at Apollo Bunder. The value of the bottom friction coefficient is now taken into account the known sandy-clay nature of the bottom surface and the available experimental data and is believed to be more accurate.

It was decided to test the realism of the model by comparing with limited tidal elevation and current data available at five stations during Dec 3-4,1986. The calculations were started with the initial condition of the state of rest. Wind forcing was neglected as its effect is known to be small for this season. Similarly river discharge from the northern river was neglected as it is known to be small during this season. *Figures 10 and 11* show good agreement at four stations especially for the lows. For the Vashibridge the departures at highs are believed due to connection to the sea though the northern end which would need enlarged computational domain to determine. Further studies are in progress.

1.1C MODELLING IN ENGINEERING

COMPUTER AIDED DESIGN AND ENGINEERING

Aeronautical Applications

GTRE was facing difficulties in obtaining a single piece airblast atomiser for the KAVERI engine to meet their design specifications either through import or by the conventional route of investment casting. This led to a sponsored project at NAL on the development of CAD/CAM techniques using CNC milling for manufacturing the airblast atomiser as a single integral piece out of a solid bar stock. The atomisers would ultimately be manufactured from Nimonic 75 material for the aeroengine. The specific objective was to manufacture six airblast atomisers of stainless steel. They would be used for ground combustor sector tests and for evaluation of the design configuration.

CNC software and CAD\CAM techniques were developed at C-MMACS under this project by scientists of the Propulsion Division using IRIS workstation. Also, technology was developed to mill an airblast atomiser as a single integral piece. Manufacturing process is quite complex as it involves CNC milling, turning, electrodischarge machining, electron beam welding and vacuum brazing. Six airblast atomisers were manufactured on schedule, and used for tests. *Figure 12* shows six airblast atomisers. The success of this project has resulted in a capability based on CAD/CAE for making integral nimonic airblast atomisers for aircraft engines.

A second aeronautical application concerns a 1/3 scale model of the first stage of the low pressure turbine of the KAVERI engine which was required for tests in the turbine rig in Propulsion Division of NAL. Such scaling gave rise to very thin turbine blades having leading and trailing edges with radii of a few hundred microns. As a test case, the blades were modelled on the C-MMACS workstation, CNC software developed, and the blades were machined. As the desired machining accuracies could not be obtained, the scale of the LPT rotor blade was changed to 3/4th again using the C-MMACS graphics workstation. The new blade will now be tested in GTRE rig. This task has led to development of CNC software for machining this blade and its platform.

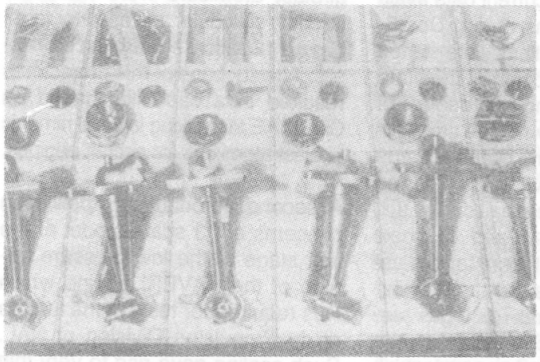
A third aeronautical application of the Iris workstation at C-MMACS has been discussed elsewhere in this report (*see pages 58-59*).

Space Applications

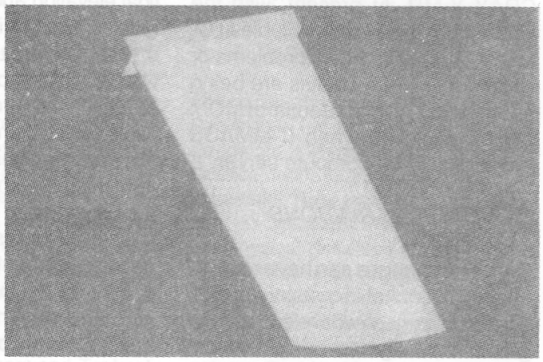
New nonaxisymmetric configurations of strap-on booster nose cones of the Geostationary Satellite Launch Vehicle (GSLV) were modelled at the on C-MMACS workstation. Each configuration was modelled, CNC software developed and the 3-D nosecones machined in the Propulsion Division and given for wind tunnel tests in NTAF.

