Slider Block Models

It is well-known that the slider block models for the generation of earthquake sequences show chaos. But quantitive comparison between the sequence of earthquakes generated by them and the sequence of empirical earthquakes has not been properly performed so far. This task has been attempted under this project jointly undertaken with NGRI. The slider-block model is defined by two differential equations and two failure conditions. It generates two synthetic point processes corresponding to the earthquake on two blocks. The conventional techniques of computation of fractal dimensions could be used only with the uniformly spaced data along some axis, and not for the point process as it is. Hence the point processes generated by the slider block models and two of their interpolations were converted into uniformly sampled processes by spectral transformation, which can be readily performed because the earthquake constitute a series of impulses. This step has the advantage of not reducing the data size by aggregation to define a time-series. It may also be noted that a linear transform does not change the fractal dimension. Comparison with earthquake catalog data could be made by going through similar steps for the cataloged earthquakes also. It was found that many different parameter sets of the slider block model can give reasonable fit with the catalog data in terms of fractal dimension. This however does not imply simultaneously good fit of the spectra or the point processes themselves. The study constitutes a criticism of both the use of fractal measures for quantitative characterization and the adequacy of simple slider block models. *(R N Singh*, V M Maru*, P S Moharir*, N K Indira, * NGRI)*

Modelling and Computer Simulation of Multi-Layered Road Systems

Determination of subsurface structure of road pavements is of considerable importance as it leads to structural capacity of inservice pavements and maintainence requirements. Amongst several techniques available, Falling Weight Deflectometer (FWD) is notable for its speed and accuracy. A project has been initiated by the Central Road Research Institute (CRRI), Delhi and C-MMACS under the sponsorship of DST for the development of a mathametical model for multilayer road-systems of types prevelant in India, and development of an indigeneous software for analysis of FWD deflection data, for estimating substructure of road from surface data, and the remaining life of pavements and the overlay requirements. The software system along with FWD data provided by CRRI, will form a core research tool for structural analysis of pavements under Indian conditions which would hopefully become an important input to pavement design and maintainence procedures.*(J Sridevi, K S Yajnik, P K Nanda*, *CRRI)*

Technique for Conformational Sampling of Cyclic Molecules: Application to 18-CROWN-6

Microcyclic ring systems are known for their selectivity in binding to guest substrates. The design and synthesis of such systems are motivated not only by their practical applications but also by the scientific challenges in understanding how certain molecules recognize guest substrates. The specificity of the cyclic host is largely decided by energetics and adoption of conformations appropriate to its environment. Host-guest complexation is prompted by the characteristic conformational features. Hence, generating all the significantly populated conformers which can be correlated with experimental results is one of the important problems in molecular modelling. Many techniques have been proposed to carry out an exhaustive search of low-energy conformers. The present work being carried out by scientists of the Indian Institute of Chemical Technology (IICT), C-MMACS and the Toyohashi University of Technology (TUT), Japan is concerned with a cyclic peptide 18-crown-6 (18C6), a member of a crown ether family, which is extensively characterised by earlier workers. Because of its conformational flexibility, 18C6 adopts to different conformers which can recognize and selectively bind to ions and other molecules, a capacity similar to that of enzymes and other biological molecules. Although extensive conformational calculations have been carried out in the past for 18C6 to find low-energy conformers, very few efforts have led to the experimentally observed structures and most of the conformers are inactive for complexation. In the present work, an alternative technique (CA) is used which is essentially evolved by using two programmes, CONFLEX and AMBER. The CONFLEX combines local perturbations involving combinations of band flips and corner flapping to generate several structures and this is then followed by geometry optimization using AMBER force fields leading generated conformers to the nearest local minimum. CA runs carried out on CONVEX C3820 required CPU time of about 150 min. Conformers upto 5Kcal/mol from the global energy minimum have been searched using the reservoir-filling algorithm. Using a threshold energy value of 2.52 Kcal/mol, 30 low-energy structures were obtained. It was gratifying to note that these low-energy conformers corresponded to those reported from comprehensive MD study by earlier workers. Ci, the structure with Ci global minimum, matches the experimental and theoretical results. Most of the conformers obtained by CA search were of Ci symmetry. An exhaustive search of the conformational space cannot be guaranteed by the CONFLEX/AMBER technique, which is only possible by grid search at a high resolution. Such a practice requires very powerful computational resources and is presently not feasible. Nonetheless, identical or at least very similar results were obtained when compared to the combined use of ellipsoid algorithm and molecular dynamics; and this implies the usefulness of the technique in searching for chemically significant regions of the large conformational space. The generation of feasible starting geometries is important in conventional calculations using molecular mechanics or molecular dynamics simulation. The present technique starts from a completely random structure using no experimental constraints to generate low-energy conformers. This method could become the method of choice for conformational sampling of cyclic peptides. *(Jagannadh*, A C Kunwar*, E Osawsa †, R P Thangavelu,*IICT, †TUT, Japan.)*