Applications to Power Sector

Damaged 3-D compressor rotor and stator blades of a 108 MW industrial gas turbine running on natural gas was sent by the Maharashtra Electricity Board. Geometric data obtained from these damaged blades were smoothened out on the C-MMACS graphics workstation and



▲ *Fig. 12 Six airblast atomisers which were manufactured by GTRE using CAD/CAM techniques developed at C-MMACS.*



▲ *Fig. 13 CAD/CAM techniques were used at C-MMACS to help the Maharashtra Electric ity Board solved a problem of damaged gas turbine blades.*

CNC programs were generated after modifying the model to achieve the design expectations. The blades were machined and found to be within acceptable tolerance. *Figure 13* shows the CAD model of the modified blade.

MODELLING OF DISPERSION CHARACTERISTICS OF THERMAL DISCHARGE FROM A THERMAL POWER PLANT IN DAHANU CREEK

A thermal power plant with production capacity of 500 Mega Watt is proposed to be constructed at Dahanu creek on Gujarat-Maharashtra border. The plant will take in cooling water through an intake and discharge hot water back into the creek.

A project has been taken up by NEERI, Nagpur with C-MMACS, to predict the temperature rise over the area of water body due to proposed discharge of the thermal power plant. A numerical model TIDAL-2D is currently being used to simulate the creek hydrodynamics and heat transfer phenomenon. An important question is whether there is the possibility of discharged hot water flowing back into the inlet.

Numerical experiments were carried out with 50x100 meter grid with discharge of 10.0 cubic meter per second at 55 deg. C. Modelling results show that the current pattern in the creek is significantly altered in the vicinity of outlet due to shallow depth. A maximum of 5.0 Degree Centigrade rise above the ambient water temperature is predicted near the outlet. Moreover due to mixing and advection the temperature rise reduces to 3.0 degree centigrade near the intake. Further modelling studies are planned for model effects of tidal conditions, discharge parameters and for comparison with observations (see *Figures 14, 15 and 16*).

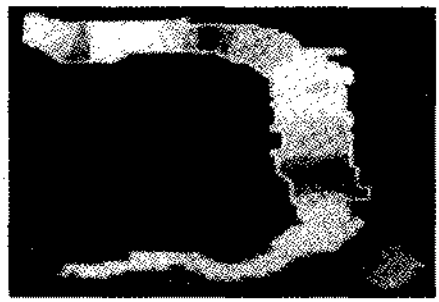
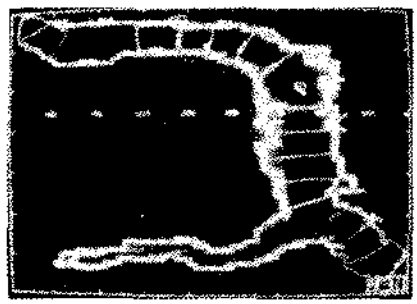
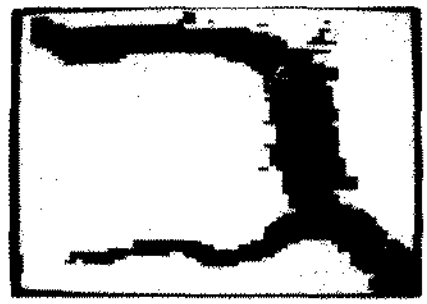
MODELLING OF ELECTROMAGNETIC ACTUATORS

C-MMACS has completed a project on modelling and simulation of electromagnetic actuators for industrial application. It was sponsored by a private sector industry. Under this project, a software was developed to calculate magnetic flux using a finite element method and to determine nonlinear dynamics of the electromagnetic actuators. The software was validated for two test cases. Training in the method was also imparted to the design engineering staff of the sponsoring industry. A technical presentation to the industry with submission and detailed technical reports' marked the end of the project (please see /CM 41,43,44/ for more details).

DEVELOPMENT OF A SOFTWARE PACKAGE FOR SOLIDIFICATION IN CASTINGS

Simulation of solidification, a project jointly taken up by RRL Trivandrum and C-MMACS, is an efficient method for determining the efficacy of feeders in avoiding shrinkage cavities in castings. The evolution of the solidification front is computed by solving for the temperature field in the casting to identify isolated pockets of liquid which lead to shrinkage cavities.

The software consists of a preprocessor, a solver and post processor. The solver is the heart of the software and it numerically solves the equations governing heat flow in the casting and the mould using the Finite Volume Method (FV). The pre processor is for the input of the casting geometry and for enmeshment of the system prior to the numerical analysis. For easy handling of complicated geometries, the solid modelling package IDEAS and the mesh generator of the IDEAS FEM package are used in the pre- processor, An interface programme has been written to read the output file of IDEAS FEM and to convert the nodal data into a form suitable for the FVM solver module. The-Finite-Volume-Method has been adapted to work with the tetrahedral volume elements

▲ *Fig. 14,15,16 Typical results from a modelling exercise of dispersion characteristics of thermal discharge from a thermal power plant in Dahanu Creek using the TIDAL-2D software available at C-MMACS. The photo on the left shows a raster plot of temperature while the figure next to it shows the contour plot.*

generated by the automatic mesh generator of IDEAS FEM. This software therefore combines the conceptual and computational simplicity of FVM with the efficient enmeshment possibilities of FEM. Work on pre-processor and solver has been completed. Work on post-processing, integration and validation is planned.

BODIES OF ARBITRARY SHAPE APPROACHING A PLANE WALL IN STOKES FLOW

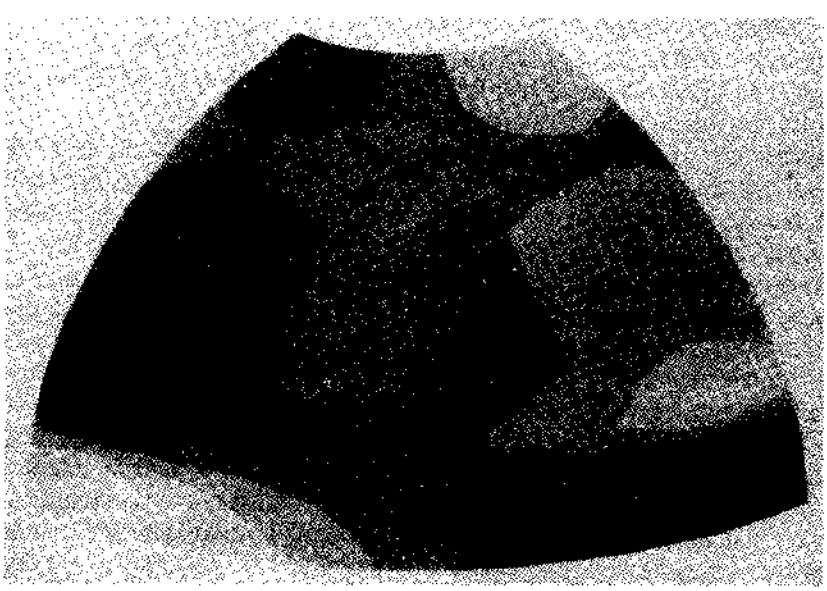
A problem of bodies approaching a wall in Stokes flow related to composites was taken up as a joint project between RRL Trivandrum and C-MMACS as it bears on metal matrix composites. An initial survey of available methods for solving similar problems showed that the method of Hsu and Ganatos (1989) appeared to be best suited. As a first step, it was proposed to make a detailed analysis of the method and to check out their results. Efforts at obtaining their published results have not been successful even after accounting for certain errors, presumably topographical. At present, the regime of applicability of their analysis is being explored. A detailed analysis is underway and a first report has been communicated for publication.

1.2 ALGORITHM DEVELOPMENT AND SIMULATION STUDIES

PRE- & POST PROCESSORS FOR FINITE ELEMENT ANALYSIS

NAL has developed a high-performance finite element software package for structural analysis. User-friendly interactive pre- & post processors for finite element analysis are being developed under a joint project between CMMACS and NAL to provide user interface to the package. This software facilitates the preparation of model data and the visualization of results. It is planned to integrate the pre- and post processors with the finite element package.

Presently pre- and post processors are being ported to MS windows graphical user interface. A program for three dimensional contour plot has been developed and incorporated into the post processor. (*see Fig.17*).