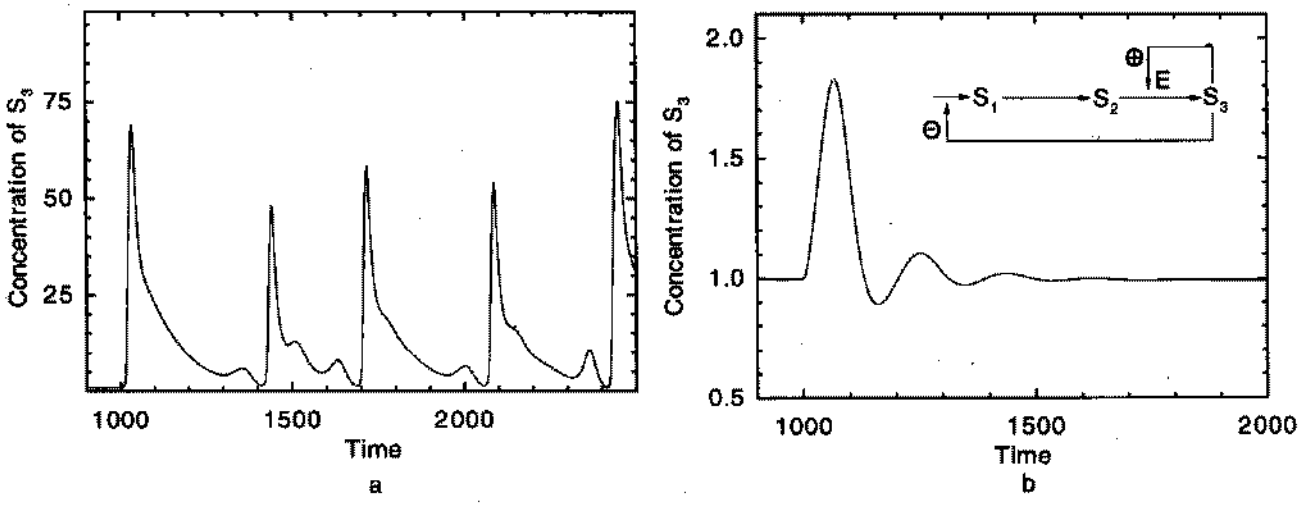

Figure 16: Behaviour of concentration of S_3, the product of the biochemical model reaction sequence, without control (a) and with control (b). Perturbation is applied to the system parameter k, the degradations rate of S_3, at 1000 time units (nondimensional).

Characterisation and Control of the Dynamics of Model Biochemical Reaction Pathways