◄ *Fig. 17 Illustration showing the contour and deformation plots obtained from the post processor.*

STUDY OF THE TRANSPORT SECTOR

Publication of the first results /CM 20/ of the study at C-MMACS on

Table 1
Projections: Civil Aviation (Indian Airlines)

Quantity & Units	Mean Annual Growth Rate	Model Predictions 2000	2010
Revenue passenger Kms (billion)	10.35	28.57 (+3.643, - 3.231)	76.48 (+ 9.751, - 8.648)
Revenue tonne Kms (billion)	8.32	1.740 (+0.2615, -0.2273)	3.869 (+0.5814, - 0.5055)
Operating revenue (billion)	17.43	57.13 (+ 15.50, - 12.19)	285.0 (+ 77.29, -60.80)

Note: The 2σ error bars are shown in brackets (see /CM20/)

transportation sector in India in *CSIR Journal* evoked considerable interest in the national press. Major national dailies carried fairly detailed excerpts from this study and, which in turn appears to have led to an enhanced awareness on the part of many individuals on the scale of the transportation problems in India and the needed solutions (see *Table 1*).

Further studies are in progress on the data with a view to ascertain interrelationship between major transportation and economic indicators. They use time series analysis and regression models.

PARALLEL ALGORITHMS

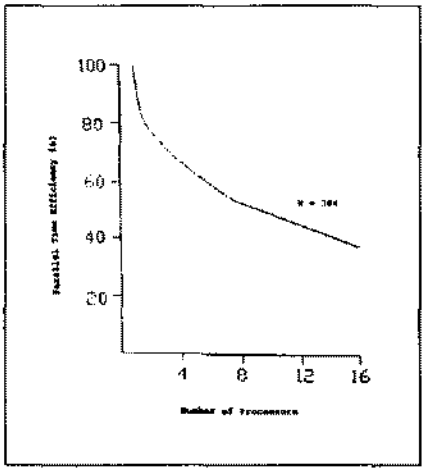
Two-dimensional panel method calculations were carried out on the 16-processor parallel computing platform at C-MMACS. Experiments were continued to examine how the parallel efficiency of a new iterative algorithm for the solution of the large-scale dense linear system Ax = b for singularity strengths varied with different topological connections of processors and communication-routing strategies. The tests indicated a marginal increase of about 1% the earlier value of 73% for 1152 panels for 16-processors connected in mesh topology. Preliminary trials conducted with a modification to the algorithm showed encouraging trends for raising parallel efficiency to higher levels.

Investigations with a three-dimensional panel method showed for a parallel Gauss-Seidel algorithm a parallel time efficiency decreasing with the number of processors (*Fig. 18*). Further work is in progress to improve efficiency.

EUGENIC ALGORITHM FOR GLOBAL OPTIMISATION

One of the important algorithms for global optimization is called the genetic algorithm and is based on the metaphor of evolution on the principle of the survival of the fittest. Such metaphors are useful as the success of genetic algorithm would illustrate. Yet a powerful metaphor carries concepts from one domain to another where it has application, rather uncritically. Thus, there is a good deal of unwarranted transfer of context from the source field to the field of application, wherein that context may even be ludicrous. For example, the genetic algorithm simulates the concepts of monogamy, chromosome swapping, binary sex, mortality and taboo against infanticide. All these concepts are irrelevant for the field of mathematical optimization. Even more importantly, the contribution of the theory of evolution was to establish that the evolution is entirely nonteleological, whereas mathematical optimization is specifically a teleological activity. Therefore, eugenic algorithm rejects all these unwarranted transfers of contest from biology and culture, while retaining the chief lesson that an interplay of chance and conscious selection can lead to rapid improvement. It also supplements the agency of chance by heuristics and theory, which are problem-specific. The

▼ *Fig. 18 Parallel performance of an iterative algorithm for Ax=b (N= problem size).*



algorithm is, at present, developed for a combinatorial problem of signal design and would later be applied to geophysical inversion /CM 11,34/.

EXPORT TRENDS: ANALYSIS, MODELLING AND FORECASTING

A thorough analysis of growth trends is required for the proper understanding of dynamics of growth and for future forecast. In the context of the analysis of export trends, we expect that the growth of total export follows S-shape curve, even though individual itemwise export may or may not follows the same. The S-shape curve can be characterized by three phases of growth: in the *initial phase* the growth is almost exponential, in the *maturity phase* the growth is around the point of inflexion, the point at which $d^2x/dt^2 = 0$, and there is finally

the *saturation phase* when growth is stagnant. Once we get the information about the shape of the growth curve, we use them for making future projections. For this purpose, we describe S-shape curve quantitatively, that is, in terms of differential equations. In the present study we have analyzed growth, both in time, and in space, and have worked out their mathematical models with an aim to make future projections. We have used these models in the study of growth of India's export to 14 major trading partners.

NONLINEAR ESTIMATION OR INVERSION

As an example of a nonlinear inverse problem, the problem of the estimation of the compounding distribution in the compound Poisson process model for earthquakes has been solved. Two important formulae derived are:

$$\mu_{n,q} = [(q-1)!] \; / \; [\Gamma(q-n)\; \mu_{n,q}\;] \text{ and } \mu_n = \mu\, f_n$$

where μ_n is the n th moment of the compound density function, μf_n is the nth factorial moment of the number of earthquakes per unit time, $\mu_{n,q}$ is the nth moment of the waiting time for the qth earthquake, and in the first formula, additional subscript q has been used as μ_n estimates obtained from for different q may not normally agree. Once the moments are obtained, any standard method for the estimation of density function can be employed. As the factorial moments and the inverse moments of the observables are involved the estimation schemes are nonlinear / CM 8/.

STEIN ESTIMATION

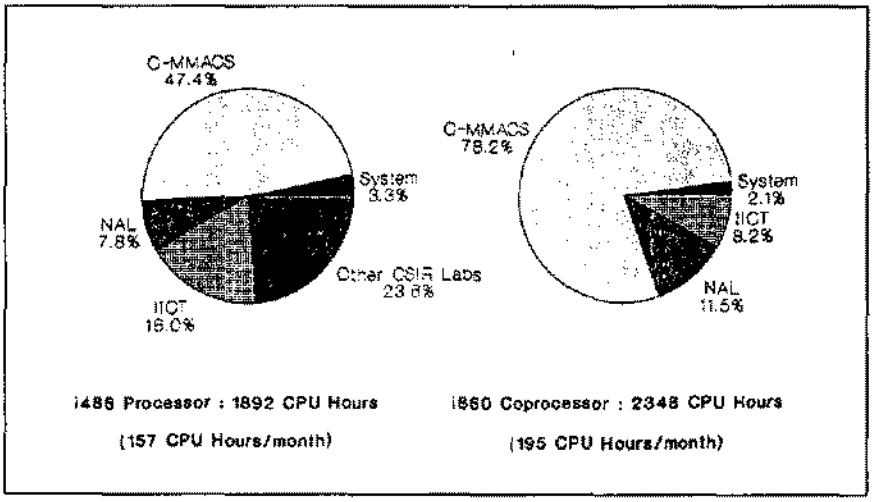
Stein estimators are nonlinear estimators for linear models. A condition for their superiority over linear estimators is that the number of parameters to be estimated must be at least three. To make Stein estimation applicable for earthquake recurrence models, rather than two-parameter slip-predictable and time-predictable models, a three-parameter size-interval relation (SIR) - predictable model has been proposed. In the process it has also been clarified that the so-called slip-predictable model has no predictability and it only states a constant relation between the waiting time for the next earthquake and the size of the next event. This relation in the so-called slip-predictable model is not contingent upon any observable quantity. In the SIR-predictable model A, the waiting time for the next earthquake can be predicted but the model is inferior to the SIR-predictable model for two reasons. Firstly, the latter model has one extra parameter and secondly a more efficient Stein estimation procedure can be used for it.

The utility of the Stein estimation procedures is further enhanced by introducing a double boot-strap estimation procedure. The first boot-strap consists of using an inferior time-predictable model to estimate the waiting time for the next earthquake, and substituting it in the size-interval relation predicted by the SIR-predictable model. As a result, the relation-predictability of the latter model is made separable in that both the size of and the waiting time for the next earthquake are predictable. The second boot-strap consists of regarding the resultant two two-parameter models as a single four-parameter model B. The ideas have been illustrated using data about a seismogenic source named Cephalonia in Greece. The work indicates that the quality of the data is normally underestimated as the estimation techniques used are not the best possible /CM 12/.