An extensive network of coupled biochemical reactions underlie all normal cellular functions. Any modifications of the network in the form of genetic and enzymatic alterations can lead to pathogenesis. Experiments have elucidated the genetic and biochemical details of the interactions but a comprehensive view of the dynamics of these coupled systems in response to modifications is yet to be emerge. Mathematical models can help in understanding coupled pathway dynamics and also predict conditions for altered behaviour, or even design new pathways which can yield better functions. A model biochemical pathway, which has been studied earlier at the Centre for Cellular and Molecular Biology (CCMB), Hyderabad and C-MMACS, incorporates one positive feedback coupled with one negative feedback process, representing enzyme activation and genetic repression. Different domains in the parameter space corresponding to steady state, limit cycles, period-doubled (period-2) oscillations and chaos had been mapped for this system. It was possible to follow the period-doubling route upto the next couple of stages, e.g. period-4, period-8 etc., but not any further because of numerical problems. It was also noticed that, for very low values of the system parameter k, reverse bifurcations to period-1 limit cycles take place. Attempts to characterise the intermediate chaotic regions acccurately using Liapunov exponents were discouraging essentially due to extreme stiffness of the equations in this region. Chaos in biochemical systems has, in general, been associated with pathogenesis and diseases. Therefore methods for controlling chaotic oscillations are increasingly assuming importance in biology. Work was initiated in CCMB and C-MMACS during the reporting period to deal with the application of algorithms used for controlling chaos to the present system. For example, the adaptive control method (Huberman & Lumer 1989 in IEEE Trans. Circuits Syst., Sinha et al 1990 in Physica D) has been applied by assuming that one of the system parameters, k, can change owing to fluctuations driven by the environment which can be interpreted as a

transient change in the enzymatic activity due to change in temperature or due to the presence of activators and inhibitors. The adaptive control is achieved when the parameter returns to the unperturbed ("goal") value through self-regulation. The process of self-regulation is modelled by introducing an additional equation for the rate of change of k; the rate of change of k is made proportional to an "error signal" which is the difference between the original, unperturbed and current, perturbed values of k. The proportionality constant, say g, determines the time taken by the system to return to its original state. A typical control scenario is shown in Fig. 16. Here the system is initially allowed to settle down to a steady state behaviour with a suitable parameter value. Perturbation is then applied to k which throws the system into a chaotic regime; time evolution is then monitored for a suitable interval. Fig. 16a shows the time variation of the concentration of the state variable S_3, first at k = 5.0 when the system shows stable equilibrium behaviour, and then at k = .0083 at which it varies chaotically. With the adaptive control turned on, the chaotic oscillations are controlled to the original stable dynamics as shown in Fig. 16b. A large value of g has been used so that the system returns to its original stable dynamics within a short time interval. Further work is in progress on alternative algorithms as well as sensitivity analysis. Such studies have potential applications in providing alternative control strategies for biological diseases and pathogenesis. *(Somdatta Sinha*, S Parthasarathy*, T R Krishna Mohan, * CCMB)*

Computer Simulation of Air-Frame and Turbomachinery Components for NC Machining

As a part of the work of the national team set up for the design and development of carbon-fibre composite wing for the Light Combat Aircraft (LCA), it was required to model and machine four numbers of "Lay-up Tools" (Moulds) for the lay-up and cusing of Carbon-fibre "Elevons" for the LCA wings. 3-D modelling of the "Elevon" and development of CNC software for machining the moulds was carried out on one of the IRIS graphics workstations in C-MMACS. The CNC programs were postprocessed to suit the control system of a MIKRON CNC machine and the lay-up tools were milled on this machine. The machined moulds were inspected by HAL and accepted to be within the machining tolerances as specified. Subsequently, they were delivered to ADA. The "Wing-Fuselage attachements" for the LCA wing were to be milled out of stressed aluminium alloy. 3-D modelling of this component was completed and CNC software for machining it was developed on the IRIS graphics workstation of C-MMACS. The CNC programs were proved on a soft material. The machining was carried out on metal at NAL. *(C.I Haque *, B B C Kumar*, * NAL)*

Strength Contours of Leather Surfaces

A project was initiated at C-MMACS on request from the Central Leather Research Institute (CLRI), Madras on developing software tools that would facilitate optimising the use of leather which have heterogeneous properties. Significant progress has been made in the development of an interactive software package for the analysis of lastometer test data to determine the lastability of glazed goat upper leather. The software has been used to visualize the strength profile of grain-crack resistance, bursting strength and distension at bursting for glazed goat upper leather. In addition, tensile strength was also determined experimentally for a side of similar type of leather. The strength of entire

leather clearly indicate that there are significant spatial variations in the properties. These variations have to be analysed carefully before cutting the shoe cut components for the manufacture of shoes. The software package is capable of calculating the percentage areas having acceptable properties for various parts of the leather. The package is expected to provide a tool for making better shoes and other products. *(B Lokanandam*, B Sivaramakrishnan*, T Ramaswami*, M I James, * CLRI)*