1.3 COMPUTING FACILITIES AT C-MMACS

The Centre offers a broad spectrum of computing facilities, comprising of computing platforms and software, for diverse research problems of CSIR laboratories. These facilities are utilised for inhouse, collaborative and sponsored projects of C-MMACS and other institutions. The ongoing developments taking place in the centre should enable with the centre to become a major hub of computing activities.

Major relocation of C-MMACS computing facilities took place in 92-93. Now all C-MMACS computing facilities are in one building, namely 9.AA, in the Belur campus and they are supplied by 110 KVA UPS, which was also relocated during this period. Despite these changes, utilisation of computing facilities showed an encouraging trend. For example,



◄ *Fig. 19 Utilisation of C-MMACS Supermini in 1992-93 by different CSIR establishments.*

the supermini clocked an average rate of 157 and 195 CPU hrs/month for processor and coprocessor respectively. Utilisation by different organisations is shown in *Fig. 19.*

Considerable efforts went in the procurement process of a large compute-server (LCS) and graphics works stations (GWs). Following raising of the global tender in October 92 and receipts of quotations in January 93, technical evaluation was taken up which involved specially designed benchmark programmes. The process is expected to be completed and the systems procured and installed in 93-94. Site preparation work was initiated during early 93 and is also expected to be completed during 93-94.

DoE has agreed to provide C-MMACS with internet connectivity which will enable it to access remote computing facilities worldwide and share its resources with R & D labs and academic institutions. The following tables (*Tables 2,3 and 4*) gives details of software available at C-MMACS.

Table 2
Graphics libraries at C-MMACS

Libraries	Platform
GINO-F, GINOSURF, GINOGRAF	PS/386
GKS2B+	COSMOS
SGGL	IRIS 3120, 3130, 4D/20GT
SUN PHIGS	SUN SPARC 1
NAG Graphics	PS/486

Table 3
Mathematical libraries at C-MMACS

Library	Area	Platform
EISPACK	Eigen System Analysis	COSMOS
ELLPACK	Solvers for Elliptic Partial Differential Equations	COSMOS
IMSL	Comprehensive Library for Numerical and Statistical Analysis	COSMOS & PS/486
ITPACK	Iterative Solvers for Linear Systems	COSMOS
LINPACK	Linear System Solvers	COSMOS
NAG *	Numerical & Statistical Analysis	PS/486
NUMERICAL RECIPES	Extensive Programs of Numerical & Statistical Analysis	COSMOS & PS/386
ODEPACK	Ordinary Differential Equation Solvers	COSMOS
SPARSEPACK	Sparse Linear System Solvers	COSMOS

Table 4
Application packages at C-MMACS

ACRPLOT	General Purpose PLotting Package	PS/486
AMBER 4*	Modelling of Peptides/ Nucleic Acids	COSMOS/SUN Sparc
AUTOCAD	Computer Aided Design	PS/386
CAMAND	Computer Aided Modelling, Analysis, Numerical Control etc.,	IRIS 3130
CHEMKIN	Chemical Kinetics	COSMOS
CSS STATISTICA	Integrated Statistical and Graphics Analysis	PS/386
DADISP	Digital Signal Processing	PS/386
DT-IRIS	Image Processing Software	PS/386
FASCOD 2	Line-by-line Atmospheric Radiative Transfer	COSMOS
LAWPM*	Limited Area Weather Prediction	COSMOS
LOWTRAN 7	Atmospheric Radiative Transfer	COSMOS
MAPINFO	Desktop Mapping Software	PS/386
MATLAB*	High Performance Matrix Computation	PS/386
MOM*	Global Ocean Circulation	COSMOS & SUN Sparc
MOPAC 6*	Molecular Orbital Calculations	COSMOS
NASASEC	Chemical Equilibrium (Combustion)	COSMOS
NEXPERT	Expert System Shell	PS/386
NISA 92*	Finite Element Analysis	PS/486
PCMODEL*	Molecular Modelling	IRIS 4D/20GT
PHOENICS*	Computational Fluid Dynamics	PS/486
PORFLOW	Simulation of Fluid Flow, Heat and Mass Transfer in Porous Media	PS/486
SDRC I-DEAS GEOMOD	Solids Modelling	IRIS 4D/20GT
SUPERTAB	Finite Element Modelling	IRIS 4D/20GT
TIDAL	Shallow Water Simulation & Pollutant Transport	PS/486

* acquired during 1992-93